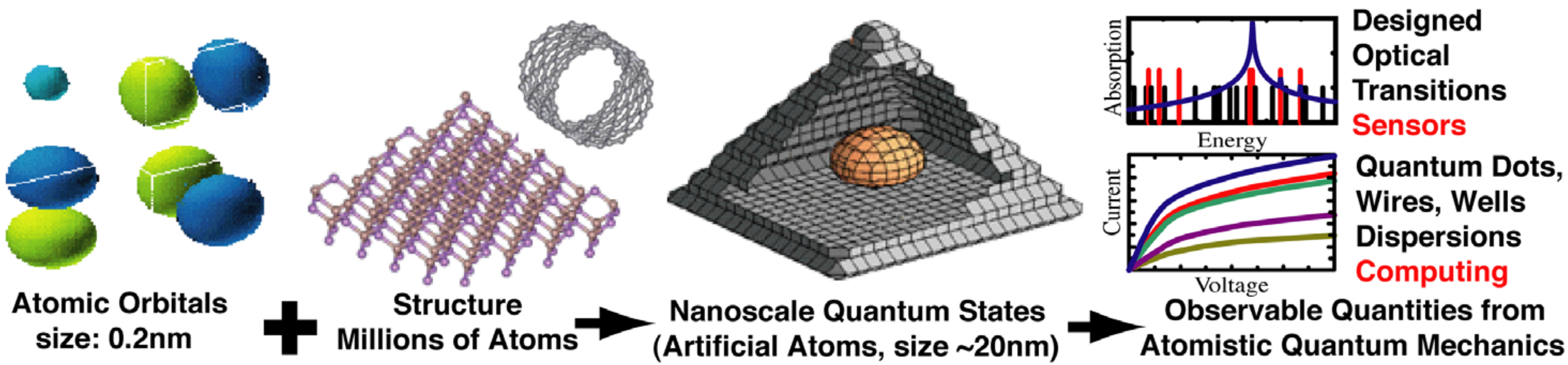
Introduction to the NEMO3D Tool

Gerhard Klimeck

NCN

NEMO 3-D Technical Approach



Problem:

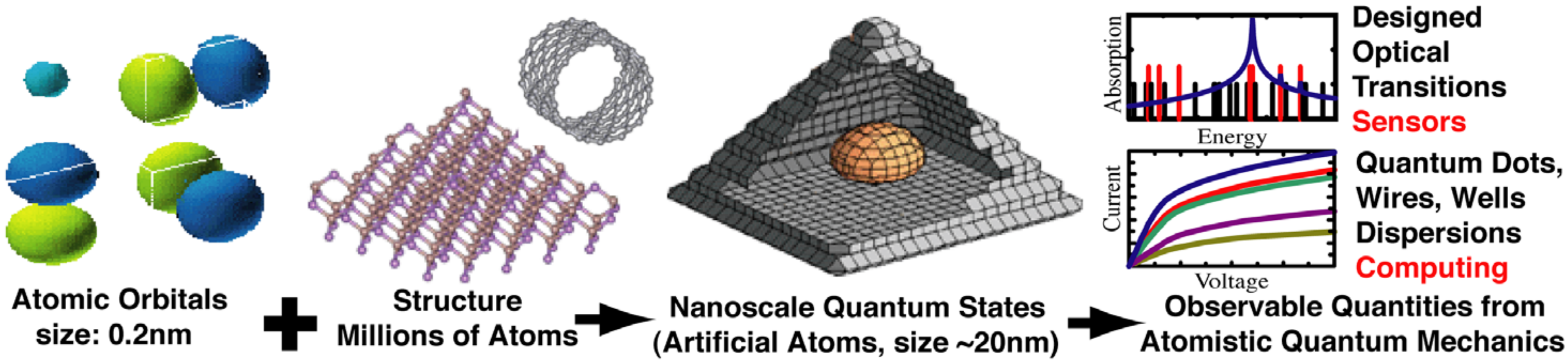
Nanoscale device simulation requirements:

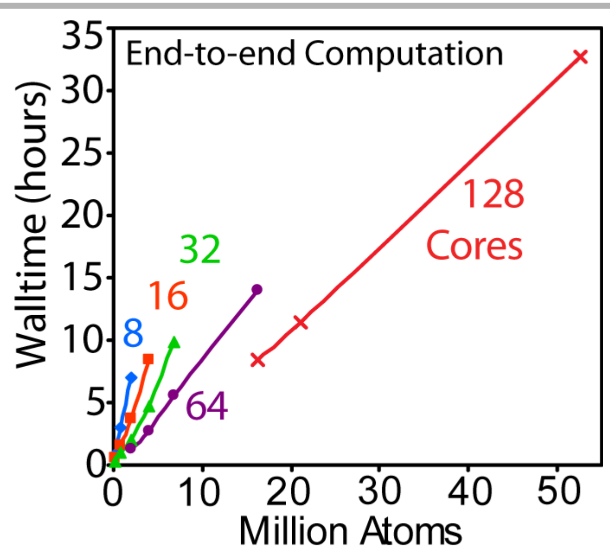
- Cannot use bulk / jellium descriptions, need description atom by atom
  => use pseudo-potential or local orbitals
- Consider finite extend, not periodic
  => local orbital approach
- Bonds in semiconductors are stable!
  => Do not need ab-initio methods!
- Need to include about one million atoms.
  => need massively parallel computers
- The design space is huge:.
  => 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

NEMO 3-D Technical Approach





Demonstration / Capability / Impact:

- 52 million atom electronic structure (101nm)^3.
- Quantum dots, nanowires, quantum computing…

Approach:

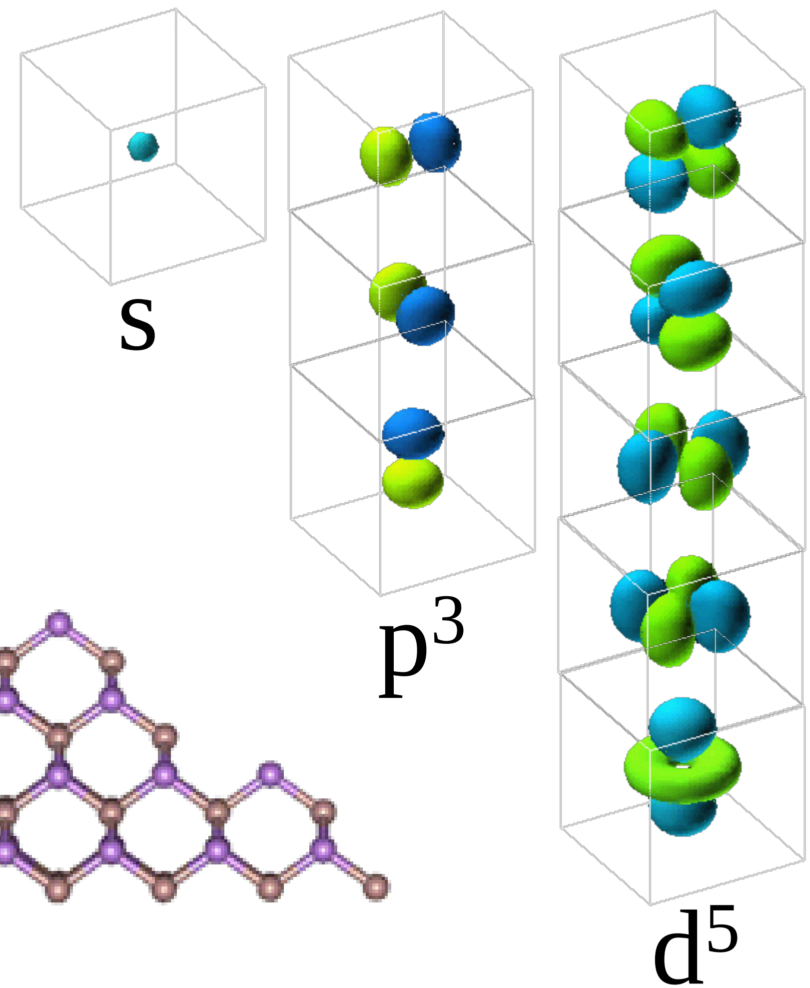
- Use local orbital description for individual atoms in arbitrary crystal / bonding configuration
  - Use s, p, and d orbitals.
  - Use genetic algorithm to determine material parameter fitting
- Compute mechanical strain in the system.
- Develop efficient parallel algorithms to generate eigenvalues/vectors of very large matrices

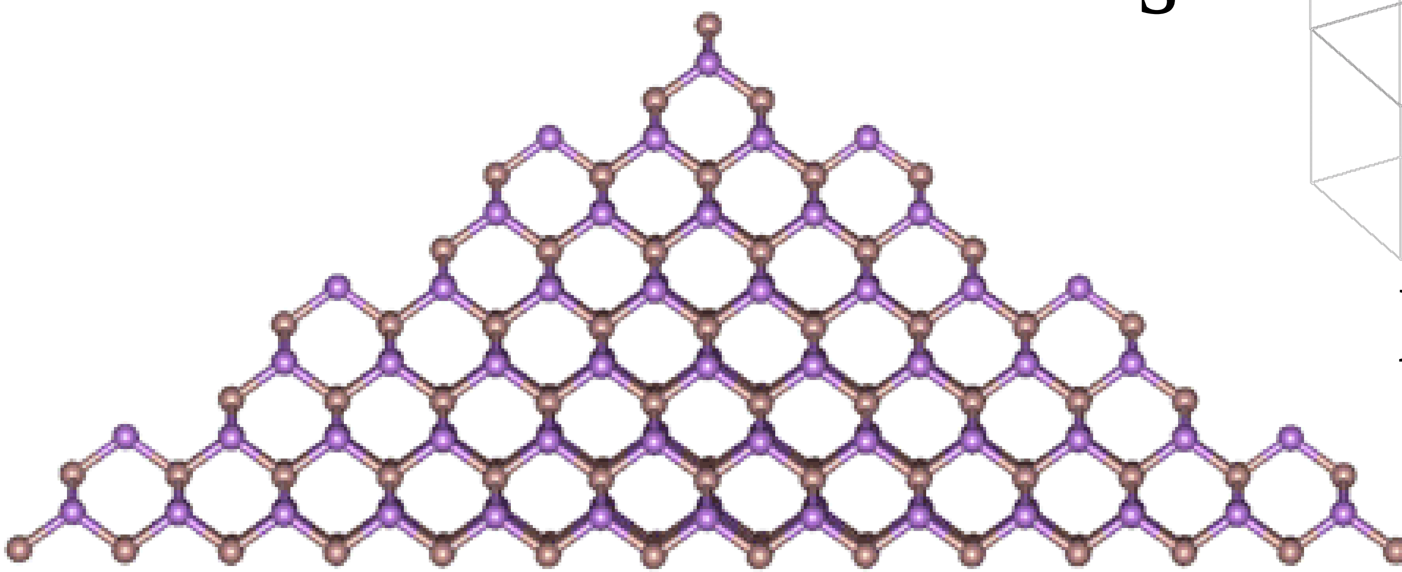
Atomistic Tight-Binding Hamiltonian

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

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

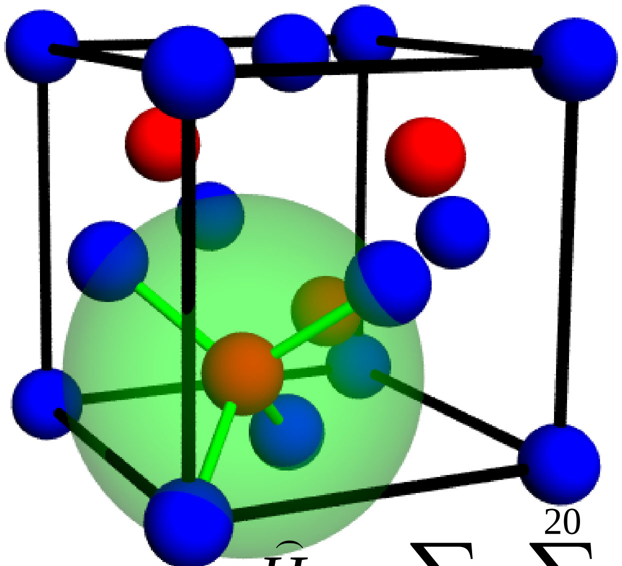
Wavefunction Basis





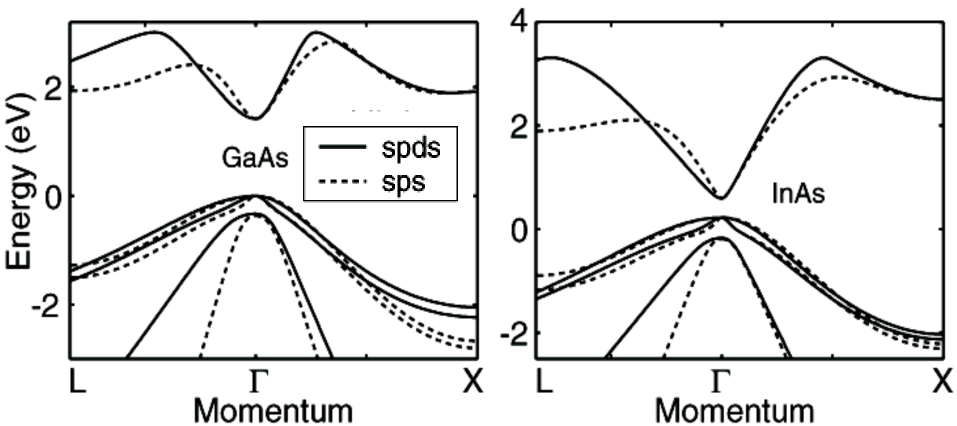
Crystalline Structure

Nearest-Neighbor sp3d5s* Model



- Realistic zinc-blende lattice
- Each atom has 10 spin-degenerate orbitals (*sp³d⁵s**)
- Each atom has 4 nearest neighbors
- TB parameters found by fitting of bulk band structure to experiment

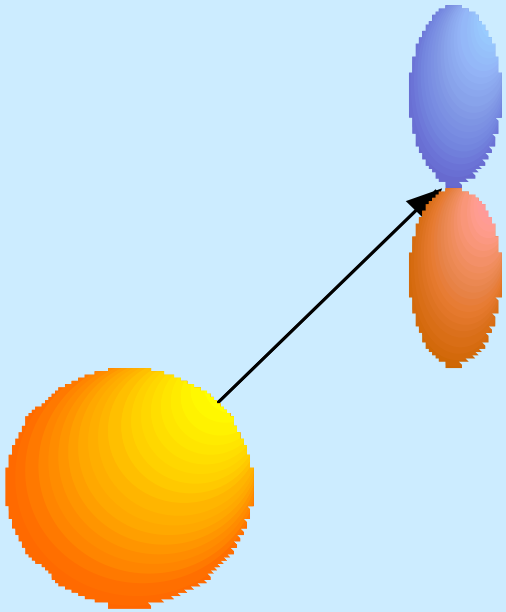
$$\hat{H} = \sum_{atoms\ R} \sum_{\substack{\alpha=1 \\ bands}}^{20} \varepsilon_{R\alpha} c^{+}_{R\alpha} c_{R\alpha} + \sum_{atoms\ R} \sum_{atoms\ R'=1}^{4nn} \sum_{\substack{\alpha=1 \\ bands}}^{20} \sum_{\substack{\alpha'=1 \\ bands}}^{20} t_{R\alpha,R'\alpha'} c^{+}_{R\alpha} c_{R'\alpha'}$$

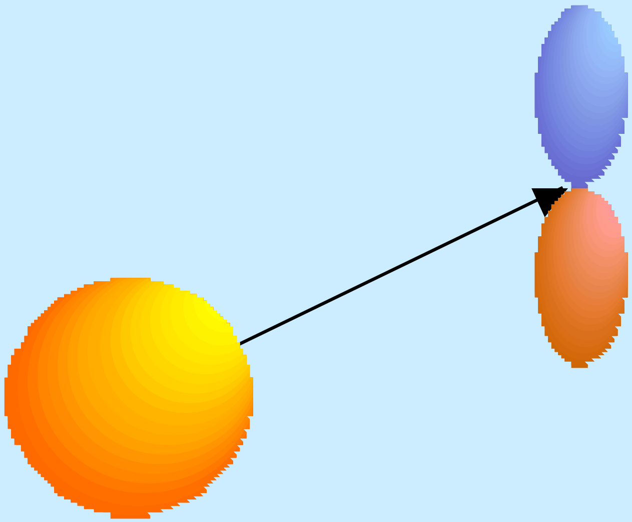


Systems with up to 52 million atoms

Matrix order: 1×10^9
Lanczos Diagonalization

Modeling Strain
Bond Lengths and Angles Change





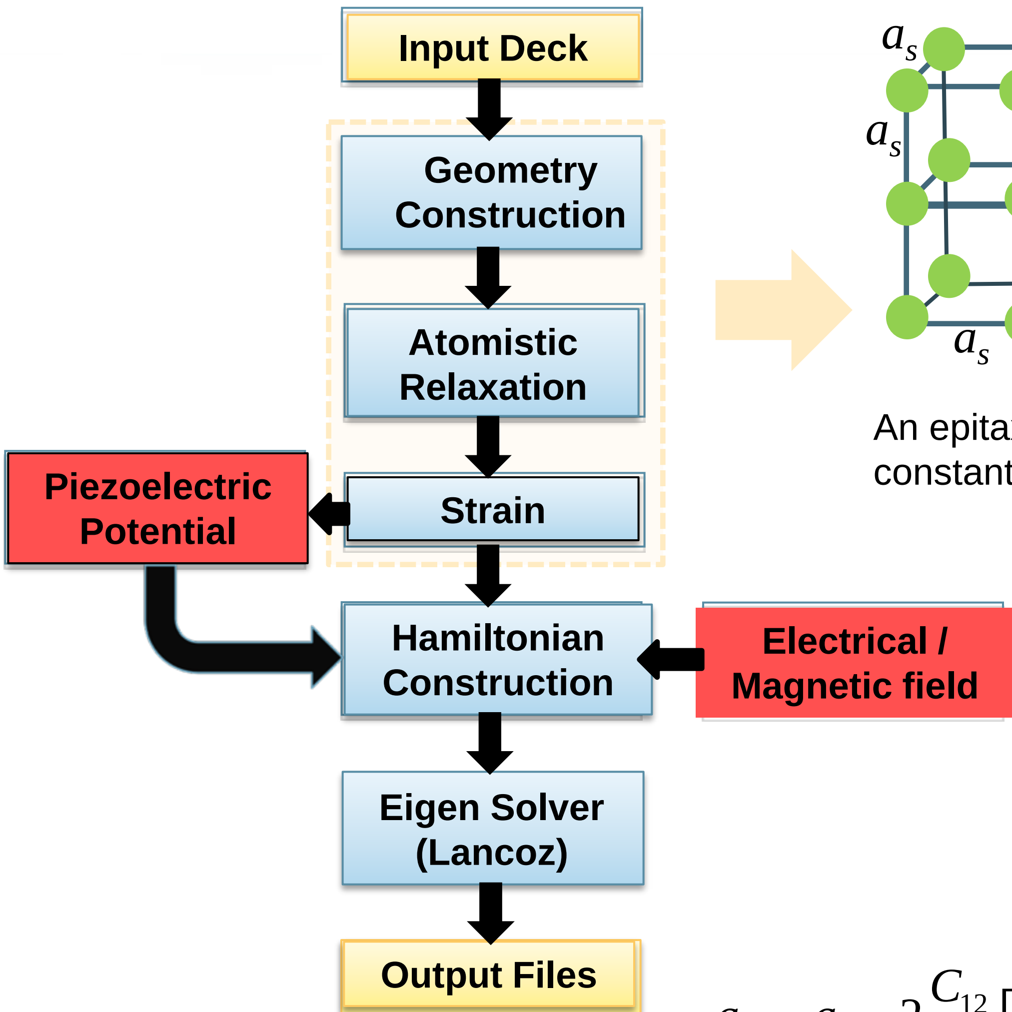
$$\mathbf{d} = d\left(l\mathbf{e}_x + m\mathbf{e}_y + n\mathbf{e}_z\right)$$

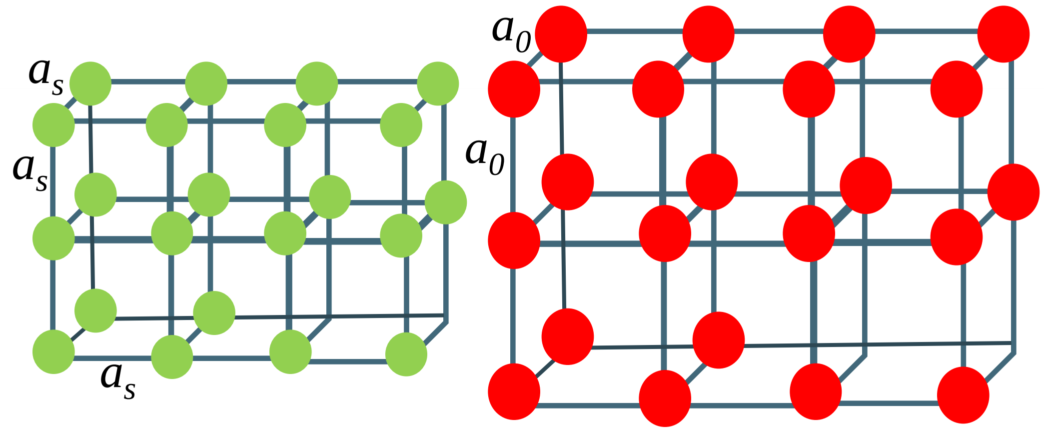
$$E_{sa,\,zc} = n V_{sa,\,pc\sigma}$$

$$\mathbf{d}' = d'\left(l'\mathbf{e}_x + m'\mathbf{e}_y + n'\mathbf{e}_z\right)$$

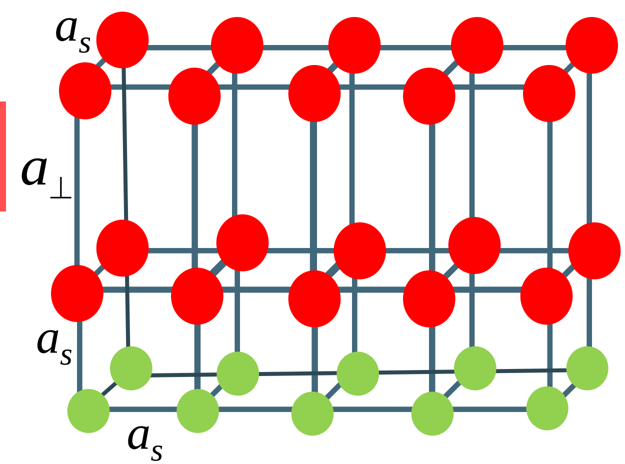
$$E_{sa,\,zc} = n' V_{sa\,,\,pc\sigma}\left(\frac{d}{d}\right)^{\eta}$$

NEMO 3-D Calculation Flow – VFF Strain Model





An epitaxial layer is grown, on a substrate with different lattice constant, the epilayer deforms (strain) :



VFF Model

$$a_\perp = a_0 - 2\frac{C_{12}}{C_{11}}[a_s - a_0] \iff \mathbf{R}' = (1 + \varepsilon)\mathbf{R}$$

Strain tensor (ε)

Strain Impact on Electronic Structure

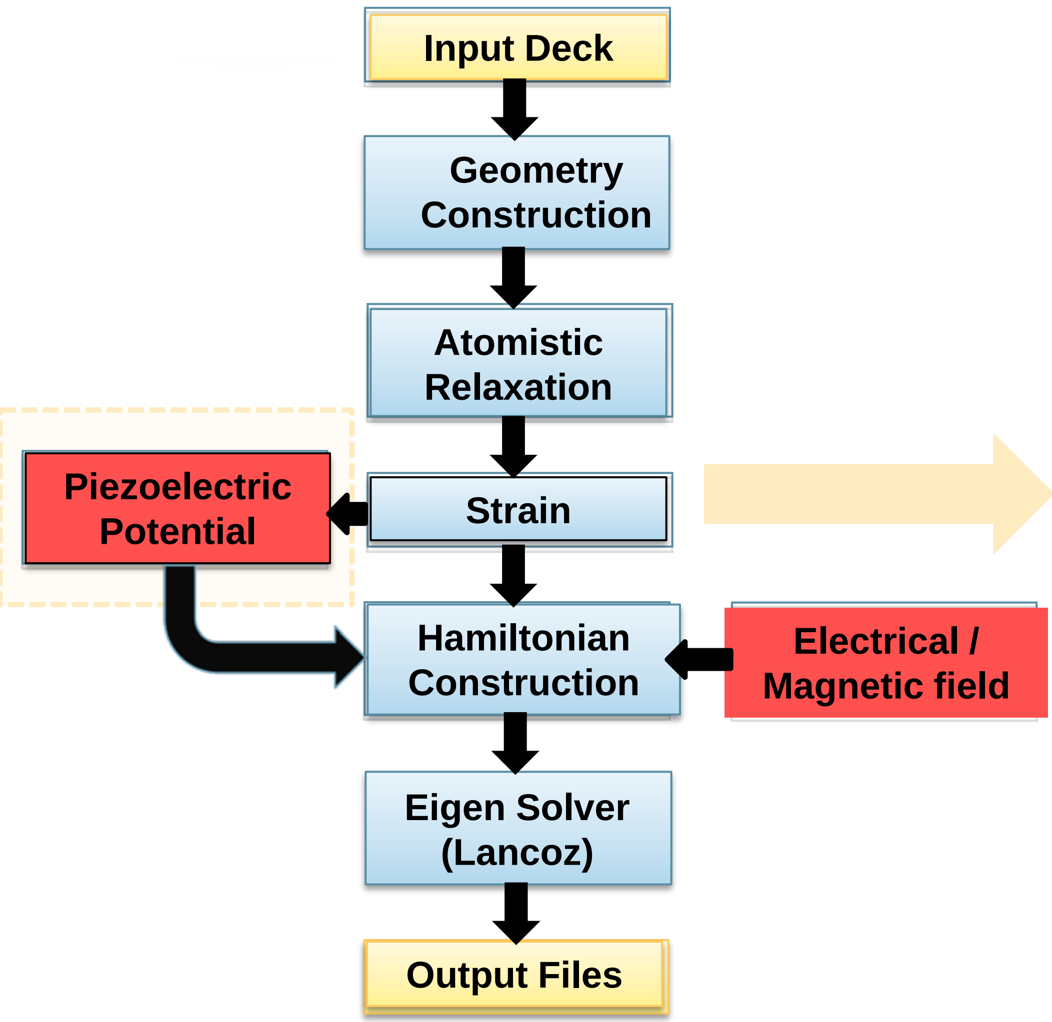
- Strain ➔ Changes bond lengths/angles ➔ deforms crystals
- Band edges are shifted and degeneracy of HH-LH is lifted
- Strain impact on electronic structure:

Conduction Band ➔ $E_c = E_{c0} + a_c(\varepsilon_{xx}+\varepsilon_{yy}+\varepsilon_{zz})$

Valence Band ➔ $E_{HH/LH} = E_{HH0/LH0} + a_v(\varepsilon_{xx}+\varepsilon_{yy}+\varepsilon_{zz}) \pm 0.5b_v\,(\varepsilon_{xx}+\varepsilon_{yy}-2\varepsilon_{zz})$

where a_c = -5.08eV, a_v=1.0eV and b_v = -1.8eV for InAs

NEMO 3-D Calculation Flow -Piezo-Electric Model



Strain tensor ➔ Polarization

$$P_1 = 2e_{14}\begin{pmatrix}\varepsilon_{yz}\\ \varepsilon_{xz}\\ \varepsilon_{xy}\end{pmatrix}$$

$$P_2 = 2B_{114}\begin{pmatrix}\varepsilon_{xx}\varepsilon_{yz}\\ \varepsilon_{yy}\varepsilon_{xz}\\ \varepsilon_{zz}\varepsilon_{xy}\end{pmatrix} + 2B_{124}\begin{pmatrix}\varepsilon_{yz}(\varepsilon_{yy}+\varepsilon_{zz})\\ \varepsilon_{xz}(\varepsilon_{zz}+\varepsilon_{xx})\\ \varepsilon_{xy}(\varepsilon_{xx}+\varepsilon_{yy})\end{pmatrix} + 4B_{156}\begin{pmatrix}\varepsilon_{xz}\varepsilon_{xy}\\ \varepsilon_{yz}\varepsilon_{xy}\\ \varepsilon_{yz}\varepsilon_{xz}\end{pmatrix}$$

Polarization ➔ Charge density

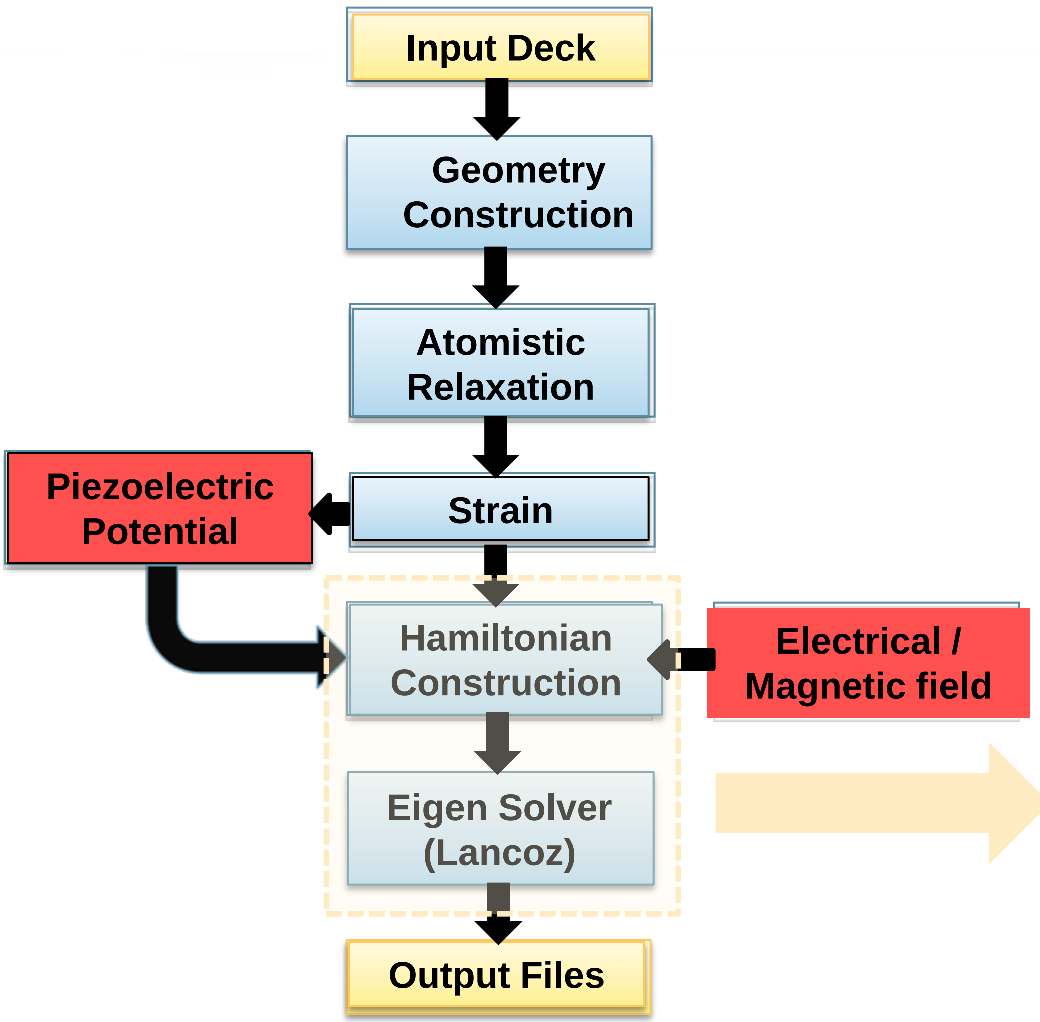
$$\rho_{piezo}(r) = -\nabla . P$$

$$P = P_1 + P_2$$

Charge density ➔ Potential

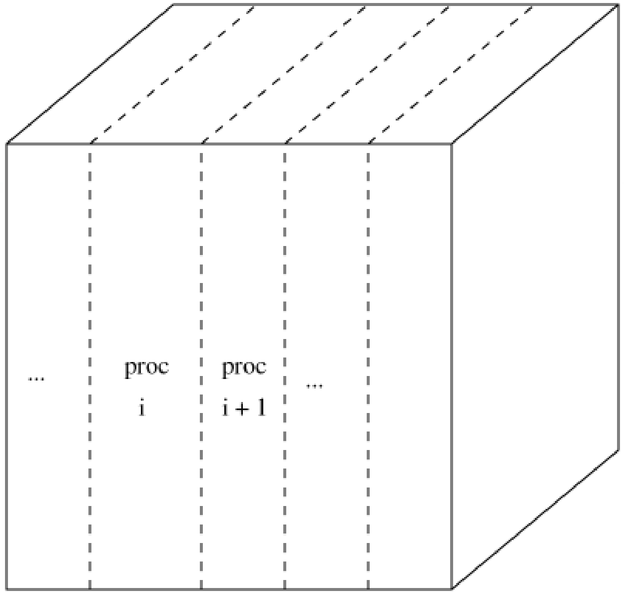
$$\rho_p(r) = \varepsilon_0 \nabla . [\varepsilon_s(r) \nabla V_p(r)]$$

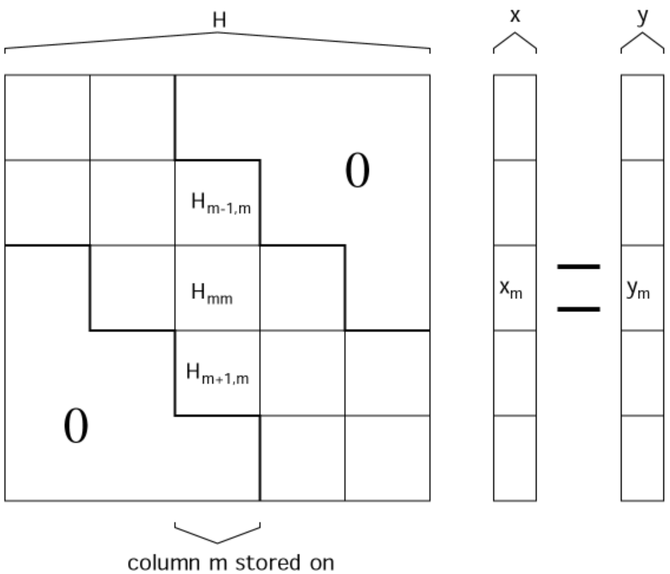
NEMO 3-D Calculation Flow - Electronic Structure Model



- Real-size QD typically involves multi-million atoms.
- *sp³d⁵s** TB requires 20 bases per each atom with consideration of spin-orbit couplings → (Natomx20) by (Natomx20) Hamiltonian.
- Need to obtain interior spectrum eigenstates
- NEMO 3-D: Designed from the bottom up to be parallel: MPI.
- NEMO 3-D code has been tested to run on (almost) any HPC cluster

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

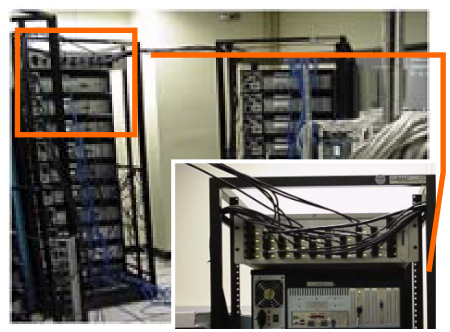
From Beowulf Concept (1998 JPL, Tom Sterling) to Commodity Products in 4 Generations

<u>Hyglac (1997)</u>
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

<u>Nimrod (1999)</u>
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

<u>Pluto (2001)</u>
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



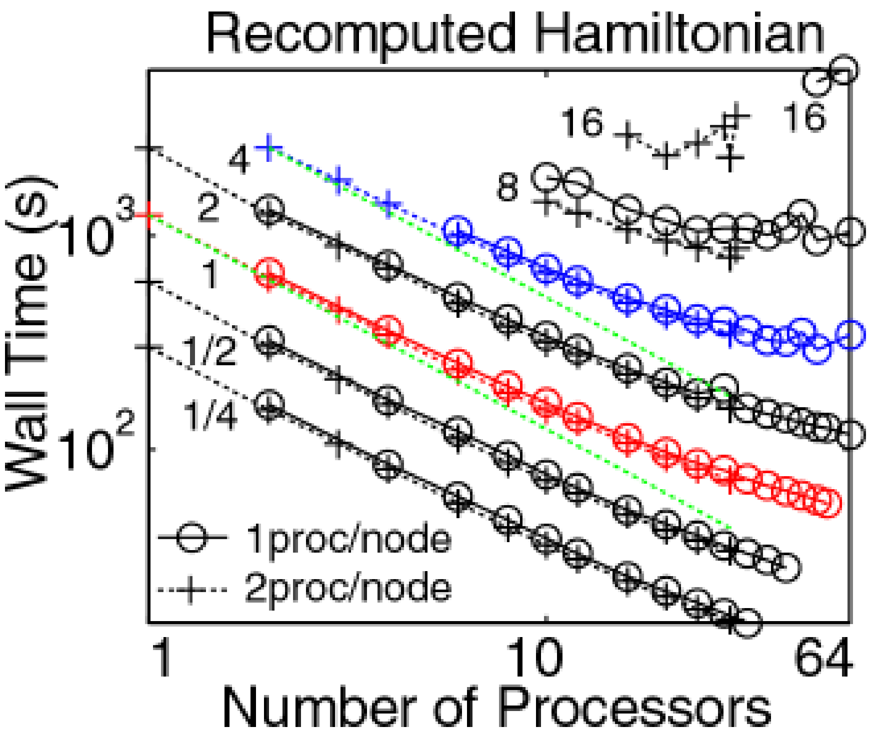
<u>NewYork (2002)</u>
66 Xserve G4 1GHz
1GB RAM per node
33 GB total
60 GB Disc per node
2 TB total
100 Mb/s ethernet crossbar
MAC OS X, MPI
495GFlops

Affordable Supercomputer for ~$100k

Parallelization Benchmarks

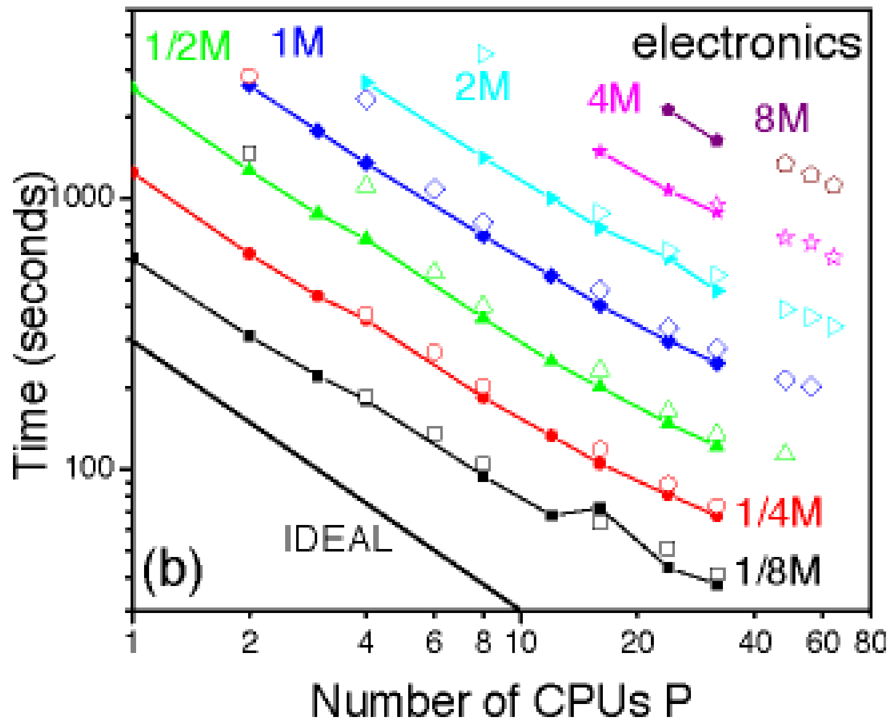
2000

32 nodes Dual Intel P3, 800MHz,
1GB RAM, 100Mbs ethernet



2003

32 node, G5 Apple cluster
2GB RAM, Dual Gigabit Ethernet.

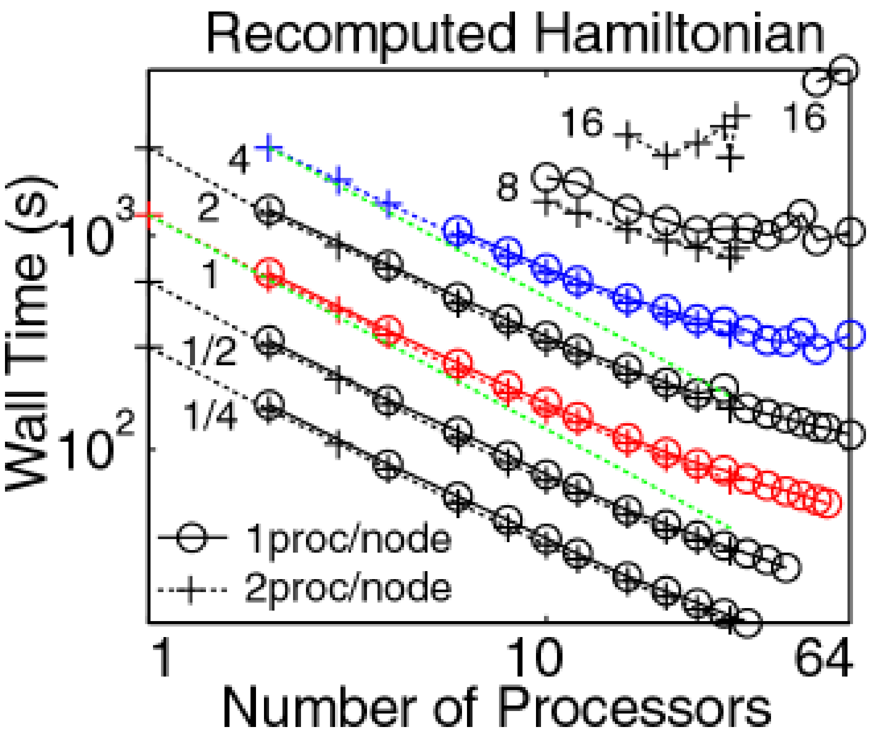


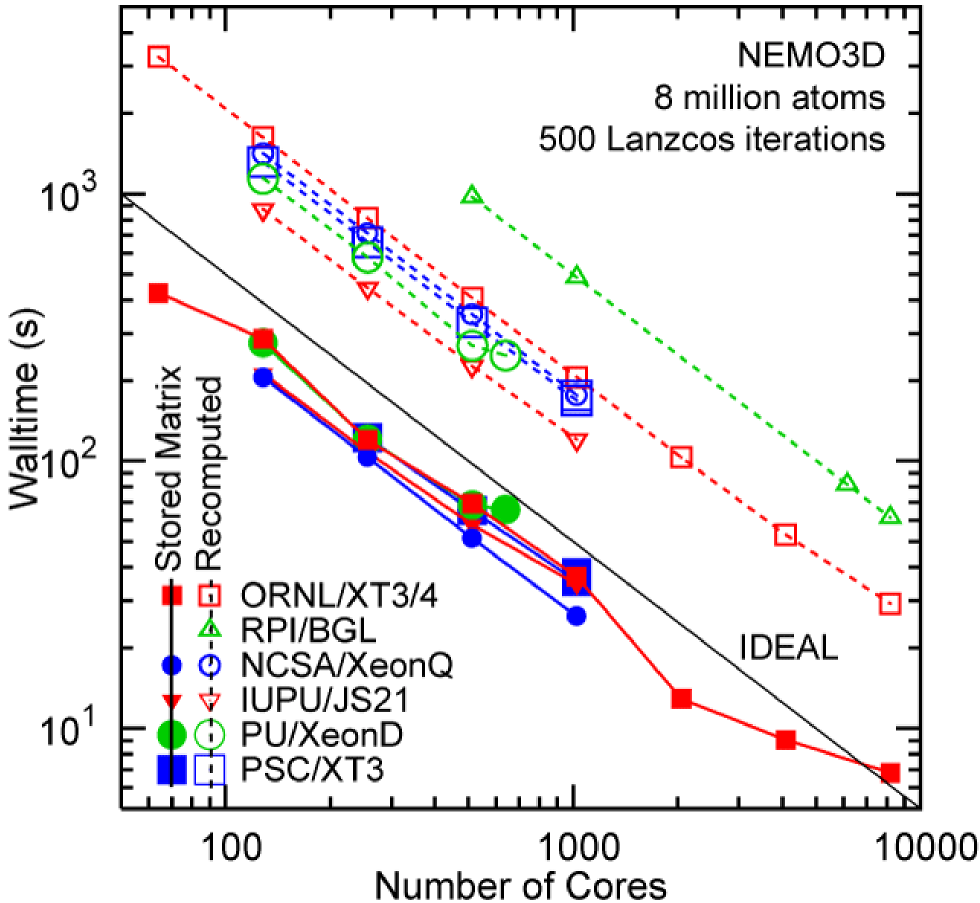
Parallelization Benchmarks

2007
IBM BGL, Cray XT3,
Intel Clusters, IBM JS21

2000

32 nodes Dual Intel P3, 800MHz,
1GB RAM, 100Mbs ethernet





Demonstrated scaling to 8,192 cores

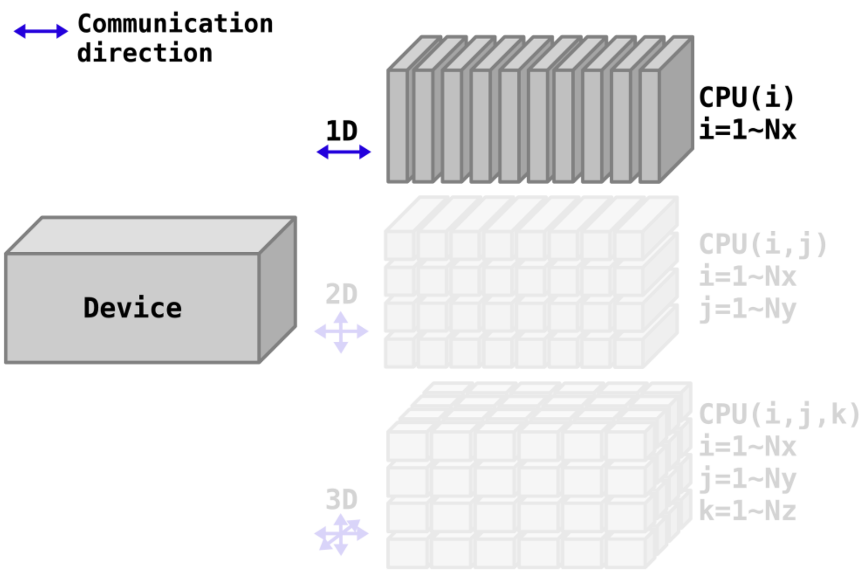
Parallelization Benchmarks

Scaling to 8,192 processors in NEMO3D

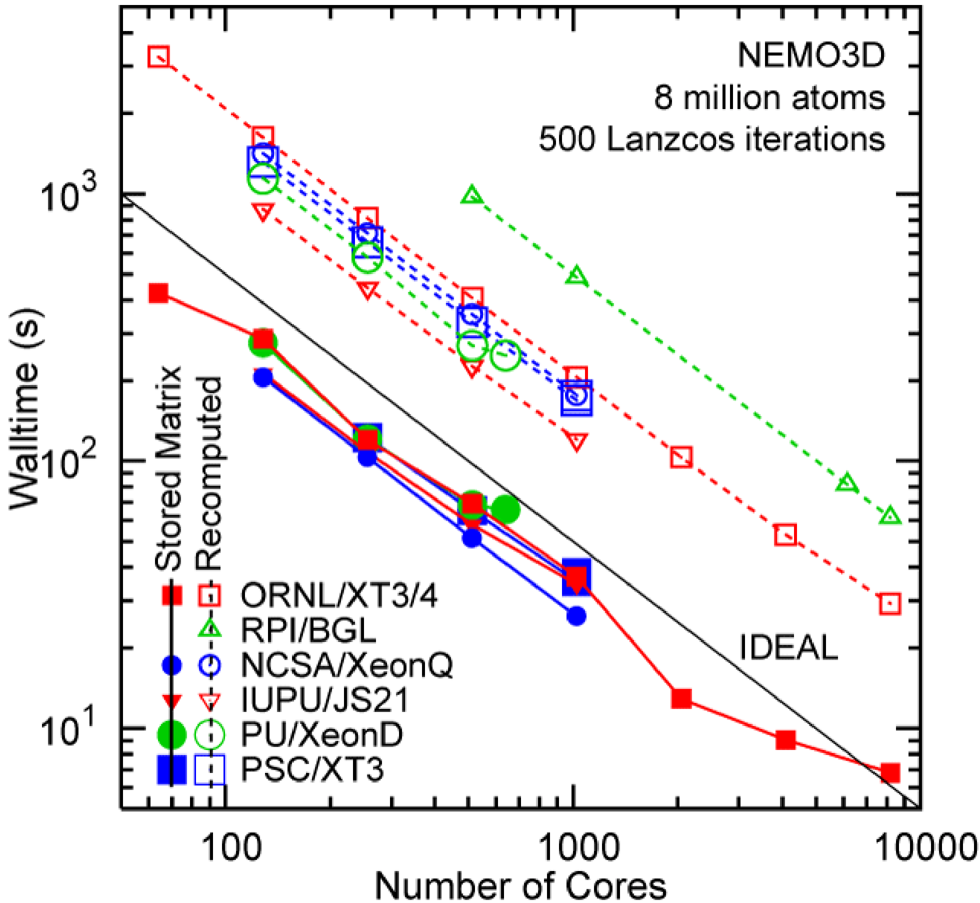
Is a bit of a cheat!
NEMO3D does a 1D decomposition!!

The domain is
a very thin and very long nanowire
NOT a Quantum Dot!

Need a 2D and 3D Decompositions



2007
IBM BGL, Cray XT3,
Intel Clusters, IBM JS21



Demonstrated scaling to 8,192 cores

NEMO Development and Scalability Study

Sunhee Lee, Hoon Ryu, Gerhard Klimeck

Objective

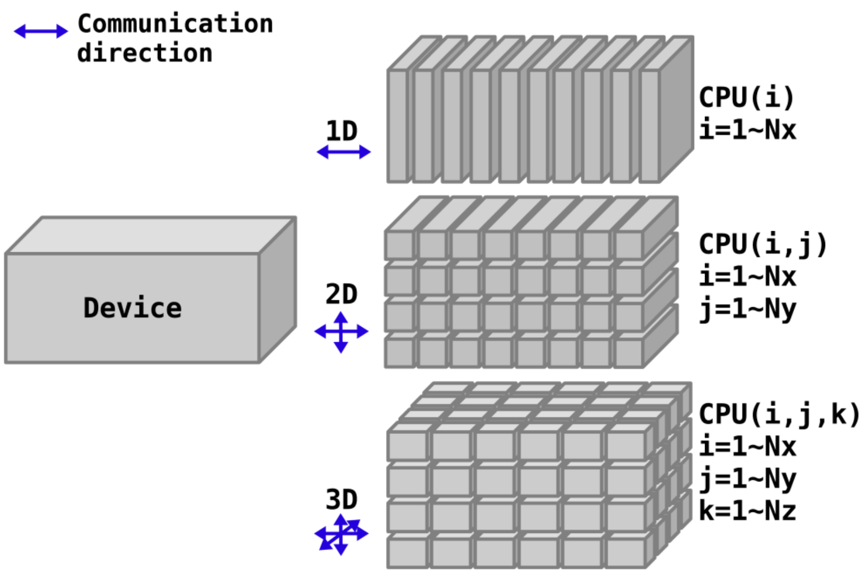
- Run large atomistic electronic structure simulations in minutes
- Represent realistically large structures atomistically
- Utilize available peta-scale computers

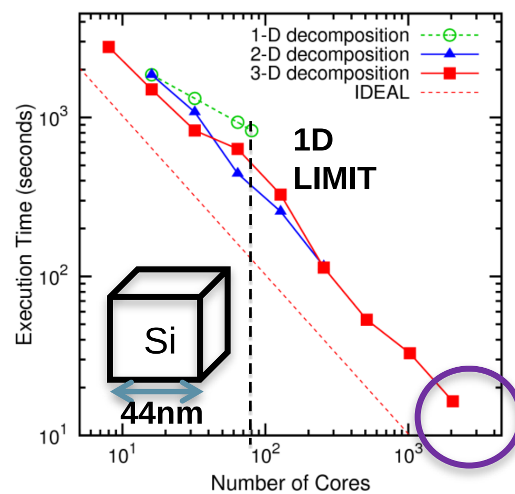
Approach

- Improve decomposition parallelism
- Include self-consistent calculations

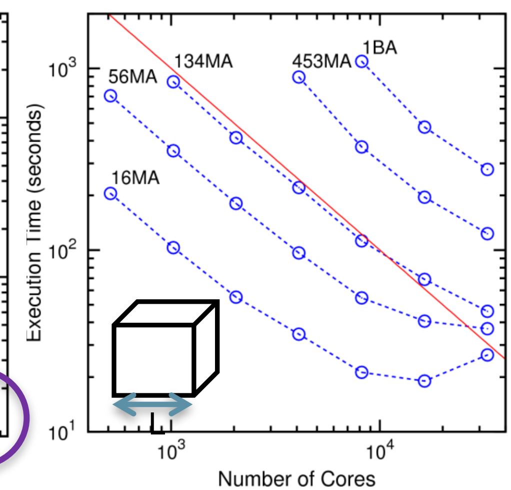
Performance / Impact

- Strong scaling of 3D decomposition
  => have overcome 1D limitation
- Utilized over 10,000 cores for realistic simulation domain size
- Expecting dramatic reduction of simulation time
  => 10hours to 20 minutes
- Published in SCIDAC proceedings, 2009, Haley, Lee et al.





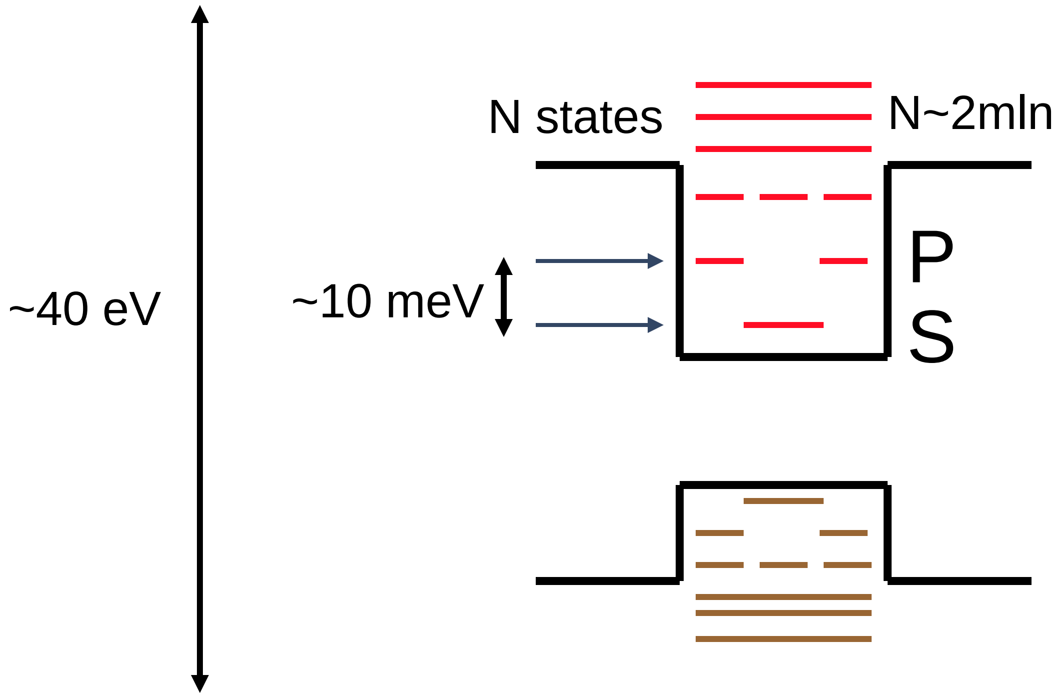
Tested on Ranger



Tested on Kraken

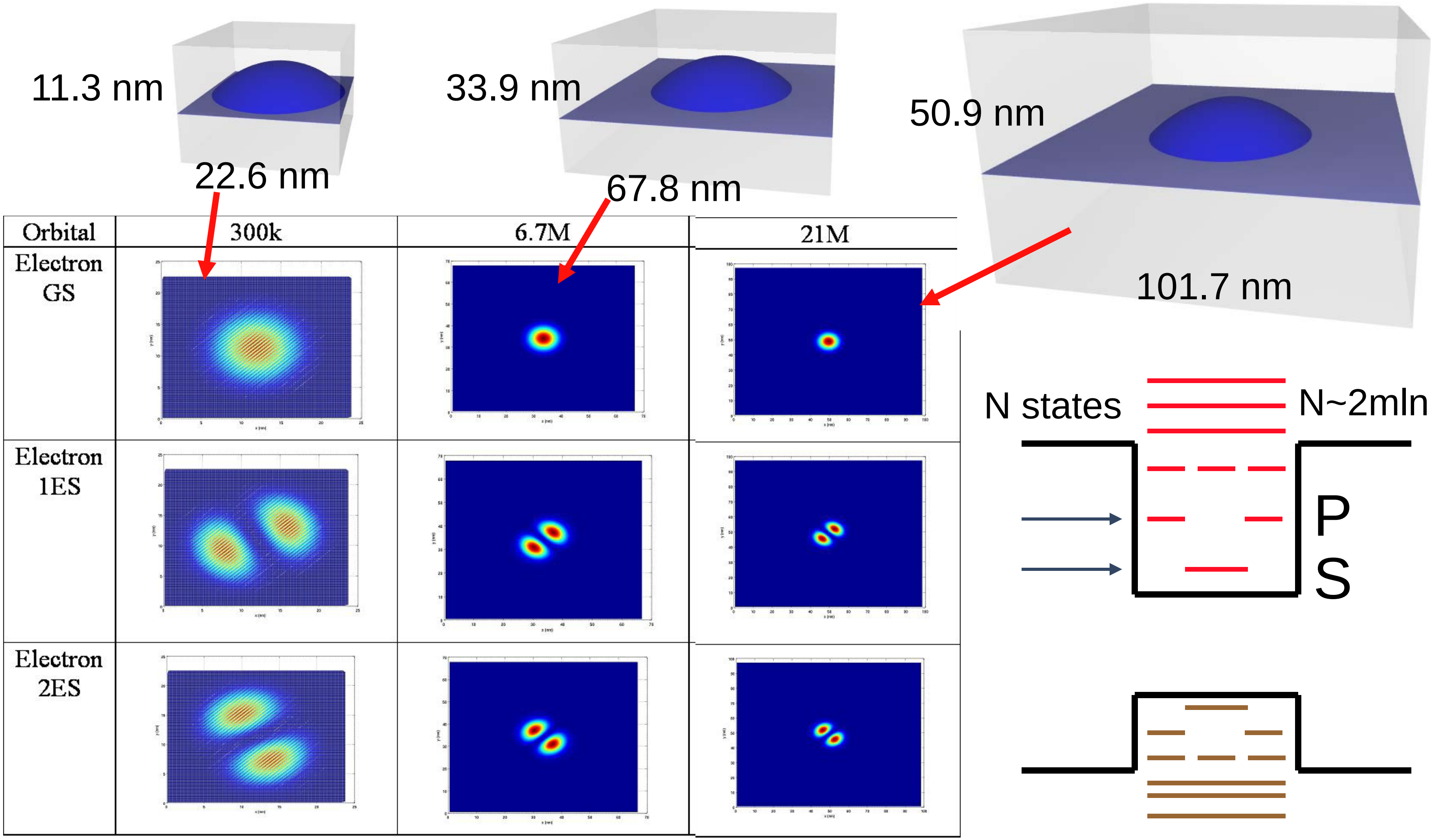
Proof of Concept

Extraction of Targeted Interior Eigenstates



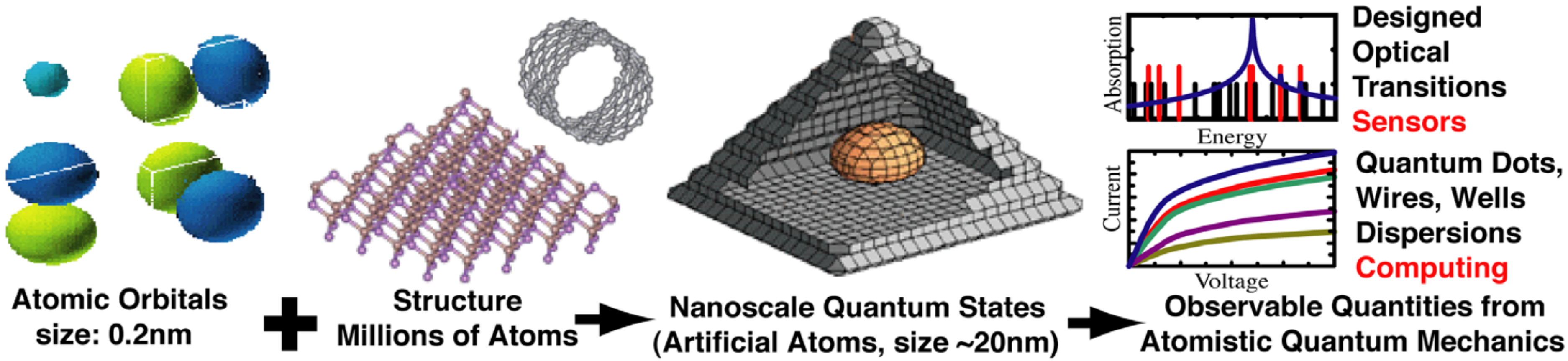
Proof of Concept

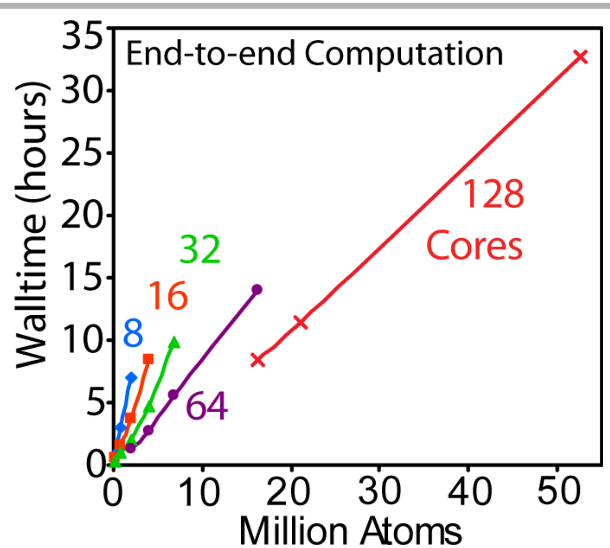
Extraction of Targeted Interior Eigenstates



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

NEMO 3-D Technical Capabilities





Demonstration / Capability / Impact:

- 52 million atom electronic structure (101nm)^3.
- Quantum dots, nanowires, quantum computing…

Capabilities:

- Arbitrary 3D zincblende, wurzite crystals
- Strain in Valence Force Fields
- Piezo Electricity through potential perturbation
- Electronic Structure with empirical tight binding

Applications:

- InAlGaAs/GaAs quantum dots
- Valley splitting in Silicon
- Alloy disorder in bulk, QD, nanowires
- Single impurities in Si

Multi-Million Atom Simulation of Quantum States and Transport in Realistically Extended Devices in Silicon for Quantum Computing

Gerhard Klimeck, Rajib Rahman, S-H Park, Hoon Ryu,
Sunhee Lee, Muhammad Usman, Neerav Kharche, **Purdue**

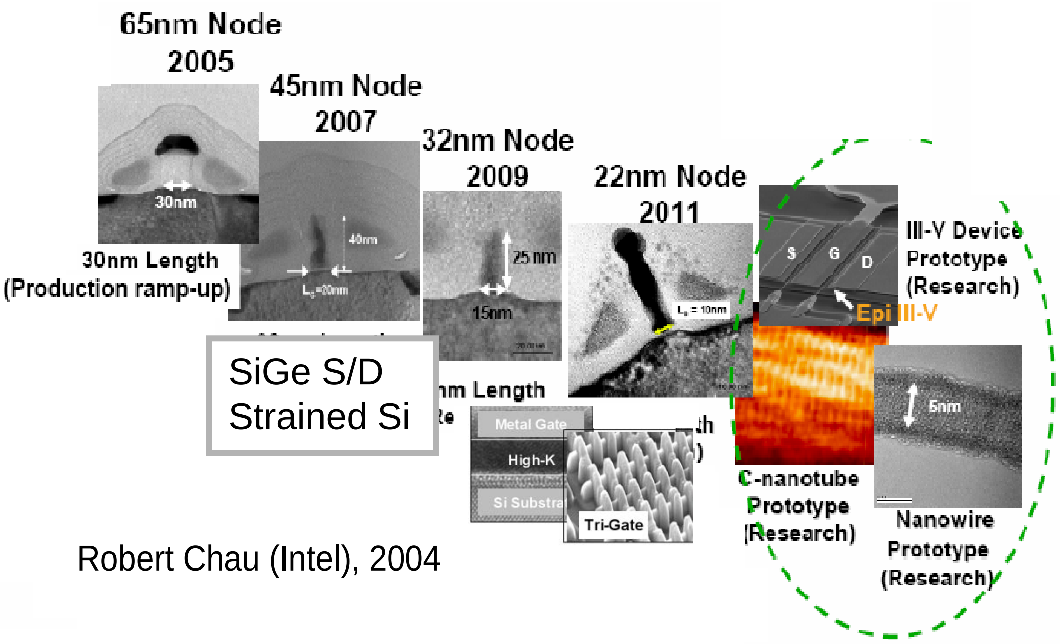
Lloyd Hollenberg, **Melbourne**

Sven Rogge, G. Lansbergen, **Delft**

Michelle Simmons, Bent Weber, S. Mahapatra, **UNSW**

Rajib Rahman, Richard Muller, **Sandia**

Industrial Device Trends and Challenges



SiGe S/D
Strained Si

Robert Chau (Intel), 2004

Observations:

- 3D spatial variations on nm scale
- Potential variations on nm scale
- New channel materials (Ge, III-V)

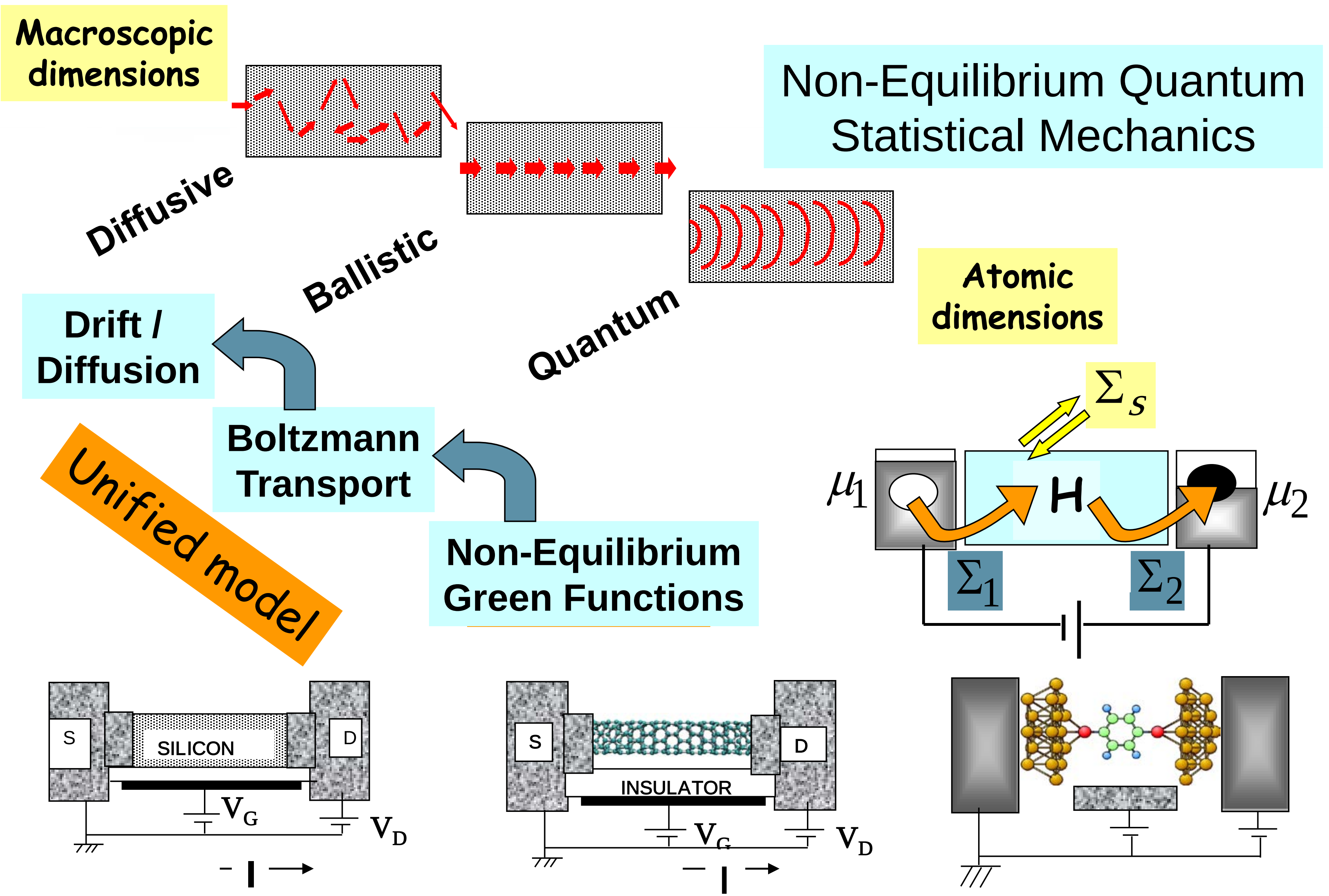
Questions / Challenges

- Strain ?
- Quantization?
- Crystal orientation?
- Atoms are countable; does granularity matter? Disorder?
- New material or new device?

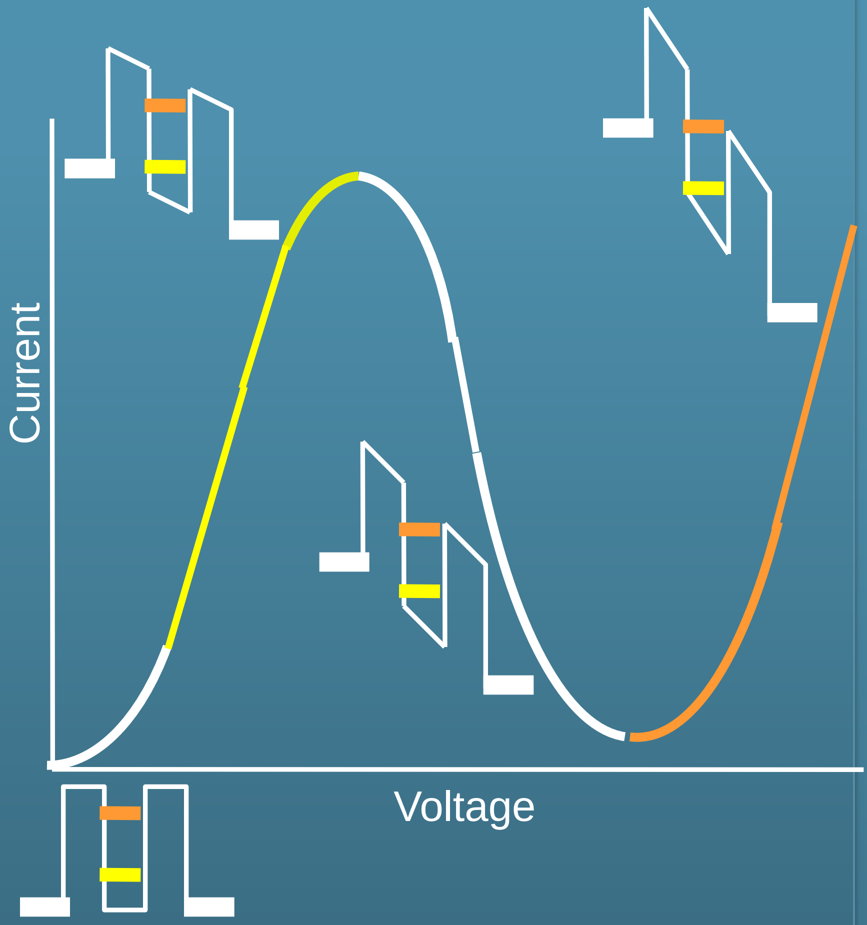
Assertions of importance

- High bias / non-equilibrium
- Quantum mechanics
- Atomistic representation
  - » Band coupling, non-parabolicity, valley splitting
  - » Local (dis)order, strain and orientation

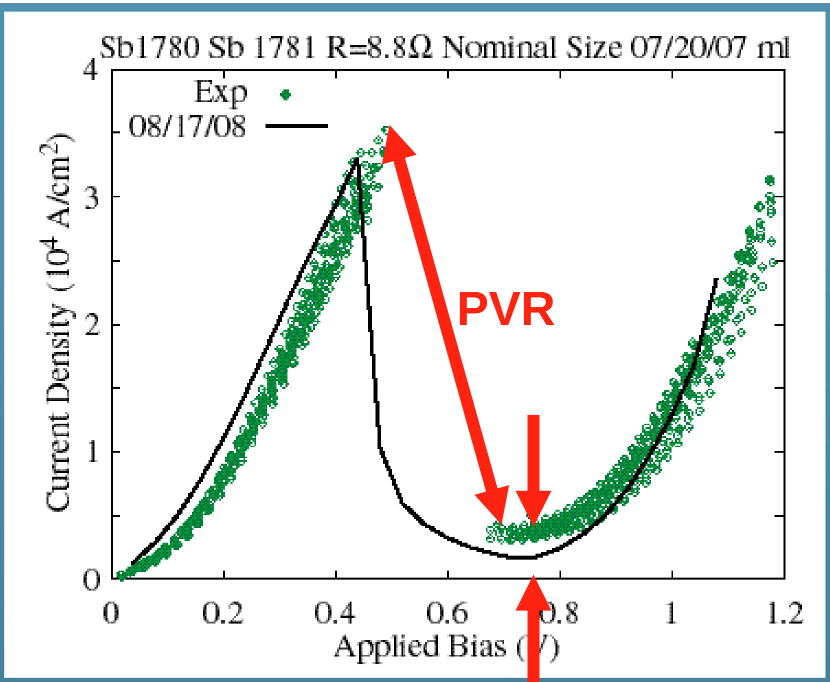
Quantum Transport far from Equilibrium



The first 300K Quantum Transport Device Controlled at Atomic Monolayers



Conduction band diagrams for different voltages and the resulting current flow



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

PVR – Peak-to-Valley-Ratio

1994: Best experiment PVR=80

=> On-Off-Ratio should to be >1,000

1994: What is the valley current physics?

1997: Can overlay experiment and theory.

What are the key insights?

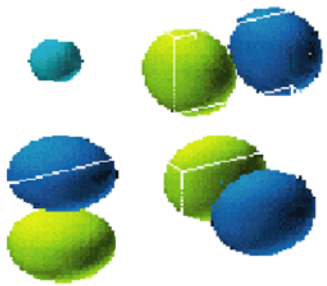
Atomistic device resolution (2-5nm dim.)

Extended contacts with scattering

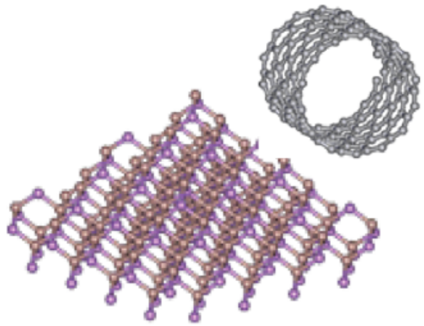
Extended electrostatics

First industrial NEGF device simulator

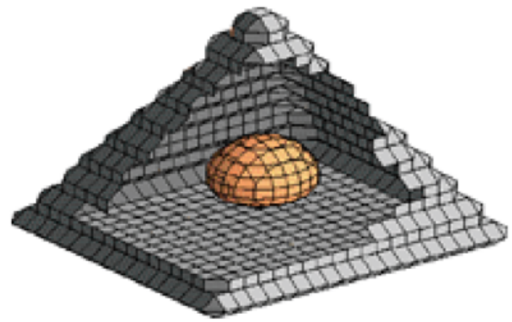
NEMO 3-D Technical Approach



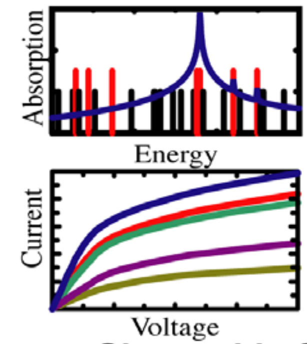
Atomic Orbitals
size: 0.2nm



Structure
Millions of Atoms



Nanoscale Quantum States
(Artificial Atoms, size ~20nm)



Designed Optical Transitions
Sensors

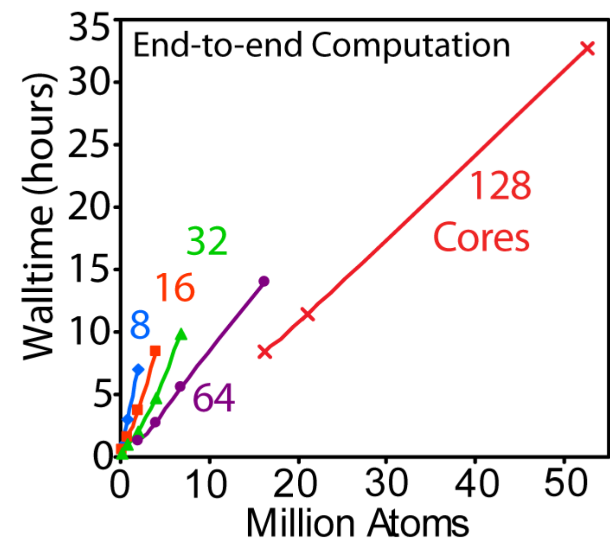
Quantum Dots, Wires, Wells
Dispersions
Computing

Observable Quantities from Atomistic Quantum Mechanics

Problem:

Nanoscale device simulation requirements:

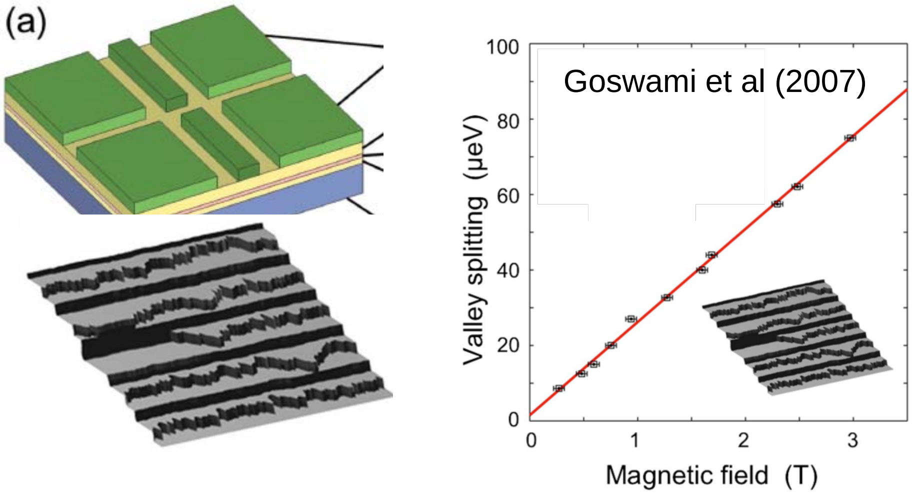
- Cannot use bulk / jellium descriptions, need description atom by atom
  => use pseudo-potential or local orbitals
- Consider finite extend, not periodic
  => local orbital approach
- Bonds in semiconductors are stable!
  => Do not need ab-initio methods!
- Need to include about one million atoms.
  => need massively parallel computers
- Tight binding in a design tool: NEMO3D



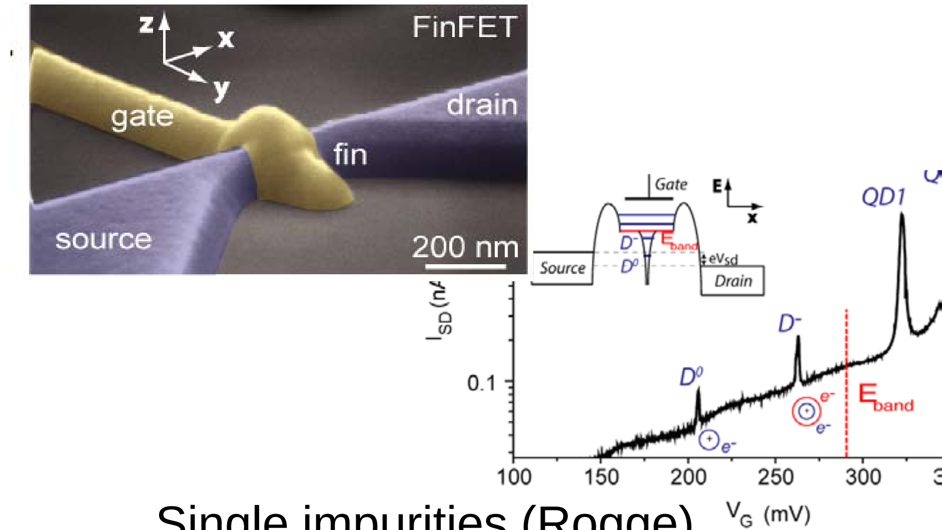
Demonstration / Capability / Impact:

- 52 million atom electronic structure $(101nm)^3$.
- Quantum dots, nanowires, quantum computing…

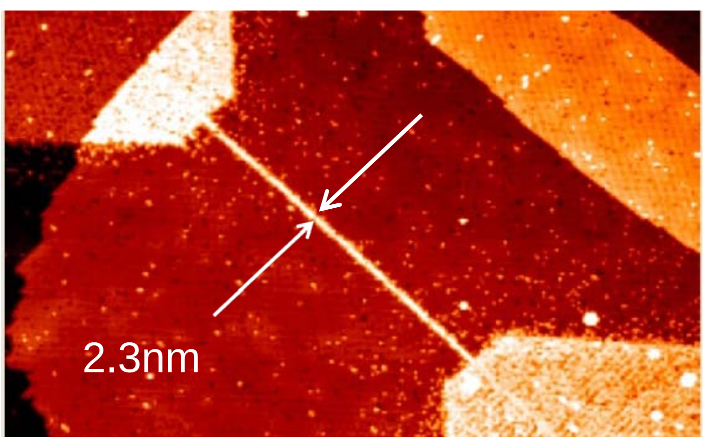
Quantum States in Silicon – Impurities / Quantum Dots



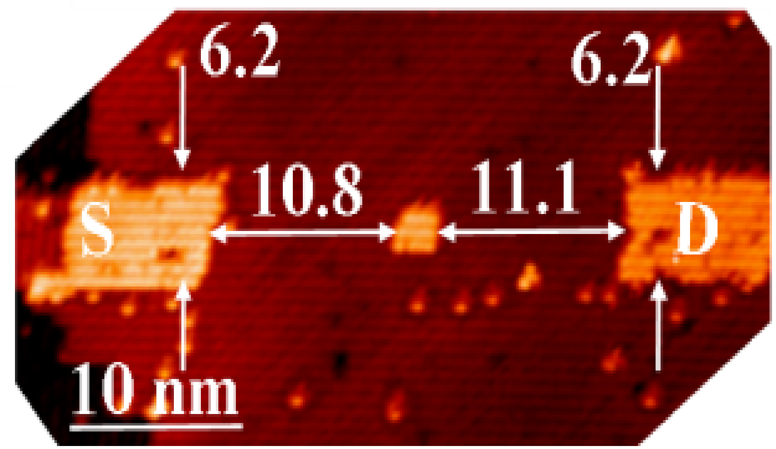
Si QD on SiGe (Eriksson)



Single impurities (Rogge)



Si:P nanowires (Simmons)



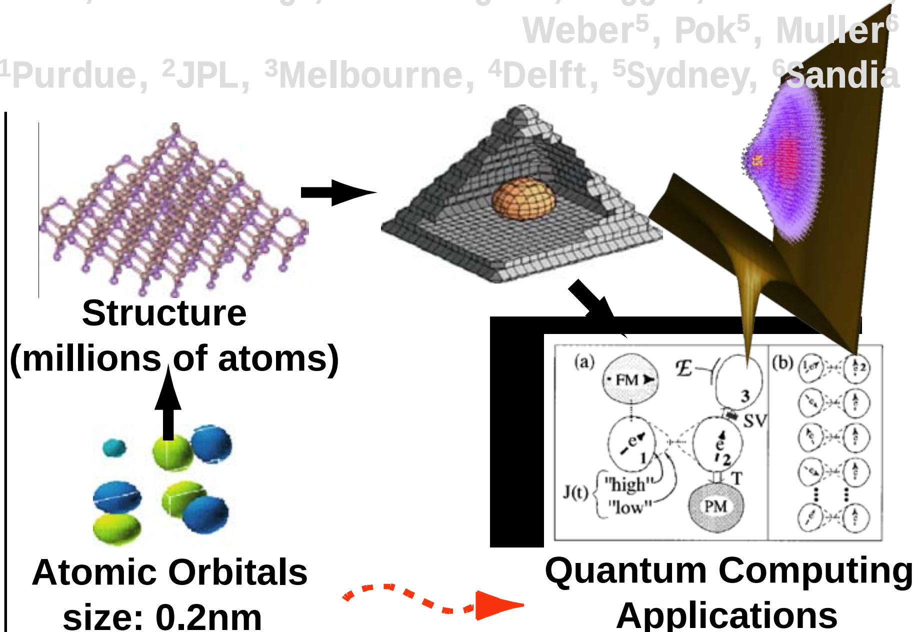
Si:P quantum dots (Simmons)

Nanoelectronic Modeling (NEMO) for High Fidelity Simulation of Solid-State Quantum Computing Gates

Klimeck[1,2], Rahman[1,6], Park[1], Ryu[1], Lee[1], Wellard[3], Cole[3], Hollenberg[3], Lansbergen[4], Rogge[4], Simmons[5], Weber[5], Pok[5], Muller[6]
[1]Purdue, [2]JPL, [3]Melbourne, [4]Delft, [5]Sydney, [6]Sandia

Objective

- Narrow experimental qubit parameter space
- Development of a comprehensive suite of modeling tools for solid state qubit devices.
- Atomic level material description.
- Model both spin and charge coherent devices.
- Magnetic field effect on electronic structure and state coherence.
- Compute interactions.



Objective Approach

- Leverage about 50,000 hours NEMO 1-D and 20,000 hours NEMO 3-D development.
- Model semicond. Quant. Comput. Syst.
  - Si on SiGe (Wisconsin / Eriksson)
  - P in Si (Australia / Dzurak)
  - Si QD in SiGe (Purdue / Rokhinson)
- Atomistic of treatment semiconductors.
- Incorporate many-body effects through Hartree & configuration interaction.

Impact / Studies

- VS in flat Si QW - (2004)
- VS in slanted Si/SiGe QW - (2007) - exp
- VS in Si/SiGe QD - (2008)
- VS in Si [111] QW - (2009) – exp
- Single impurities in Si transport (2008) - exp
- Single impurities in Si Stark Eff (2008) - exp
- Single impurities g-factors (2009)
- Single impurities CTAP design (2009)
- Single impurities Wavefunction Map (2009)
- Dense impurities in Si QW – ongoing - exp
- Dense impurities in Si Wire – ongoing - exp

Thanks to

NRI

Nanoelectronics • Architectures
MIND
MIDWEST INSTITUTE FOR NANOELECTRONICS DISCOVERY

SRC

FCRP

SCIENCE TO SHAPE THE FUTURE OF THE ARMY
ARMY RESEARCH OFFICE
1951

NSF

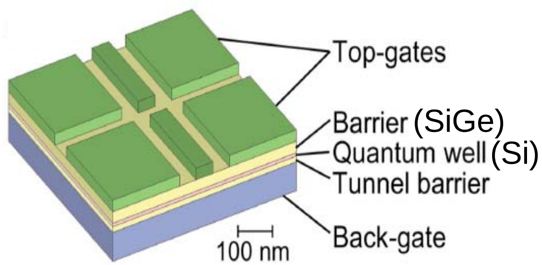
Multi-Million Atom Simulation of Quantum States in Realistically Extended Devices in Silicon

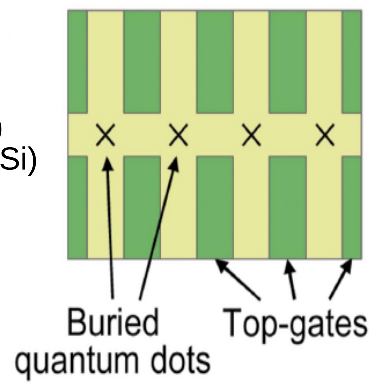
- Motivation
- NEMO Numerical Engine
- Valley splitting
  - »Si quantum wells
  - »Si Quantum Dots
- Single impurities in Si
  - »Metrology – impurity identification
  - »Wavefunction mapping
  - »g-factor engineering
  - »CTAP
- Dense impurities in Si – Si:P
  - »Infinite sheets
  - »Infinite wires
  - »Gating, transport through wires
  - »Impurity-based quantum dots

Valley-splitting in strained Silicon quantum wells on a miscut substrate

Authors: **Neerav Kharche**, Marta Prada, Timothy Boykin, and Gerhard Klimeck

Spin based quantum computing in Si/SiGe heterostructures





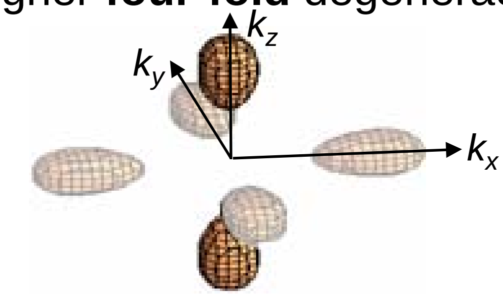
Friesen et al. Phys. Rev. B, **67**, 121301(R) (2003)

Potential problem: Valley degeneracy

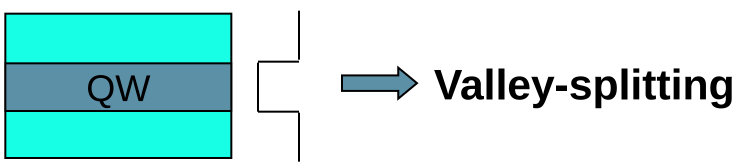
- Six-fold degenerate valleys lead to spin decoherence

Biaxial strain splits **six-fold** valley-degeneracy into

- Lower **two-fold** degeneracy
- Higher **four-fold** degeneracy



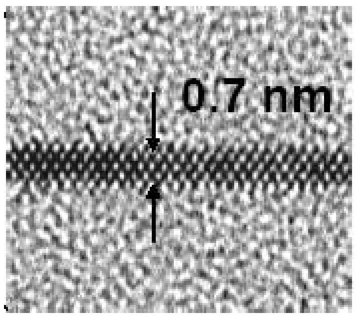
- Lowest two-fold degenerate **valleys split** in the presence of sharp confinement potentials in QWs.

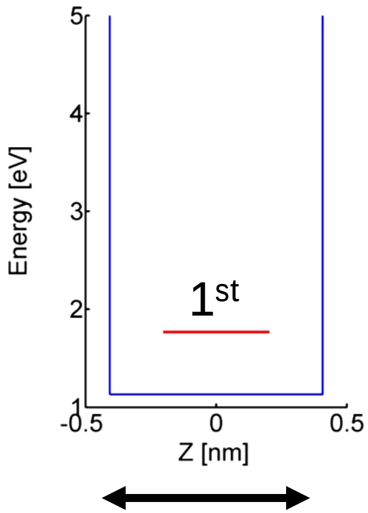


- Valley-splitting is a critical design parameter for QC devices.

Ultra Thin Body SOI:
A traditional Quantum Well?

Five Atomic Layer
Si (001)
IEDM, Uchida





Most basic quantum mechanical problem: Particle in a box!

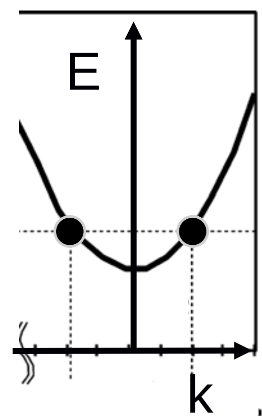
Expect / Remember:
- State quantization
- 2 counter-propagating states
- 1 bound state
- $E \sim 1/L^2$

Schrödinger Equation

$$\left(E - \frac{\hbar^2}{2m^*}\frac{d^2}{dz^2} - V(z)\right)\Psi(z) = 0$$

$$E = \frac{\hbar^2 k^2}{2m^*}$$

Parabolic Dispersion



$$k_1 = \frac{\pi}{L}$$ quantize

$$\Psi(z) = e^{-ik_1 z} \quad \Psi(z) = e^{+ik_1 z}$$ 2 propagating states

$$\Psi(z) = \sin(k_1 z)$$ 1 bound state

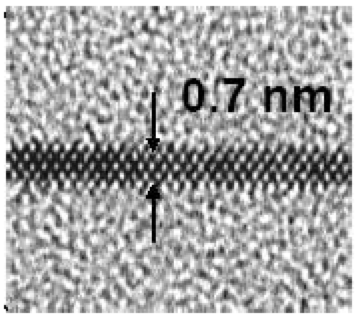
$$E = \frac{\hbar^2}{2m^*}\frac{\pi^2}{L^2}$$

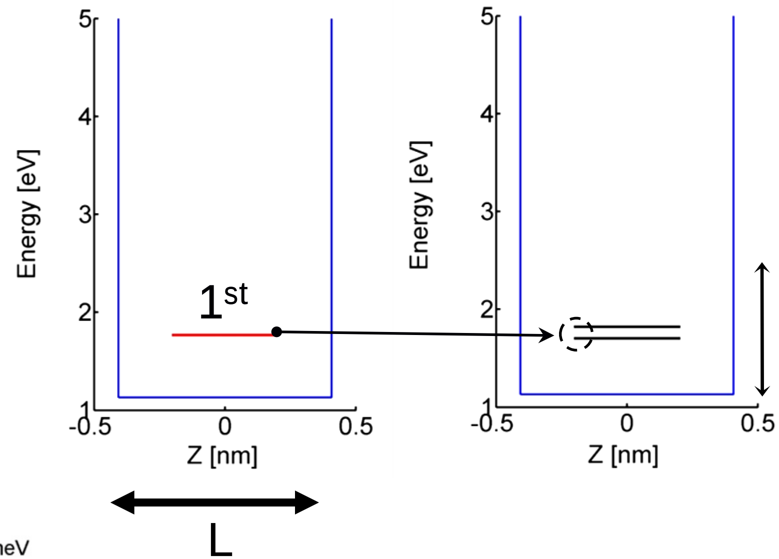
$$E \sim \frac{1}{L^2}$$

Quantum Wells

Special Considerations in Si

Five Atomic Layer
Si (001)
IEDM, Uchida

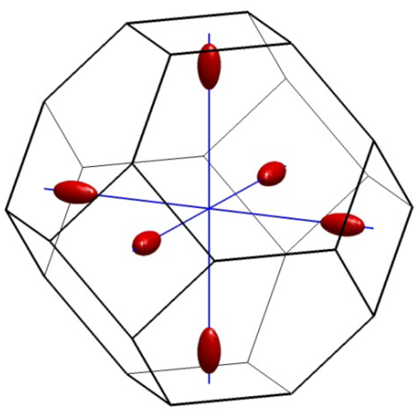


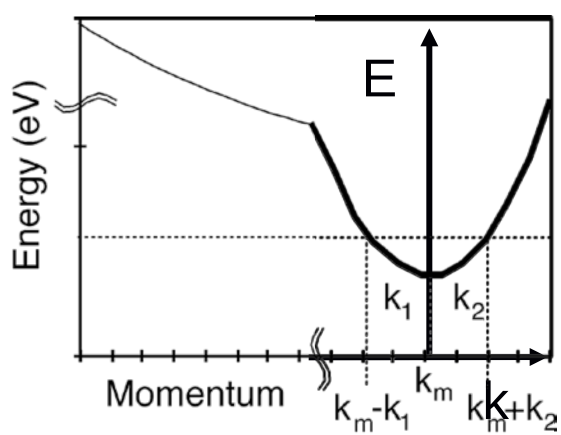


Envelope:
$k_{1/2}$ ~ a/na
a: lattice constant
n: QW layers (L=na)

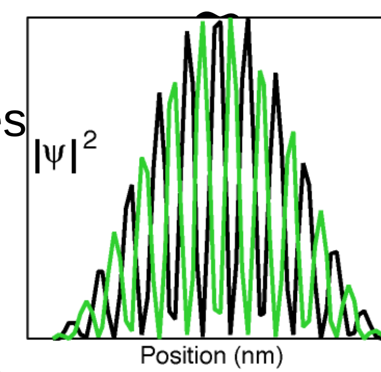
Phase control:
k_m ~ 0.85 a/a
Depends on
atomic overlaps

$sp^3s^*d^5$ (Klimeck *et al*) CB, ΔE_c=+100 meV



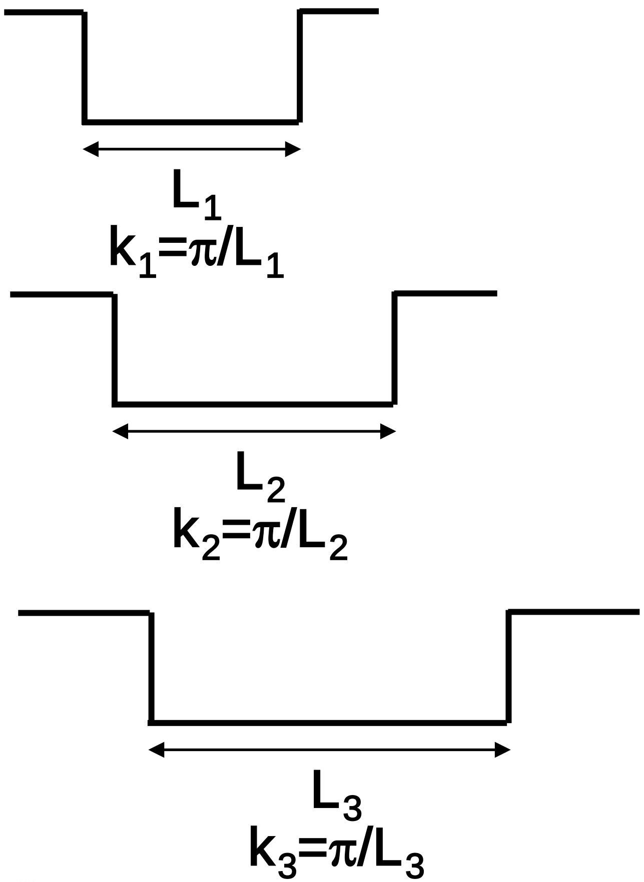


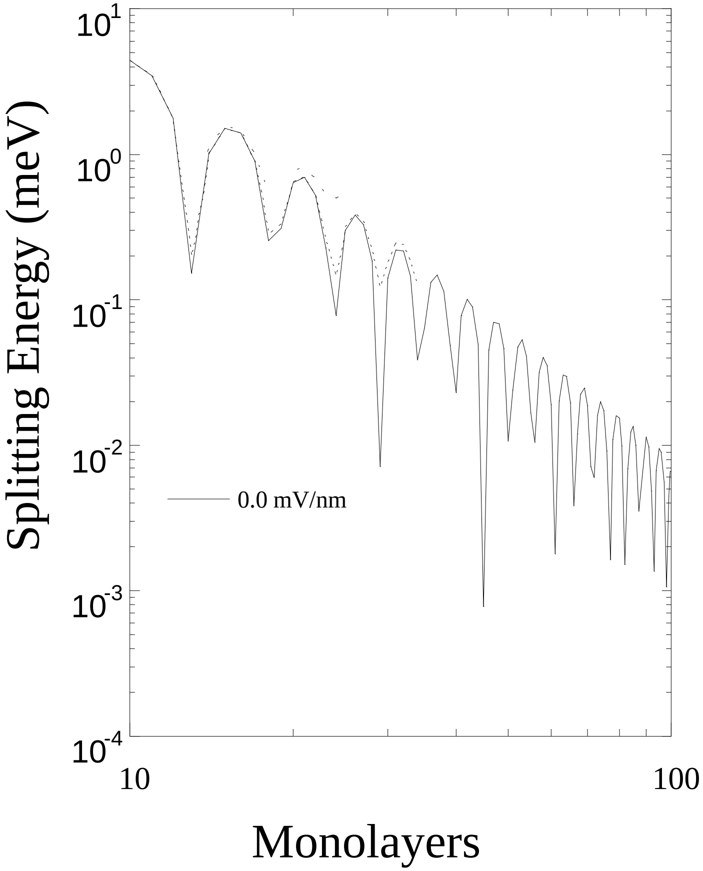
2 valleys
4 propagating states
↓
2 bound states
$k_{1,2}$ envelope
k_m fast oscillations



Splitting Behavior With Quantum Well Width

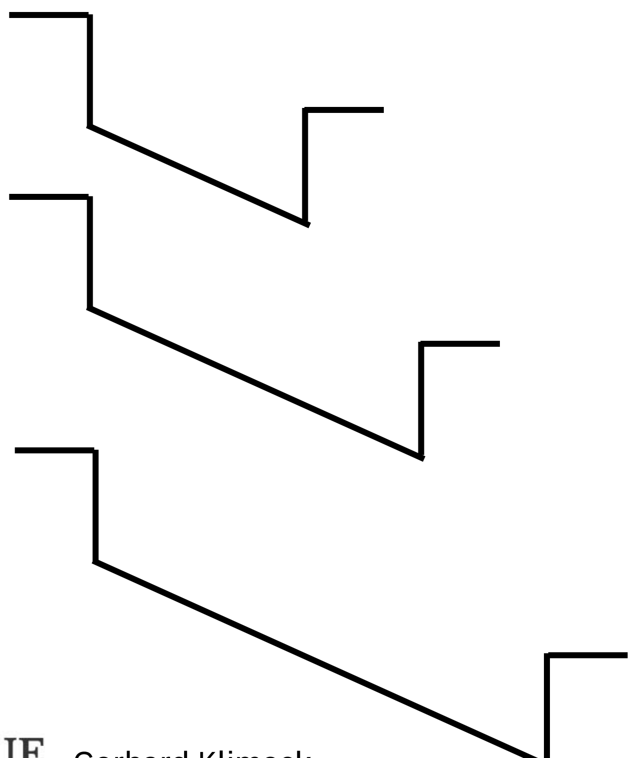
- Strained Si QW, Hardwall BCs
- Oscillations with Monolayers (decay as ML^{-3}) - published analytical results

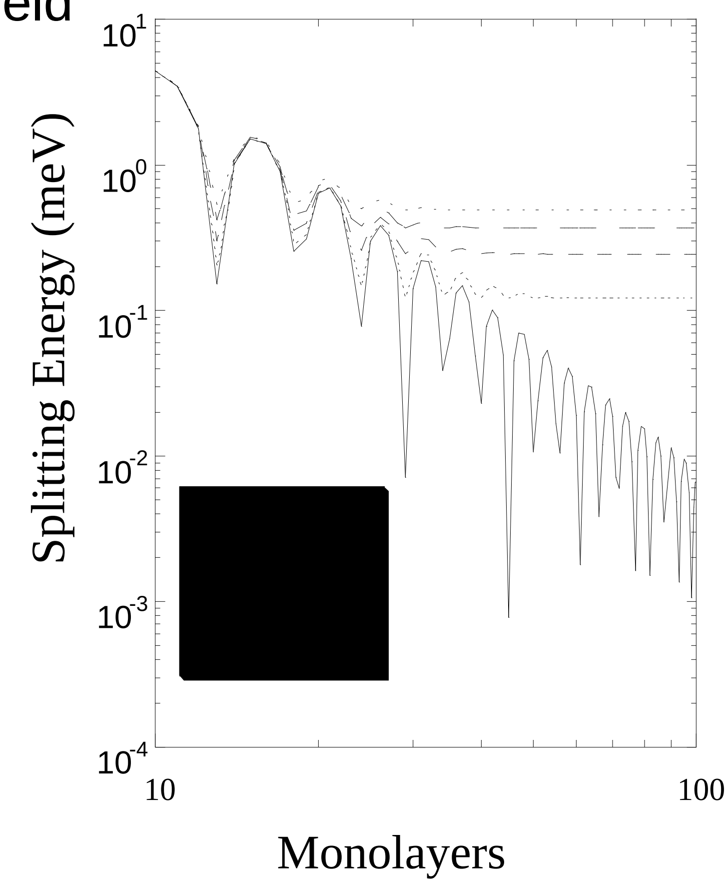




Splitting Behavior With Quantum Well Width and Electric Field

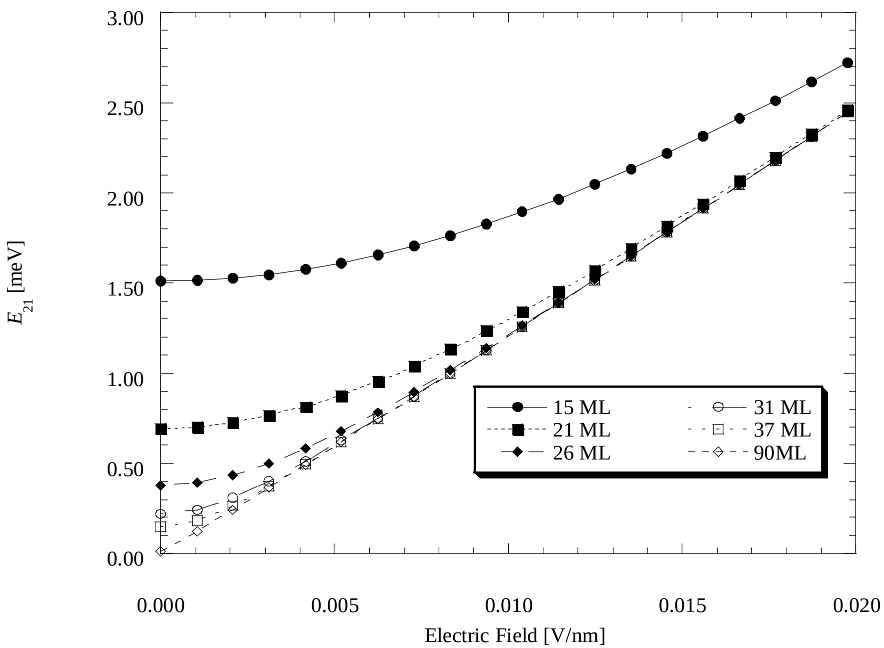
- Strained Si QW, Hardwall BCs
- Oscillations with Monolayers
- Oscillations decay with increasing Field
- Decay significant once drop/ML is of order zero-field splitting

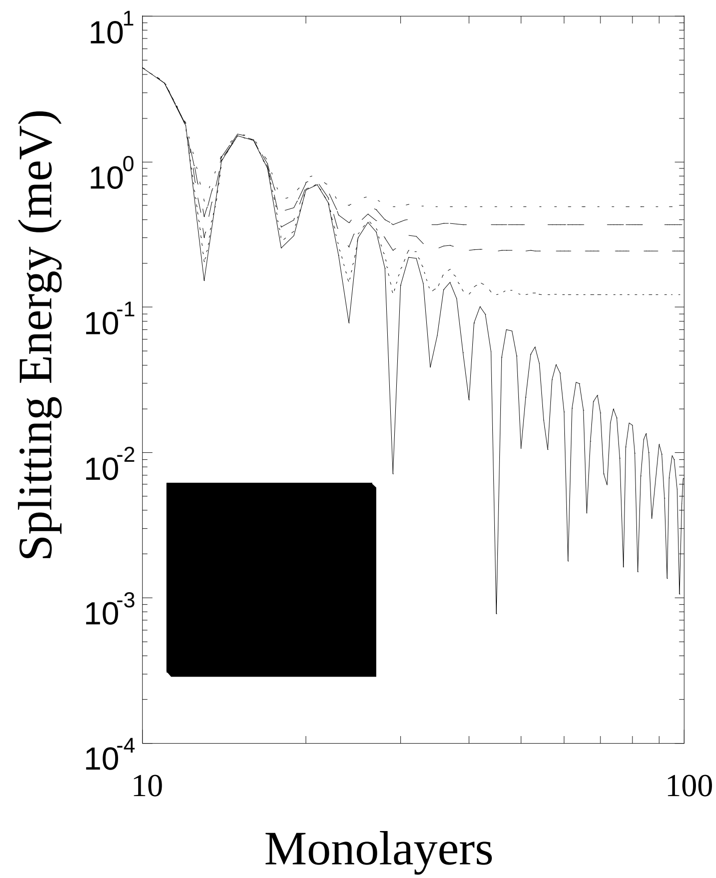




Splitting Behavior With Quantum Well Width and Electric Field

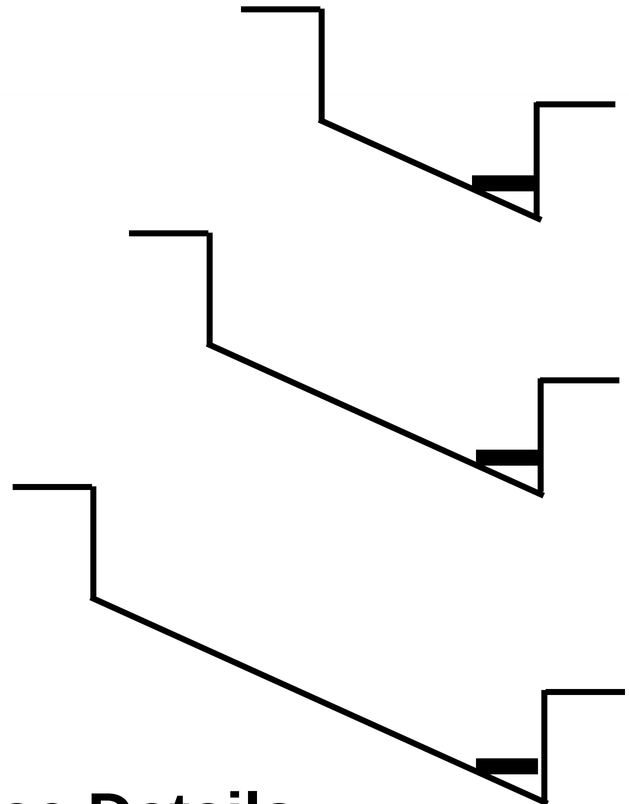
- Strained Si QW, Hardwall BCs
- Oscillations with Monolayers
- Oscillations decay with increasing Field
- Decay significant once drop/ML is of order zero-field splitting
  - For fixed *L*, splitting linear at high field, nonlinear at low field

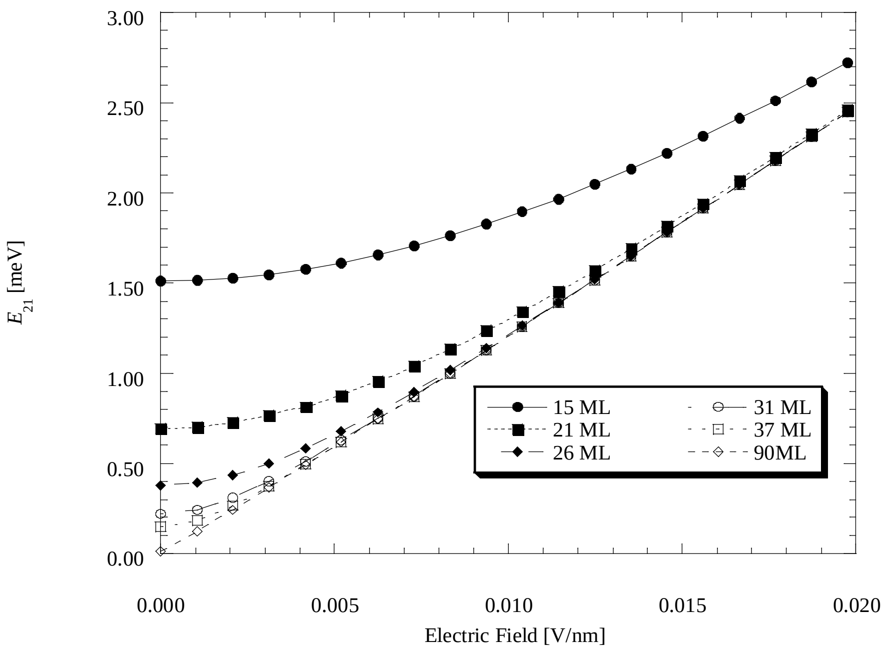




Splitting Behavior With Quantum Well Width and Electric Field

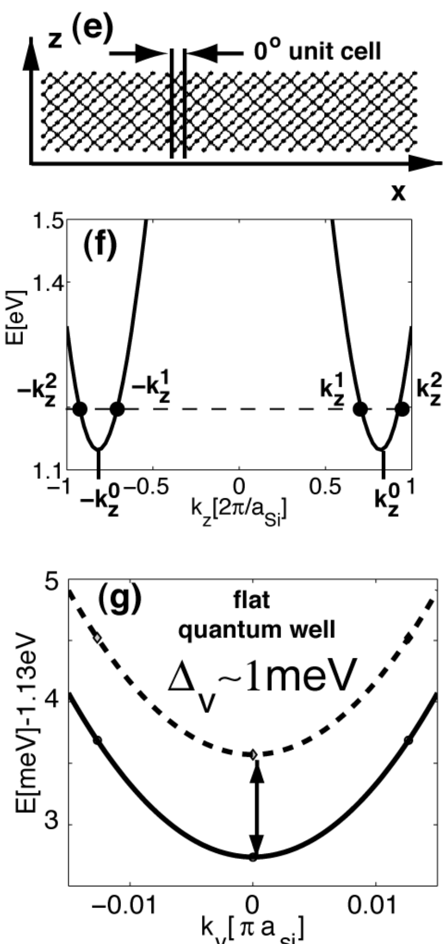
- Strained Si QW, Hardwall BCs
- Oscillations with Monolayers
- Oscillations decay with increasing Field
- Decay significant once drop/ML is of order zero-field splitting
- For fixed *L*, splitting linear at high field, nonlinear at low field

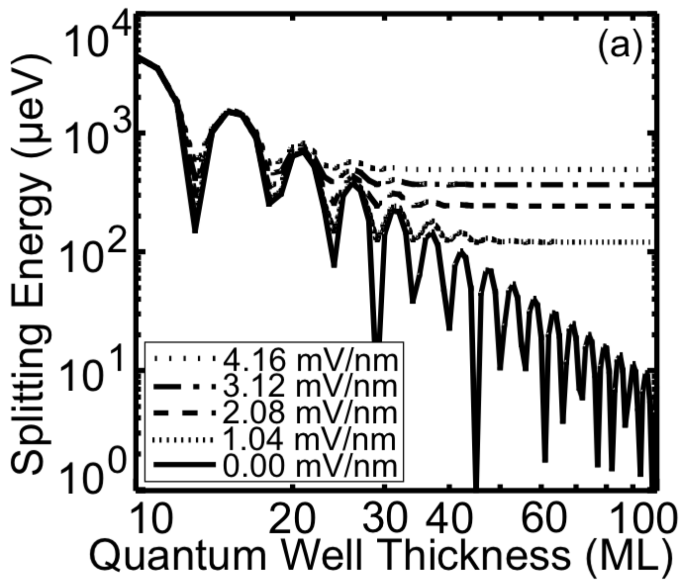


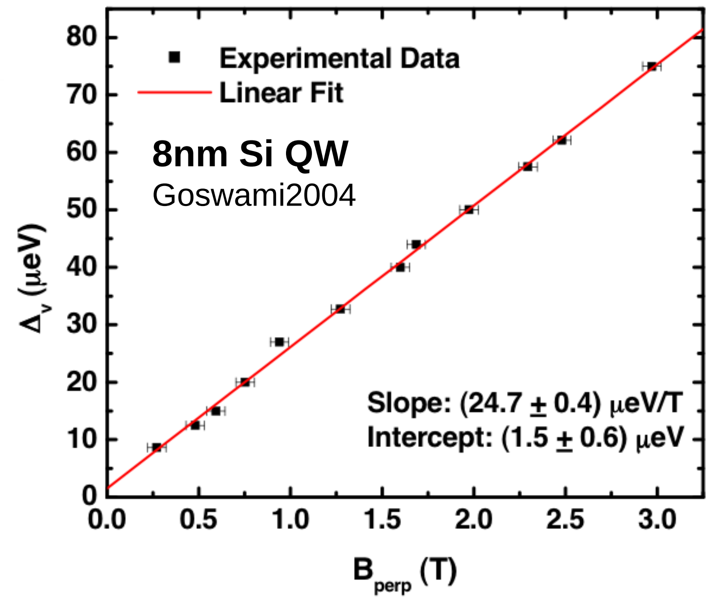


Device Details (structure, materials, local fields,) determine energy splitting

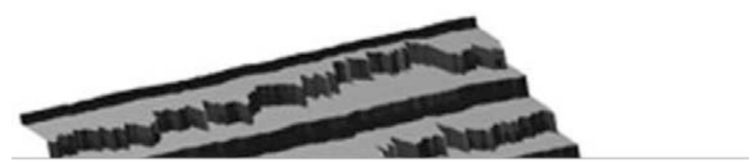
Valley Splitting Physics Flat Quantum Well







Why is the experimental valley splitting so much smaller?

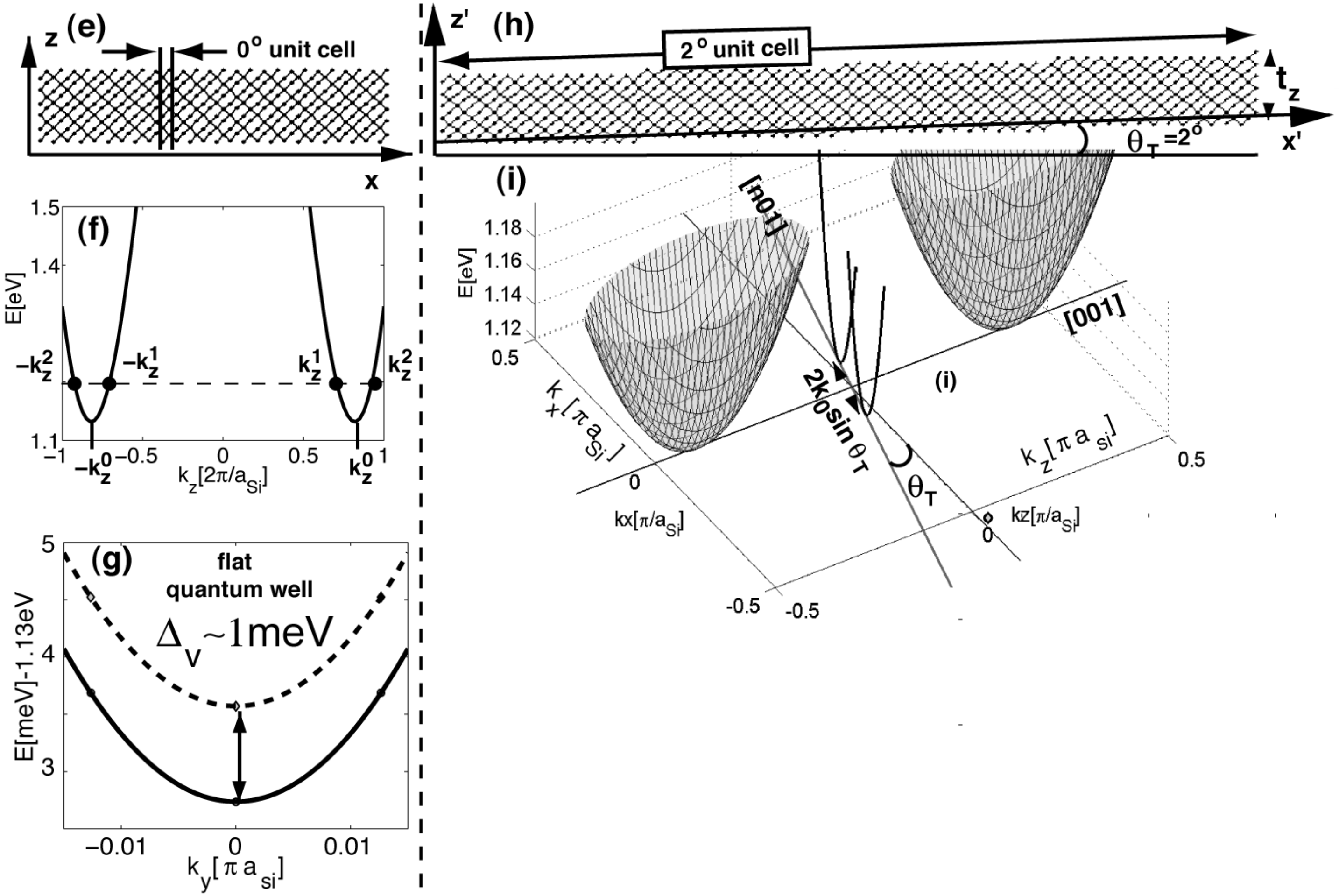


Well Understood

APL, Vol. 84, pg. 115-117, 2004

Phys. Rev. B. Vol. 70, 165325 (2004),

Valley Splitting Physics
tilted quantum well

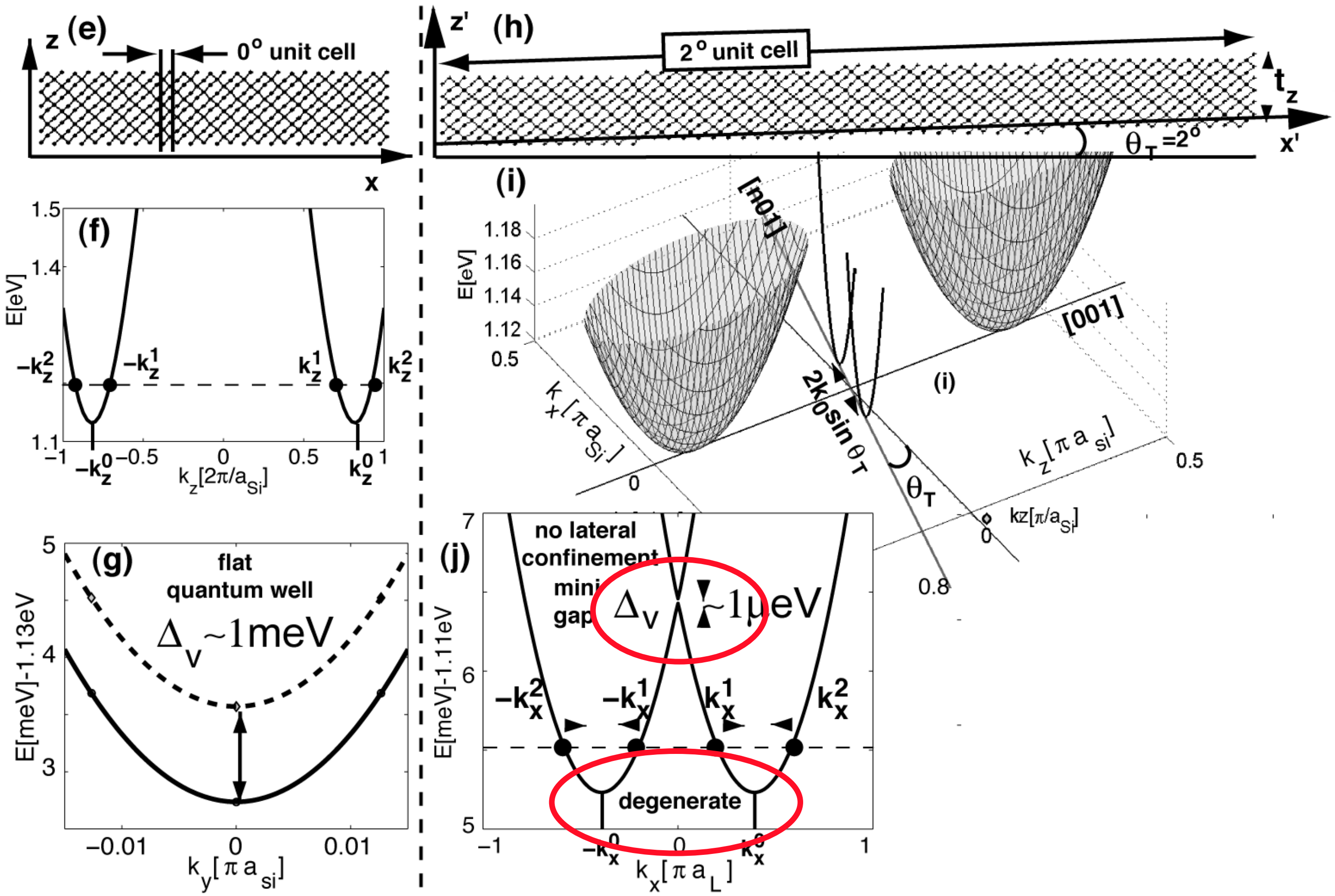


Well Understood

What happens with a tilted substrate?
"Parabolas" do not overlap perfectly on the plane!

Valley Splitting Physics

ideal tilted quantum well - zero valley splitting

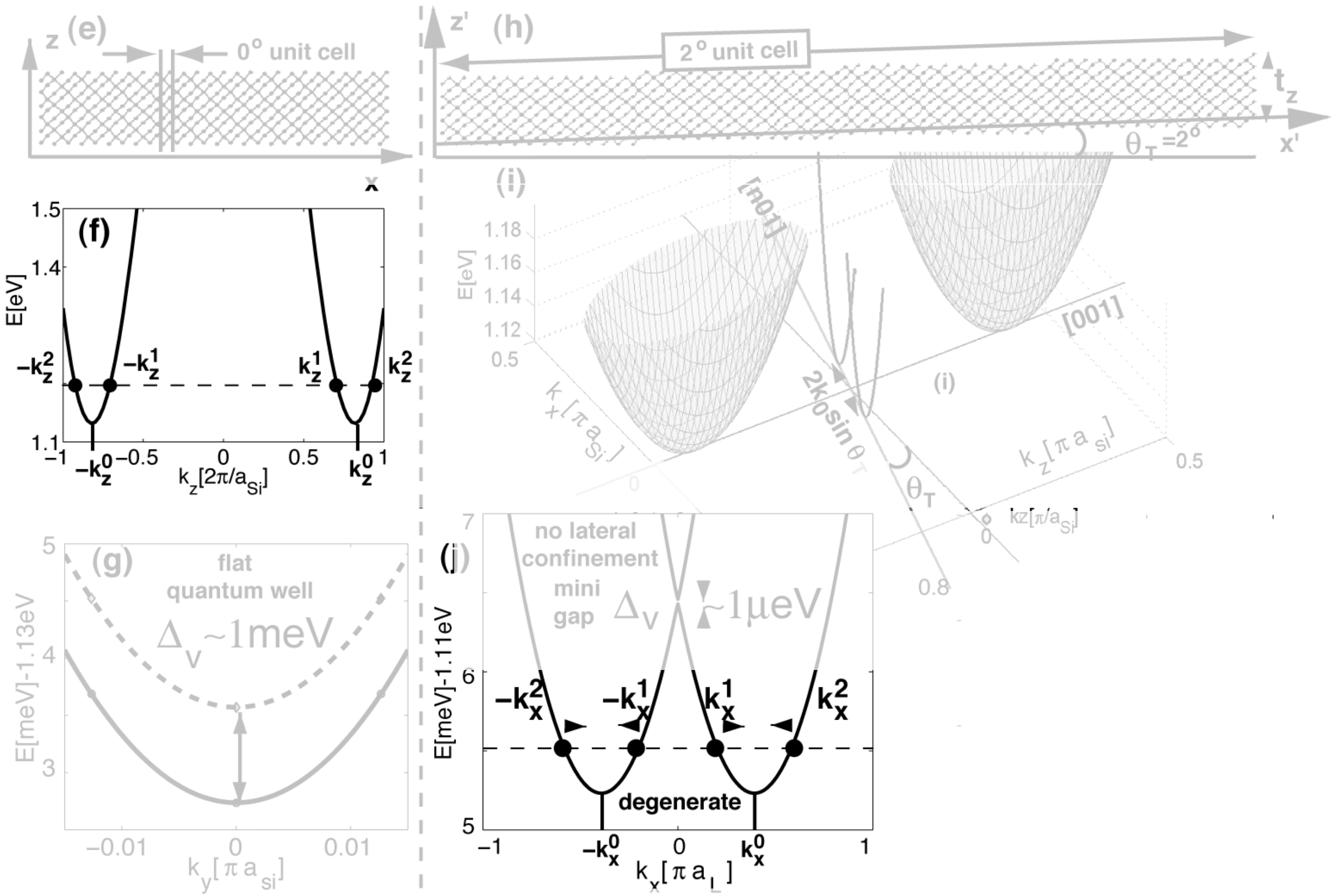


Well Understood

What happens with a tilted substrate?
"Parabolas" do not overlap perfectly on the plane!
Coherent overlap only at k=0 leads to minigap!
Valley Splitting is ZERO!

Valley Splitting Physics

need symmetry breaking to induce valley splitting



Well Understood

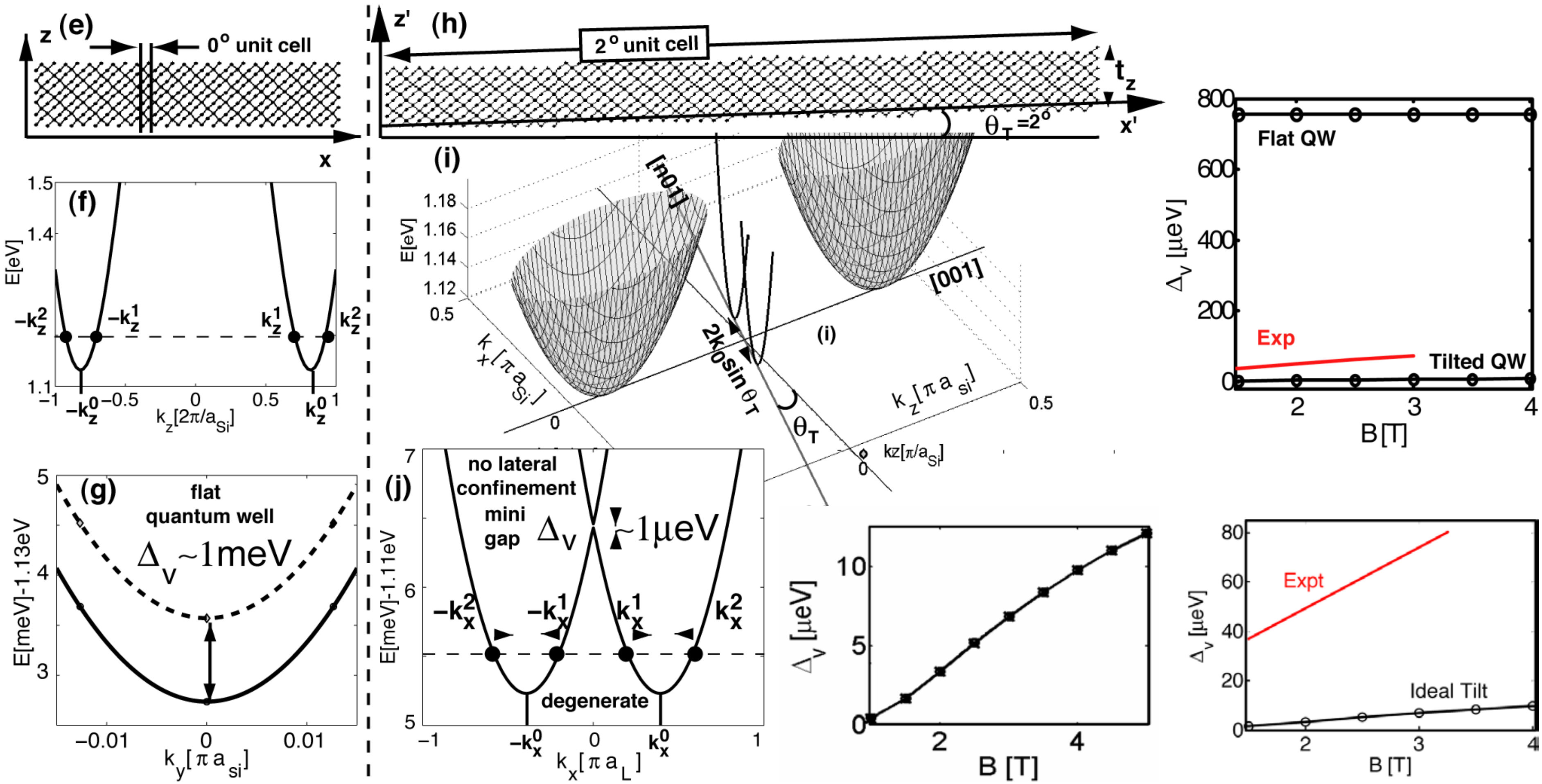
What happens with a tilted substrate?

"Parabolas" do not overlap perfectly on the plane!

Need symmetry breaking in x-direction to get valley splitting!

2 pairs of counter propagating states will create valley splitting!

Valley Splitting Physics
magnetic field confinement



Well Understood

What happens with a tilted substrate?

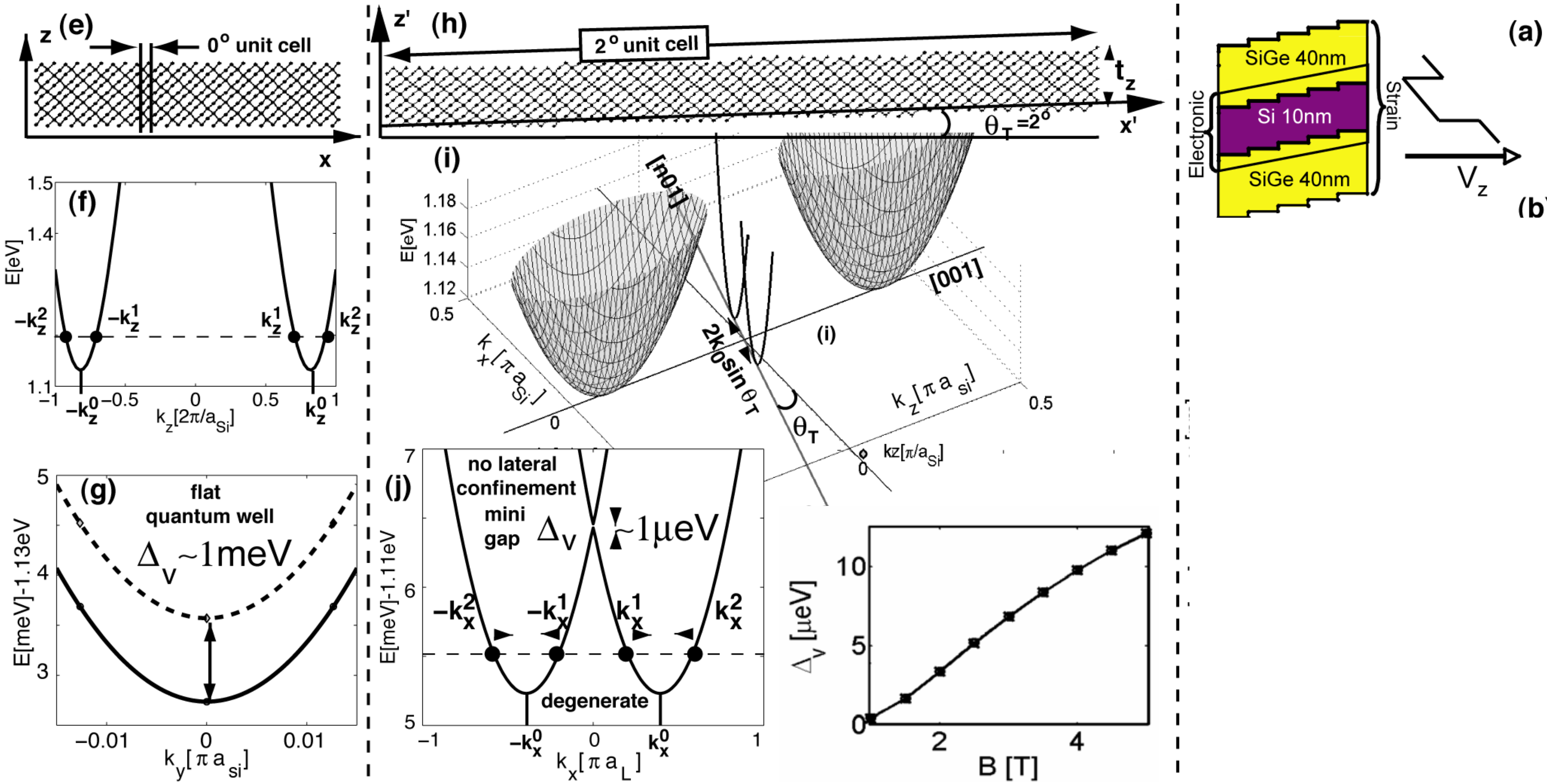
Need symmetry breaking in x-direction – confinement / mag.field

Ideal tilted QW underpredicts,

Ideal flat QW overpredicts VS!

Valley Splitting Physics

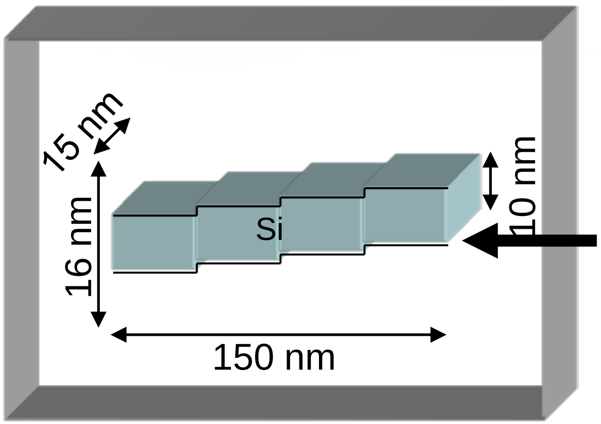
Other symmetry breaking mechanisms



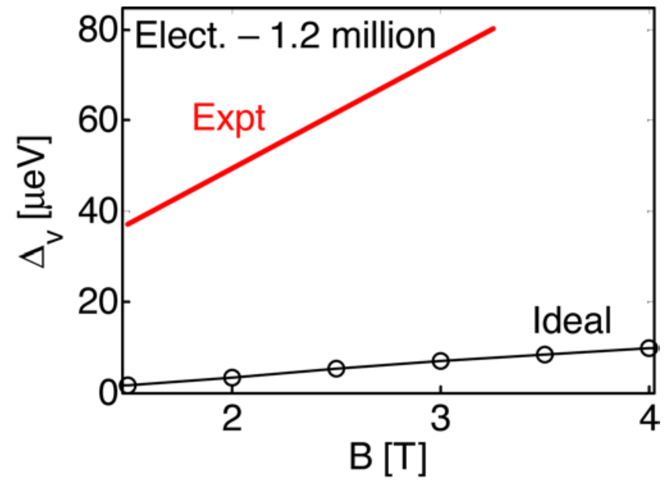
Well Understood

What happens with a tilted substrate?
Are there other symmetry breaking mechanisms?
Step disorder (happens on an atomic scale)
Alloy disorder (happens on an atomic scale)

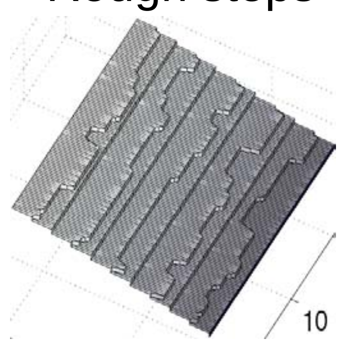
Effect of disorder on valley-splitting
step roughness

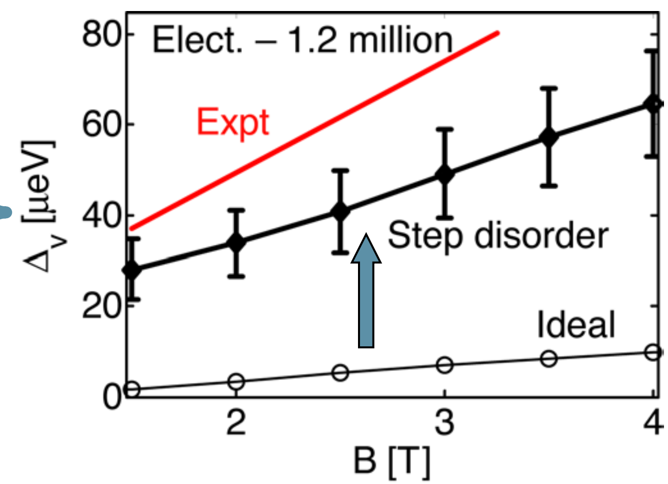


Elect. – 1.2 million
atoms



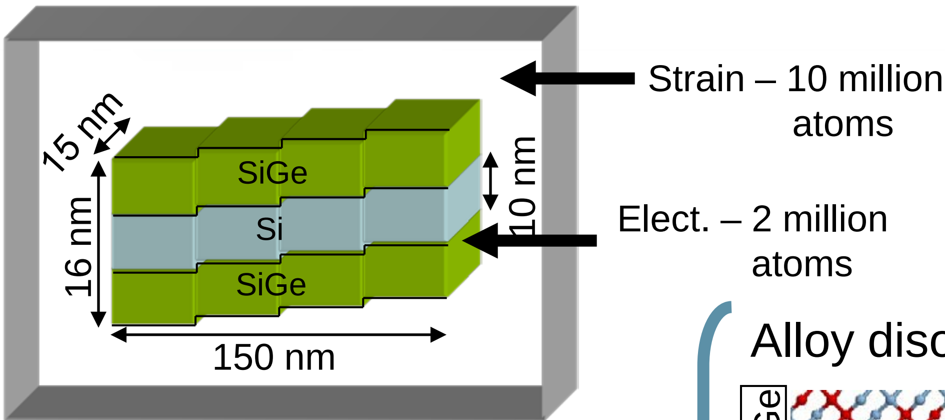
Rough steps

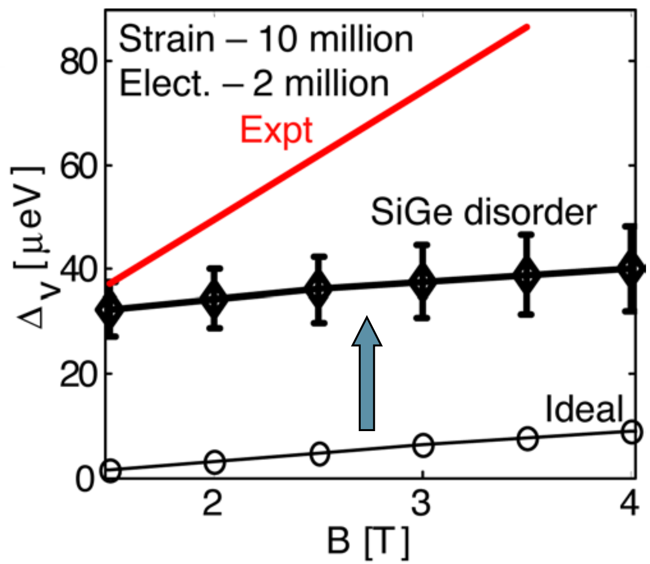


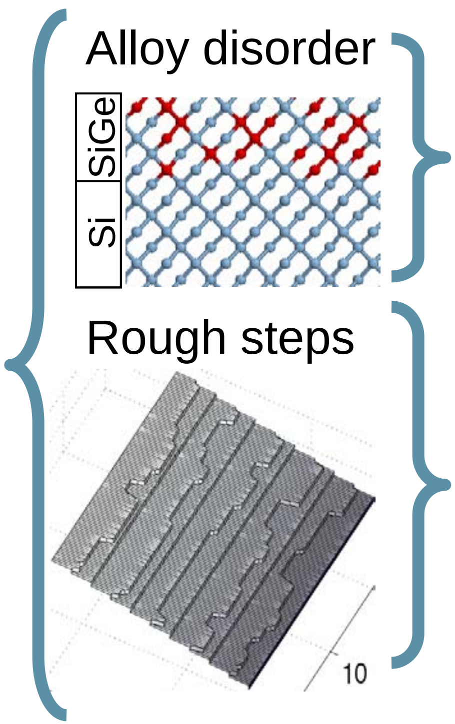


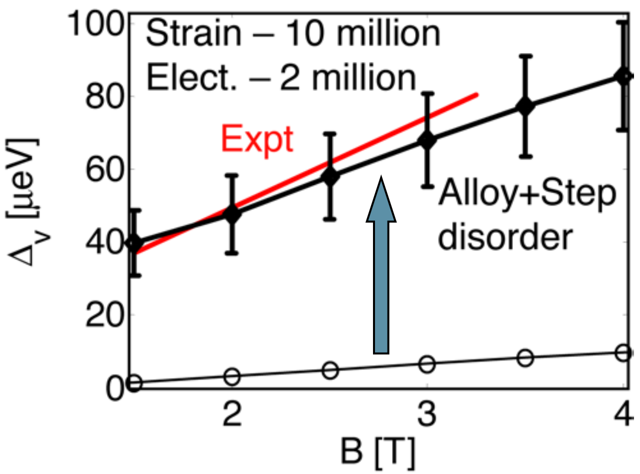
Kharche et al. Appl. Phys. Lett. **90**, 092109 (2007)

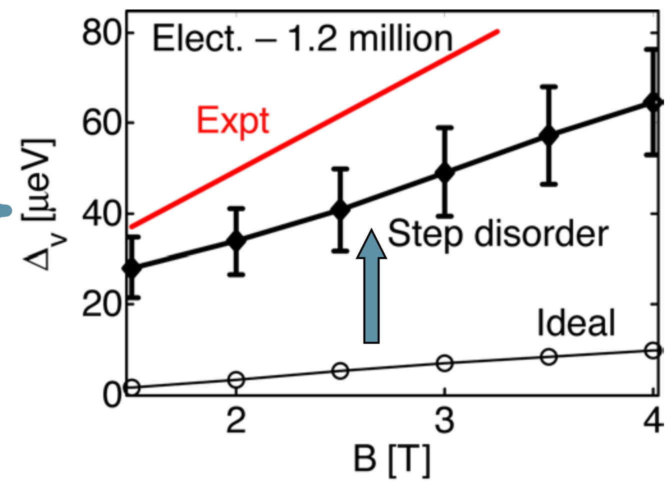
Effect of disorder on valley-splitting
step roughness and alloy disorder







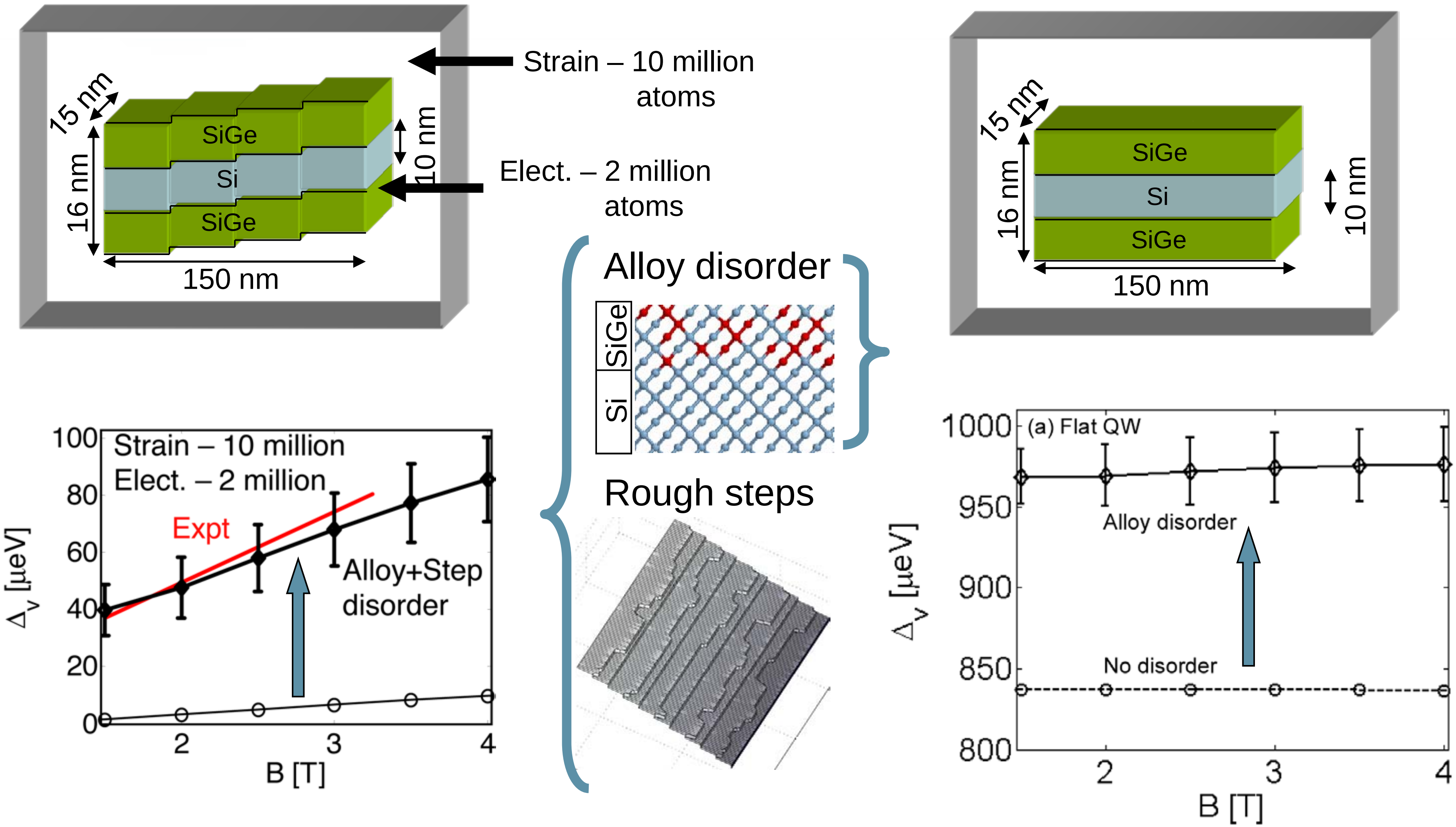




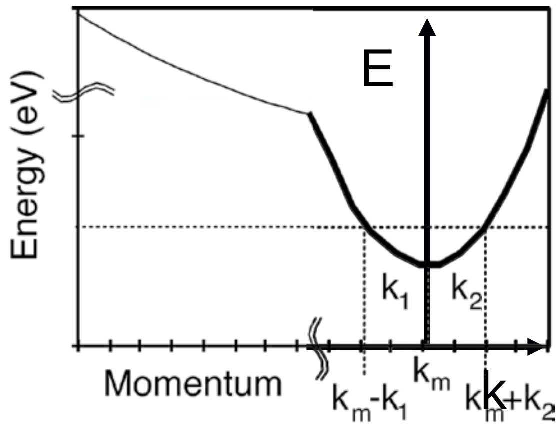
Kharche et al. Appl. Phys. Lett. **90**, 092109 (2007)

Effect of disorder on valley-splitting

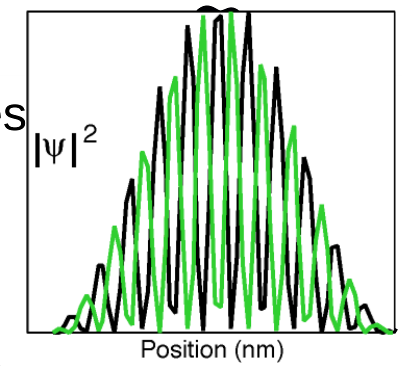
step roughness and alloy disorder



Quantum Wells
Special Considerations in Si



2 valleys
4 propagating states
↓
2 bound states
$k_{1,2}$ envelope
k_m fast oscillations



Envelope:
$k_{1/2} \sim$ a/na
a: lattice constant
n: QW layers L=na

Phase control:
$k_m \sim$ 0.85 a/a
Depends on
atomic overlaps

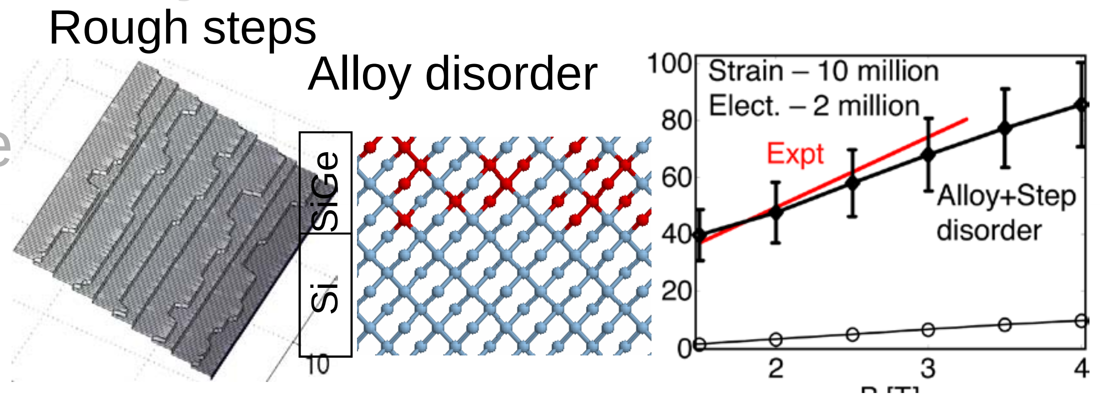
Rapid oscillation, k_m
⇒**sensitivity to atomic details** at the interface

Have demonstrated as critical understanding:
⇒Disorder in Barriers: Alloy and Step
Appl. Phys. Lett. **90**, 092109 (2007)

Analytical expressions for structures with fields:
JAP, Vol. 97, pg. 113702 (2005).

Analytical expressions for finite barriers:
Phys. Rev. B, Vol. 77, 245320 (2007)

Multi-Million Atom Simulation of Quantum States in Realistically Extended Devices in Silicon



- Motivation
- NEMO Numerical Engine
- Valley splitting
  - »Si quantum wells
  - »Si Quantum Dots
- Single impurities in Si
  - »Metrology – impurity identification
  - »Wavefunction mapping
  - »g-factor engineering
  - »CTAP
- Dense impurities in Si – Si:P
  - »Infinite sheets
  - »Infinite wires
  - »Gating, transport through wires
  - »Impurity-based quantum dots

Silicon Quantum Dots in SiGe Matrix

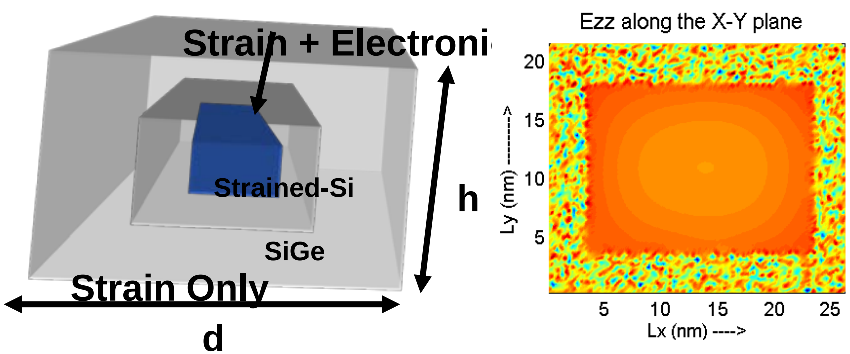
Srikant Srinivasan, Leonid Rokhinson, Gerhard Klimeck

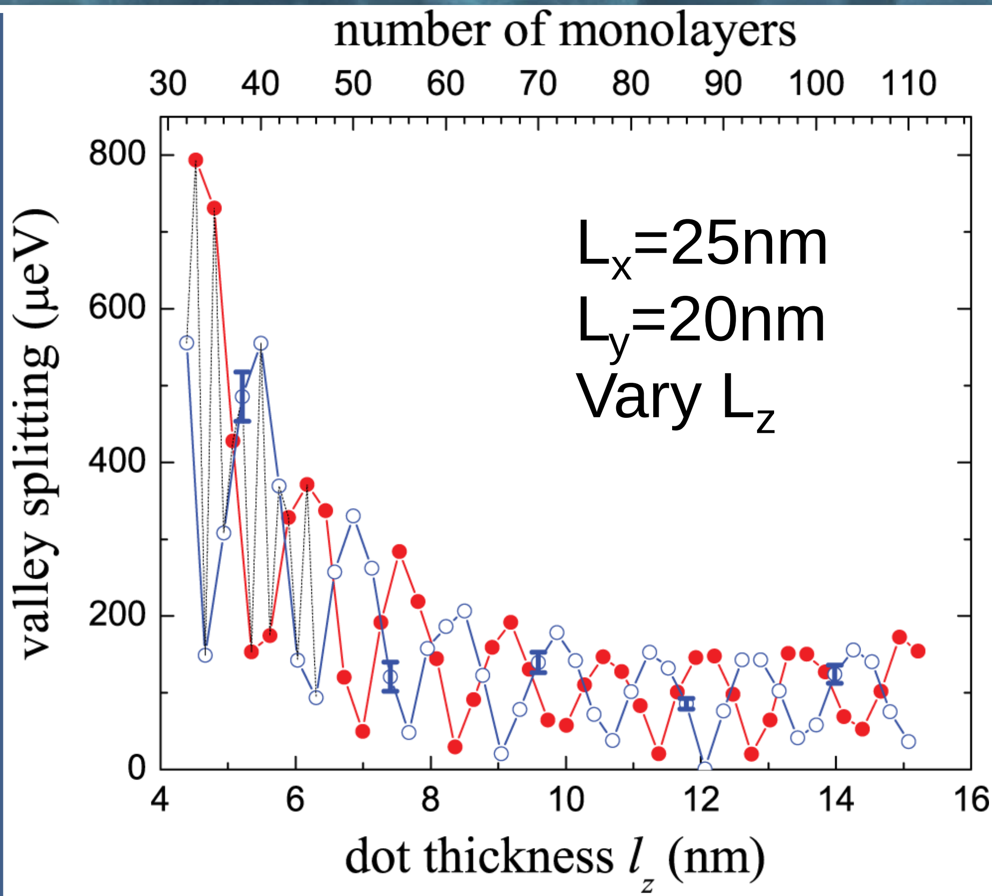
Objective:

- Prepare experiments (Rokhinson)
- Study realistic/large embedded Si QD
- Aid in understanding and design, buffer randomness, interfaces, Valley Splitting
- Explore size and disorder dependence

Approach:

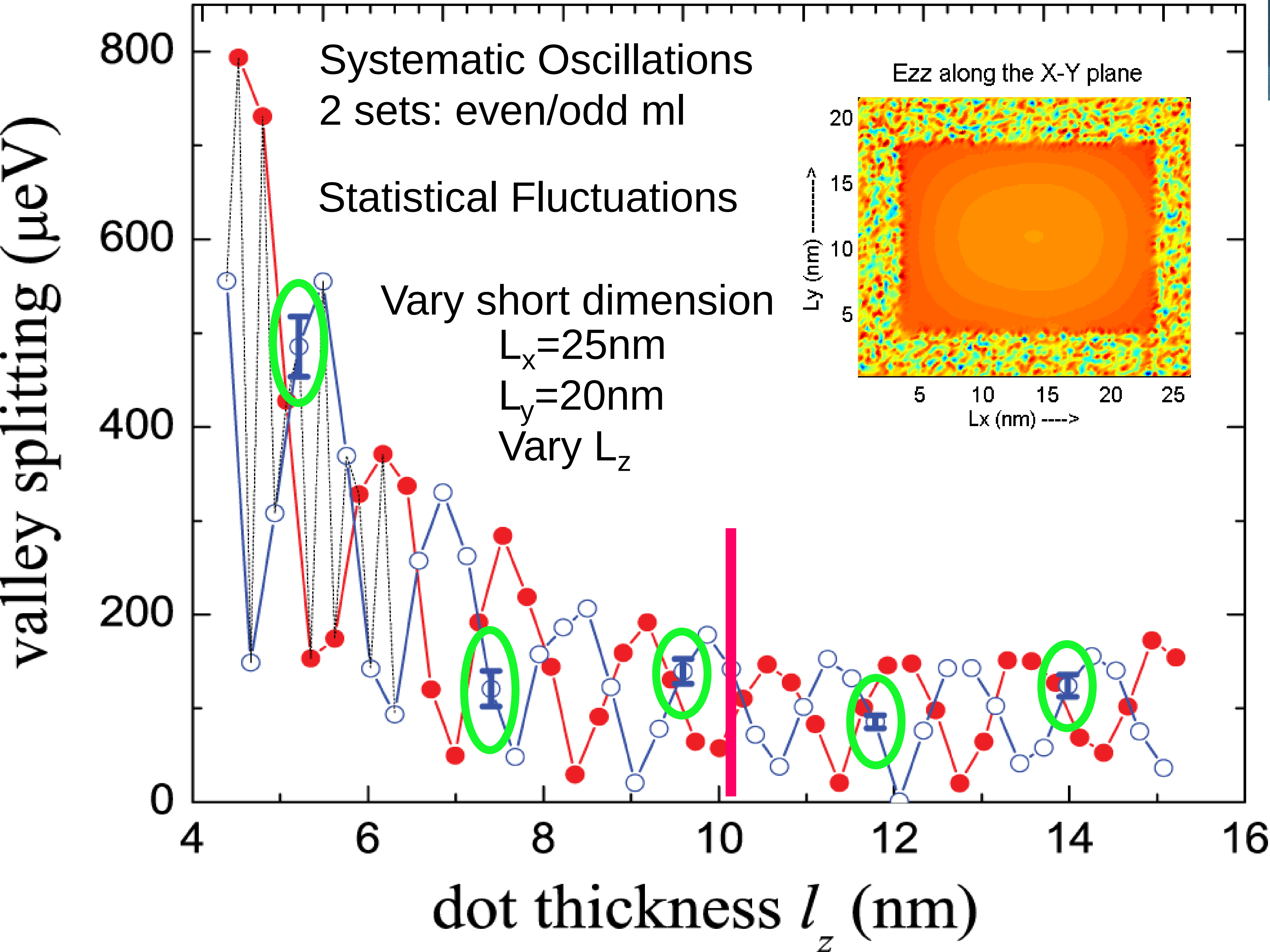
- No NEMO 3D modifications needed
- Strain penetrates 40nm into SiGe => 50 million atom strain sim..
- Typically 365.000 atoms in electronic domain



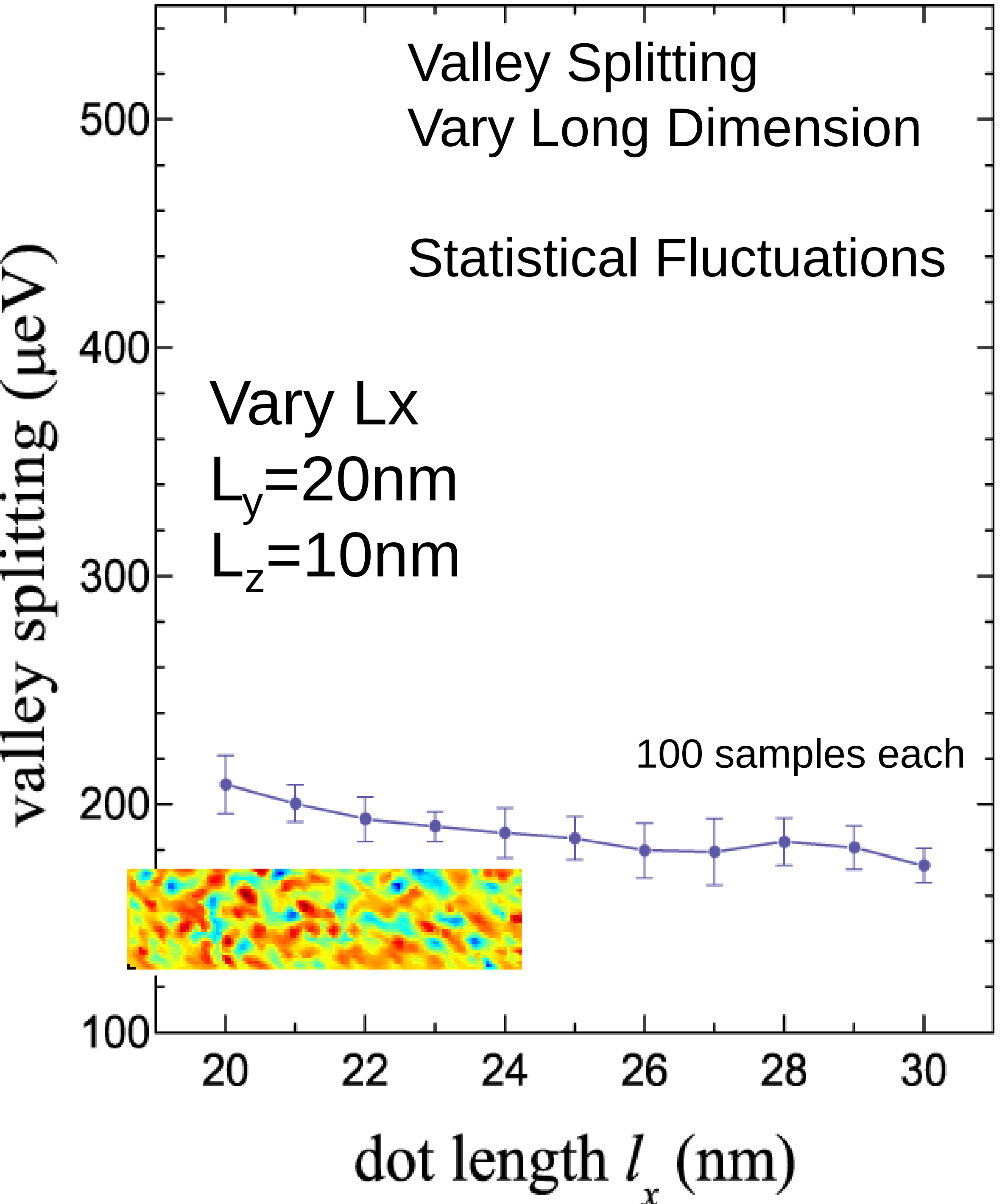


Results / Impact:

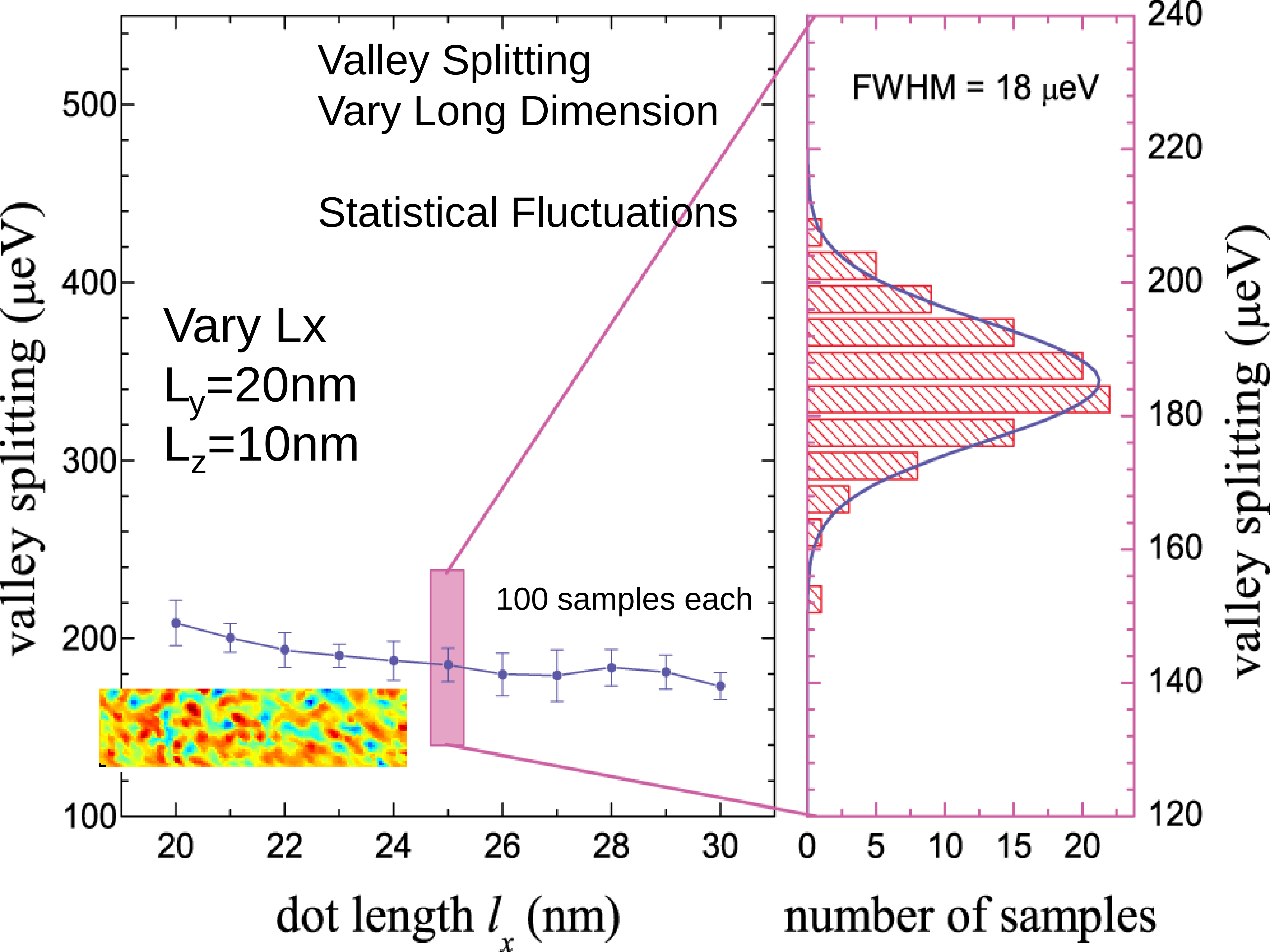
- Fluctuations with quantum dot size like 1D



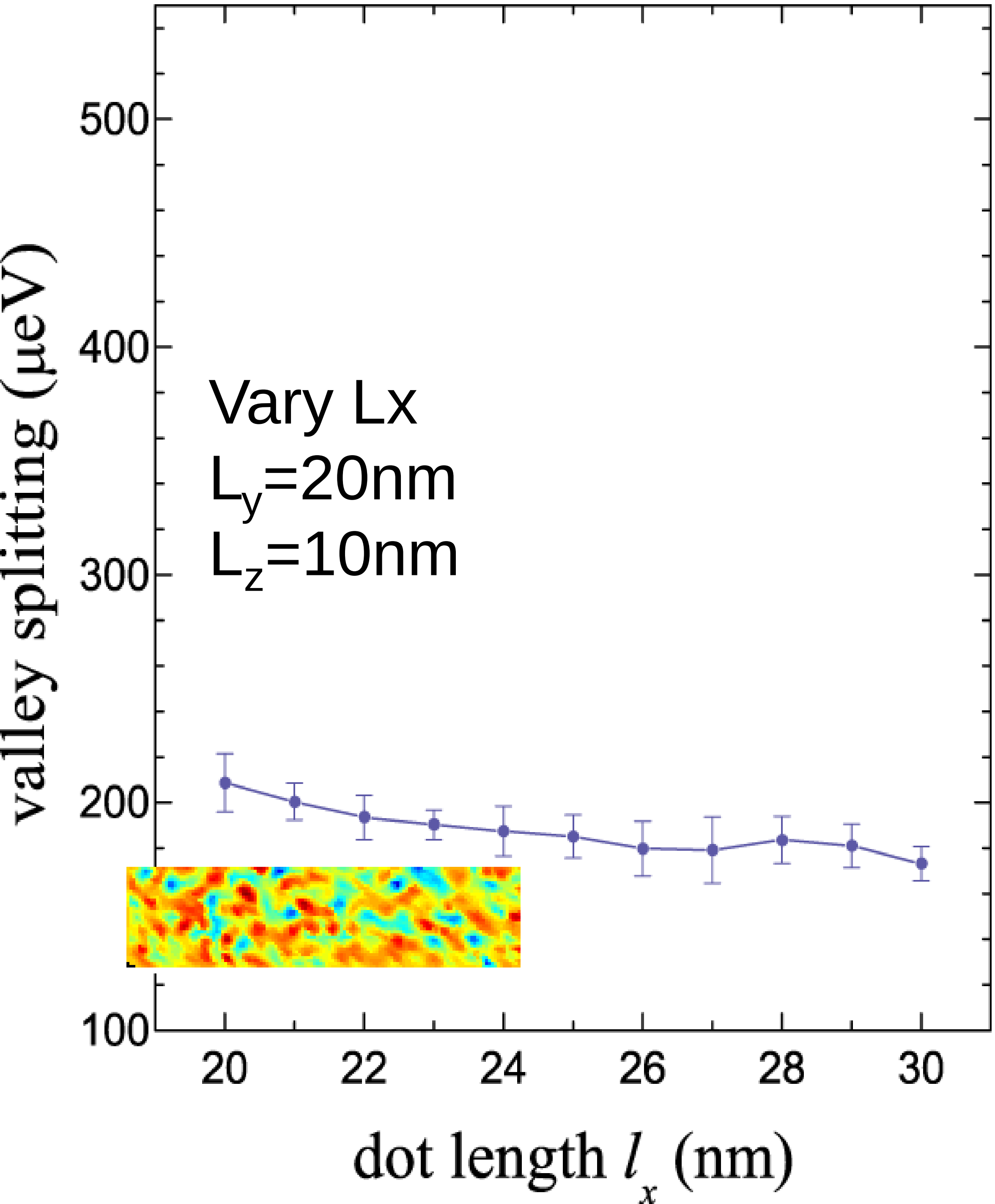
Systematic Oscillations
2 sets: even/odd ml
Statistical Fluctuations
Vary short dimension
L_x=25nm
L_y=20nm
Vary L_z
Ezz along the X-Y plane
Ly (nm) ------->
Lx (nm) ---->
valley splitting (μeV)
dot thickness l_z (nm)
0
200
400
600
800
4
6
8
10
12
14
16
5
10
15
20
25

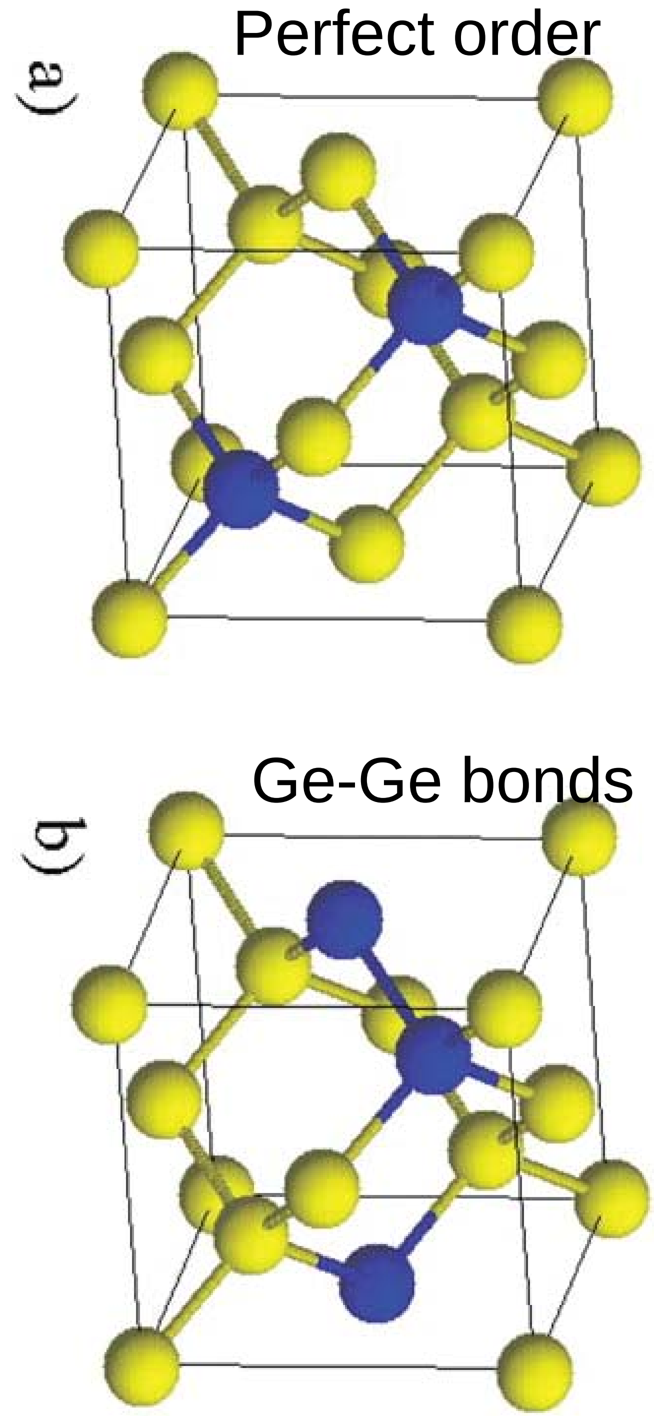


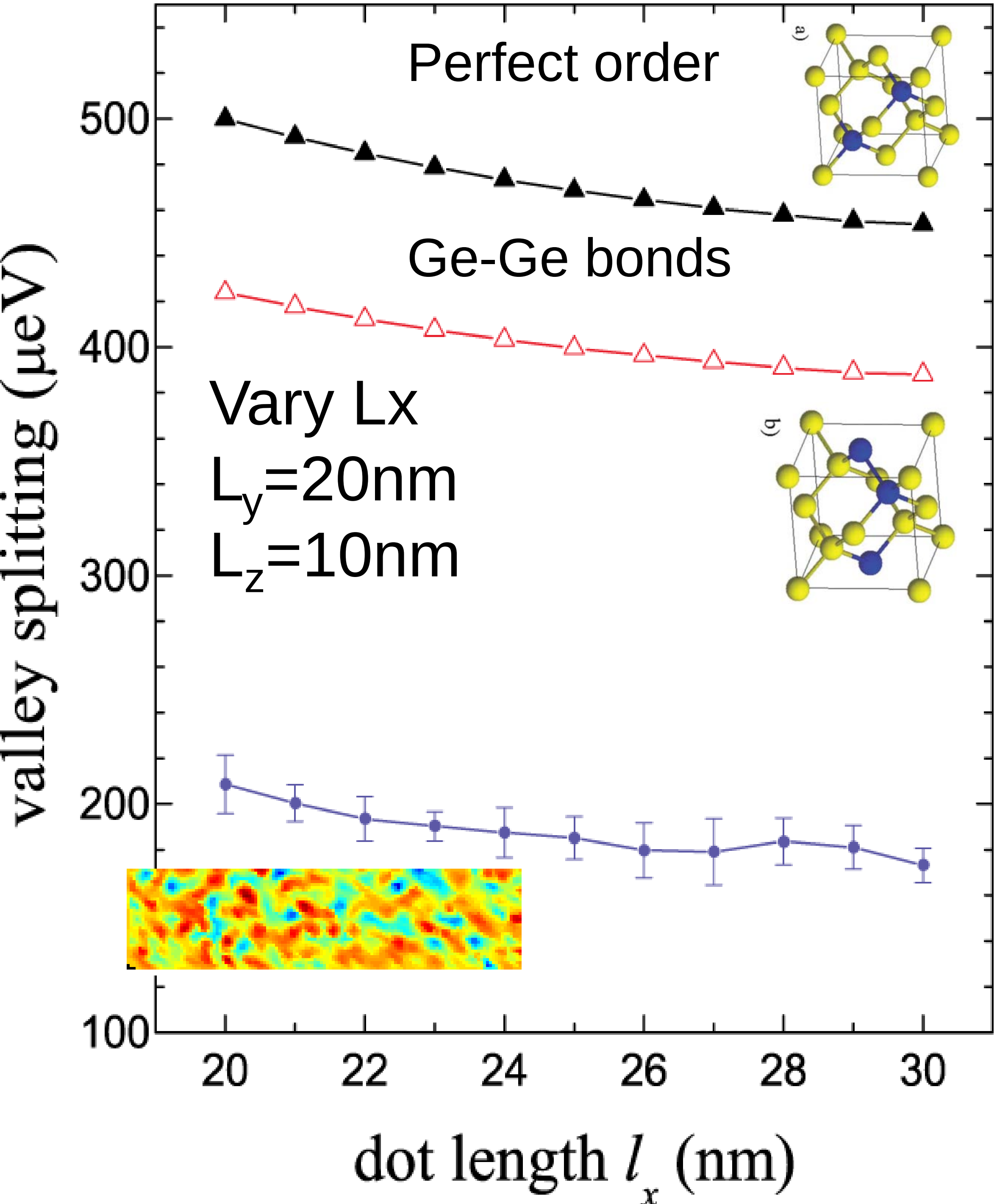
Valley Splitting
Vary Long Dimension
Statistical Fluctuations
Vary Lx
L_y=20nm
L_z=10nm
100 samples each
valley splitting (μeV)
500
400
300
200
100
20
22
24
26
28
30
dot length l_x (nm)



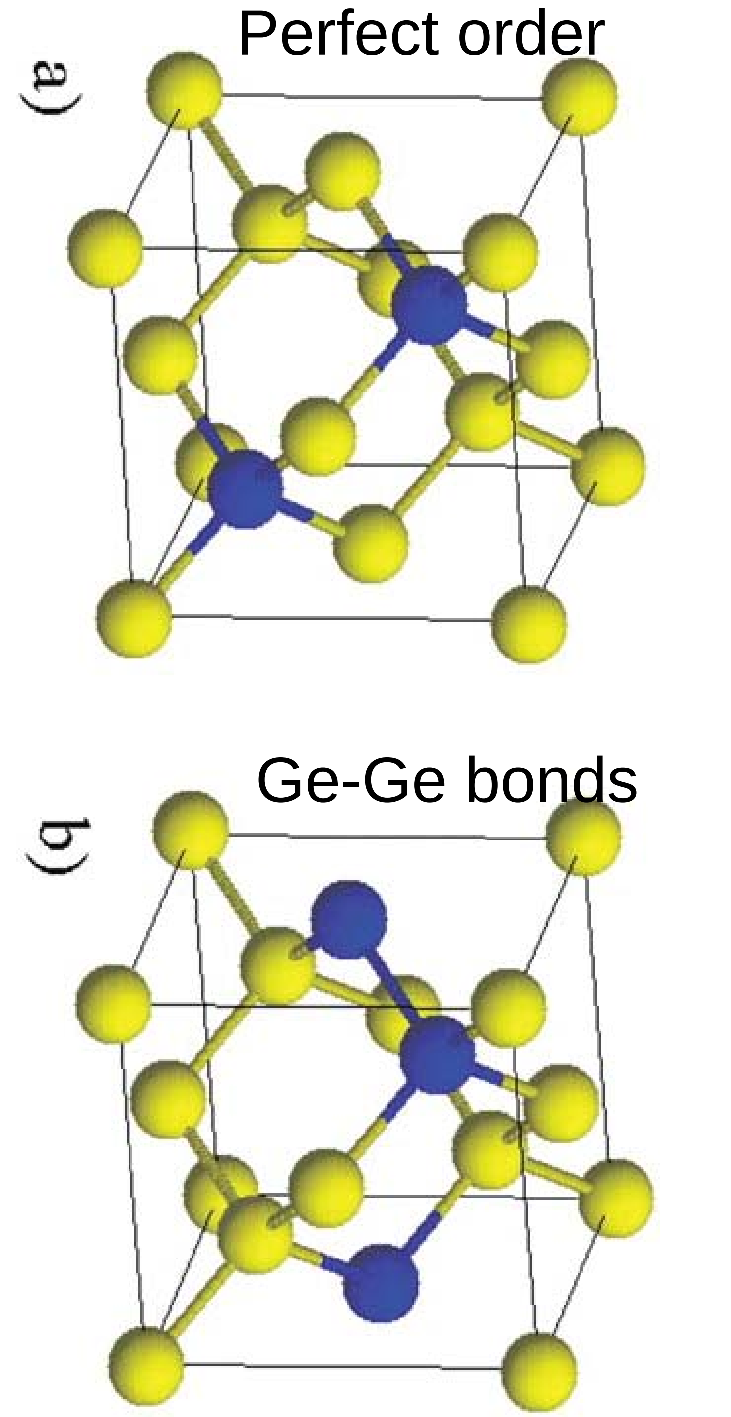
Valley Splitting
Vary Long Dimension
Statistical Fluctuations
Vary Lx
L_y=20nm
L_z=10nm
100 samples each
FWHM = 18 μeV
valley splitting (μeV)
500
400
300
200
100
20
22
24
26
28
30
dot length l_x (nm)
0
5
10
15
20
number of samples
240
220
200
180
160
140
120
valley splitting (μeV)


valley splitting (μeV)
500
400
300
200
100
Vary Lx
L_y=20nm
L_z=10nm
20
22
24
26
28
30
dot length l_x (nm)


Perfect order
(a)
Ge-Ge bonds
(b)

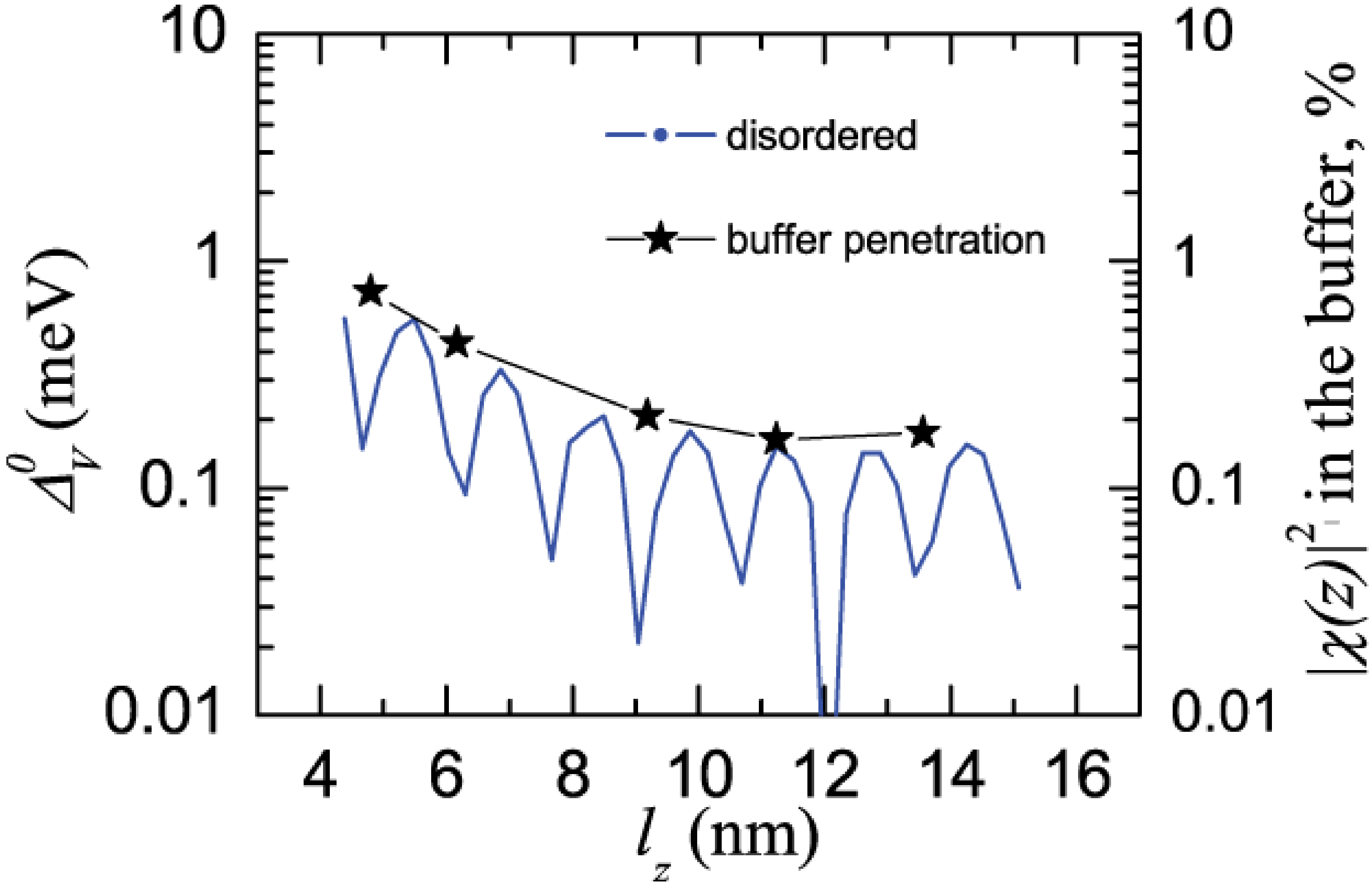


Perfect order
Ge-Ge bonds
Vary Lx
L_y=20nm
L_z=10nm
valley splitting (μeV)
dot length l_x (nm)
100
200
300
400
500
20
22
24
26
28
30



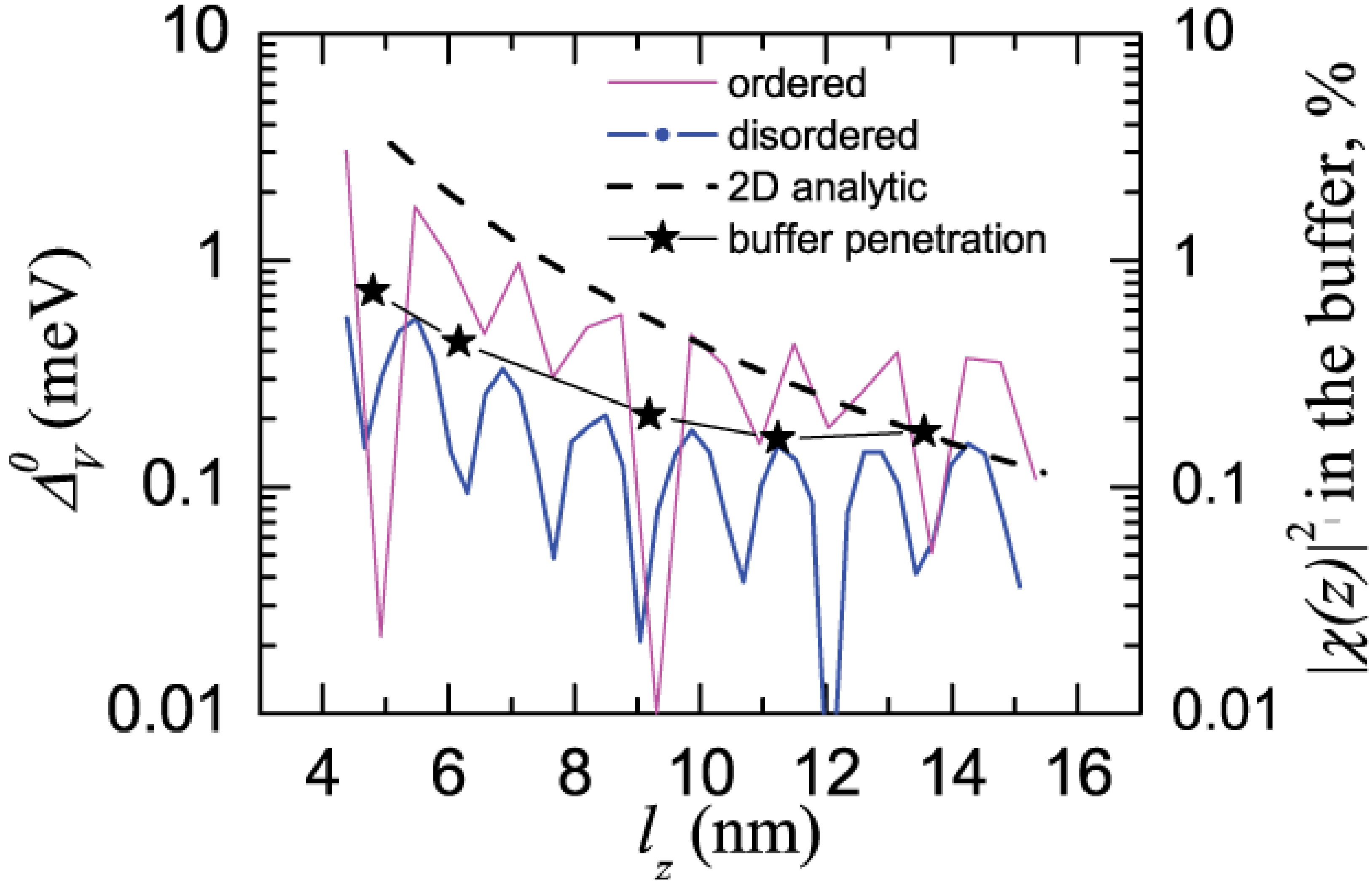
Perfect order
Ge-Ge bonds

Wavefunction Penetration



Valley Splitting is an INTERFACE DOMINTED phenomenon

Wavefunction Penetration Analytical Expressions



Valley Splitting is an INTERFACE DOMINTED phenomenon

Analytical formulas help, but cannot really guide the decision process

Silicon Quantum Dots in SiGe Matrix

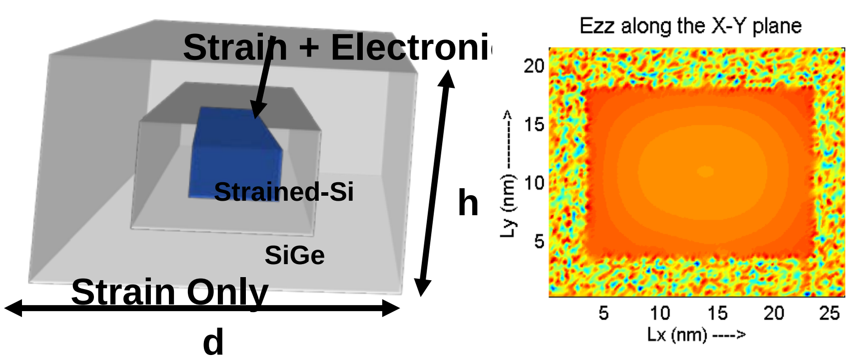
Srikant Srinivasan, Leonid Rokhinson, Gerhard Klimeck

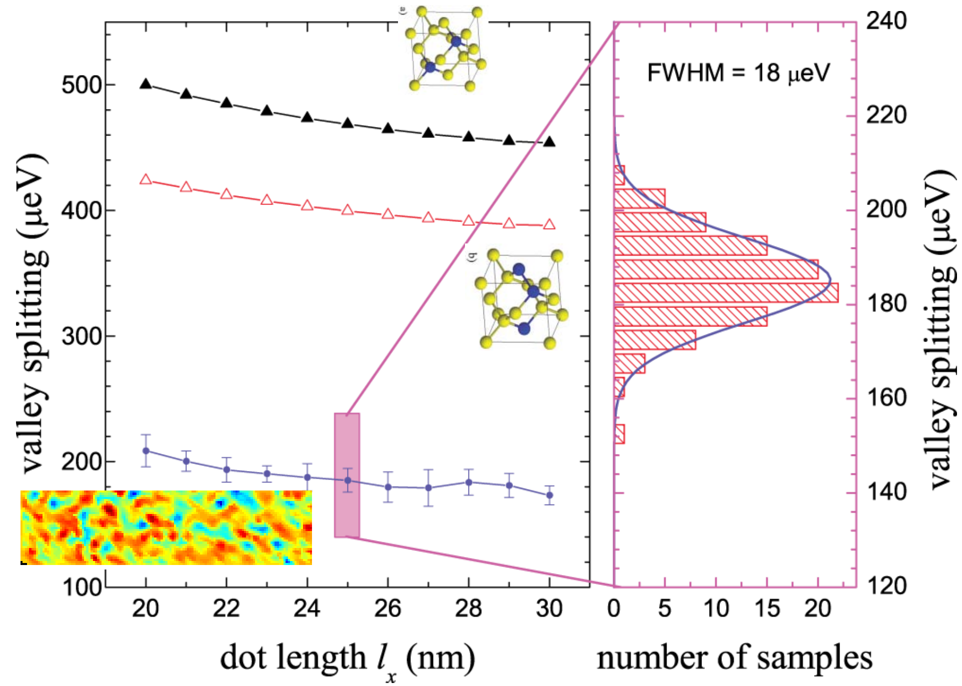
Objective:

- Prepare experiments (Rokhinson)
- Study realistic/large embedded Si QD
- Aid in understanding and design, buffer randomness, interfaces, Valley Splitting
- Explore size and disorder dependence

Approach:

- No NEMO 3D modifications needed
- Strain penetrates 40nm into SiGe => 50 million atom strain sim..
- Typically 365.000 atoms in electronic domain





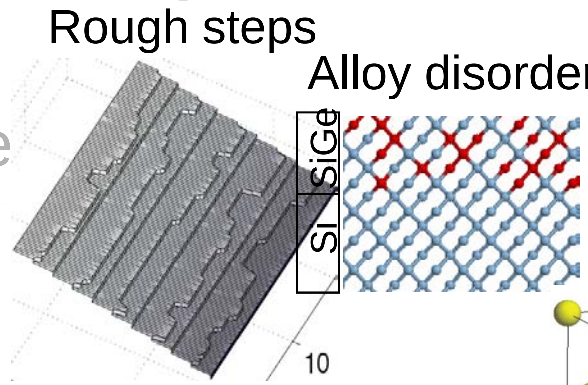
Results / Impact:

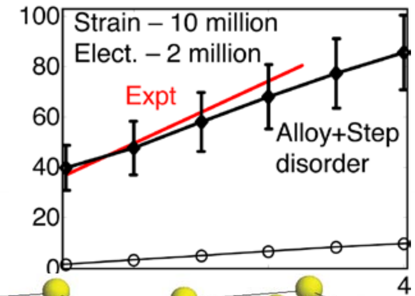
- Fluctuations with quantum dot size like 1D in short simensions
- VS controllable in long dimensions
- Disorder and Order matters
- Analytical formulas cannot provide quantitative experimental guidance

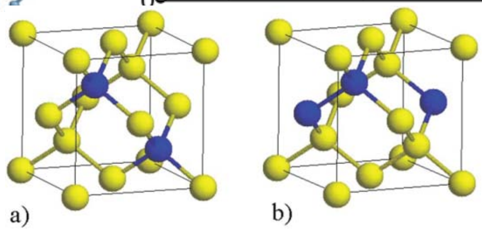
APL, Vol. 93, pg. 112102 (2008),

Multi-Million Atom Simulation of Quantum States in Realistically Extended Devices in Silicon

- Motivation
- NEMO Numerical Engine
- Valley splitting
  - »Si quantum wells
  - »Si Quantum Dots
- Single impurities in Si
  - »Metrology – impurity identification
  - »Wavefunction mapping
  - »g-factor engineering
  - »CTAP
- Dense impurities in Si – Si:P
  - »Infinite sheets
  - »Infinite wires
  - »Gating, transport through wires
  - »Impurity-based quantum dots



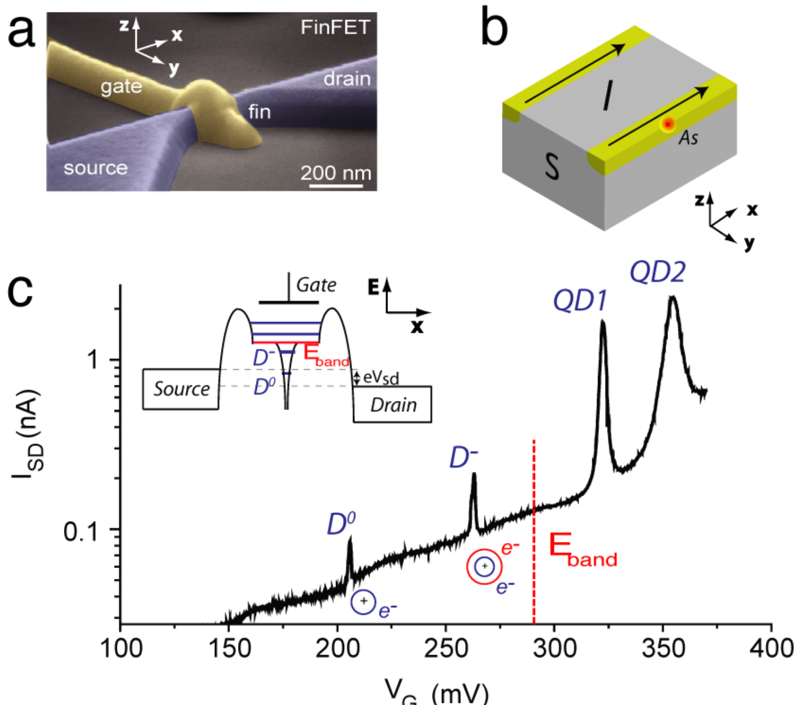




Metrology with multimillion atom simulations
Excited States are Critical!

Objective:

- Support single impurity spectroscopy

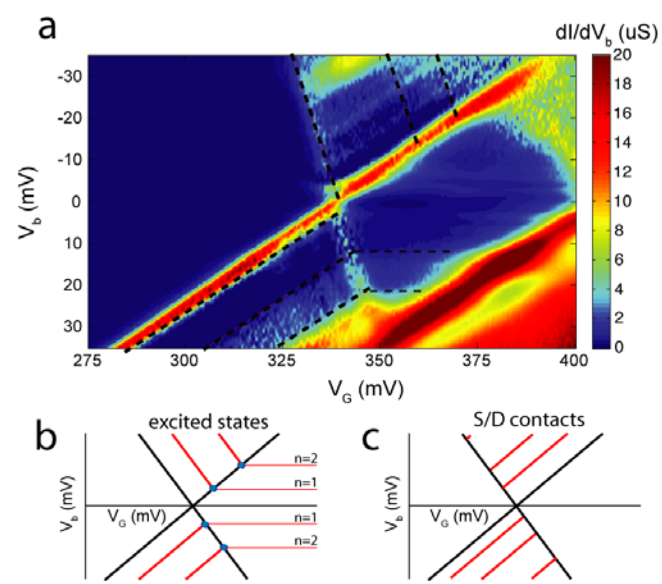


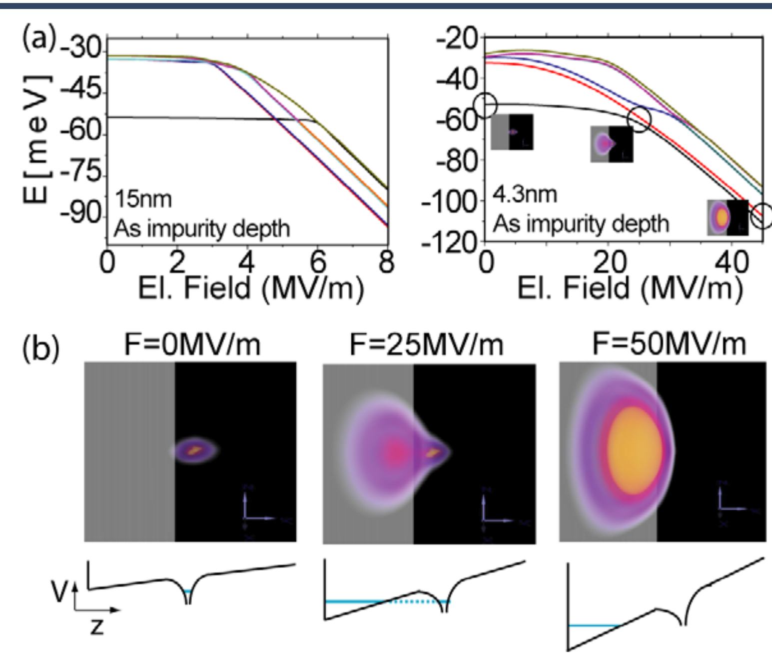
Approach:

- Experiments & NEMO3D (on 3 continents!)

Results / Impact:

- Identify Impurities as As not P
- Determine depth of impurities from interface
- Nature Physics, V4, p 656 (2008)

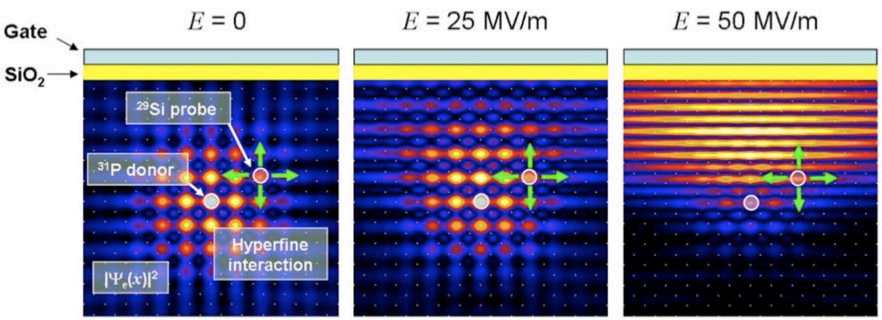




Mapping Donor Wavefunctions

Seung Hyun Park, Rajib Rahman, Gerhard Klimeck, Lloyd Hollenberg

Need for high precision control of WF in QC



Hyperfine Interaction Tensor (A)

$$A_{ij} = \gamma_I \gamma_S \hbar^2 \left(\frac{8\pi}{3} \left|\Psi(0)\right|^2 \delta_{ij} + \left\langle \Psi \left| \frac{3x_i x_j - r^2\delta_{ij}}{r^5} \right| \Psi \right\rangle \right)$$

$\gamma_{I,S}$=gyromagnetic ratio, x_{ij} = (x,y,z)

Originally measured in 1969

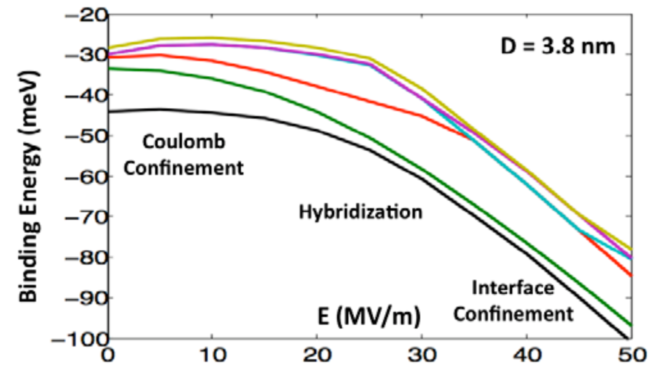
ESR Experiments can measure A_{ij}

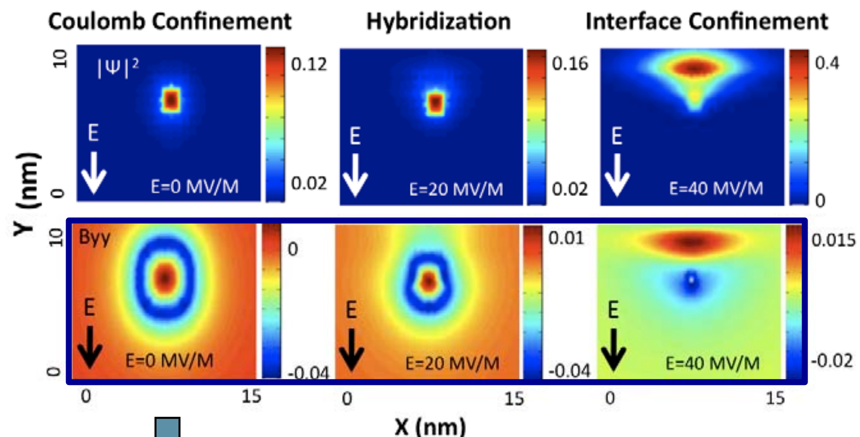
➔ Indirect measure of WF

Park, PRL (2009)

arXiv:0902.1515v1

Stark Shift Spectrum of a P donor at 3.8nm from an oxide interface in Si





Corresponding Hyperfine Maps in the forms of B_{yy} tensor component

Spin-Orbit Stark Effect in Donors

Rajib Rahman, Seung Hyun Park, Timothy B. Boykin,
Gerhard Klimeck, Sven Rogge, Lloyd Hollenberg

Objective:

- Study Stark Shift of the g-factor for an isolated donor w.r.t. expt in Si and Ge.
- g-factor shift for interface-donor system.
- Probes spin-orbit effects with electric fields and symmetry change.
- Effect of relative orientations of B and E field.

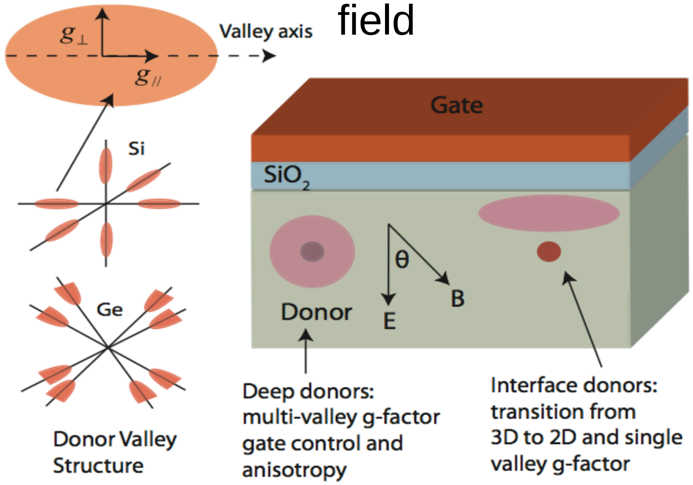
Approach:

- The 20 band nearest neighbor sp3d5s* spin model captures SO interaction of the host.
- Same atom p orbital energy between spin orbitals.
- g-factor obtained from orbital and spin angular momentum operators.
- Donor wfs with E-field are obtained from NEMO

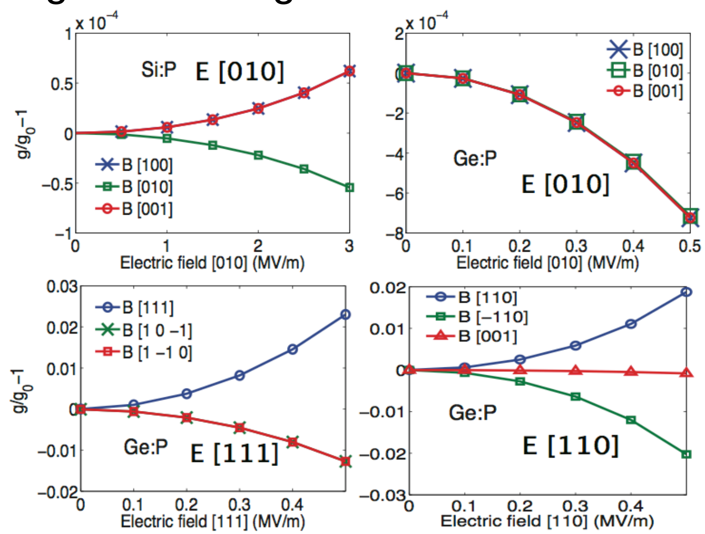
Results / Impact:

- Quadratic Stark coefficient from TB agrees with measured value in magnitude.
- Relative E and B orientations seem to affect g-factor shift. Linear for shallow donors.
- Stark shift of Zeemann splitting may become comparable to hyperfine shift at modest B fields.
- Understanding of the B field dynamics of the donor electron.

WF and g-factor of donor engineering by EM field



Change of donor g-factor for various EM-field



R Rahman in Phys Rev. B (2009)

arXiv:0905.3200v1

Coherent Transport Adiabatic Passage (CTAP)

Rajib Rahman, Seung Hyun Park, Jared Cole, Andrew Greentree,
Richard P. Muller, Gerhard Klimeck, Lloyd Hollenberg

Objective:

- Investigate CTAP in realistic setting.
- Include Si full band-structure, TCAD gates, interfaces, excited states, cross-talk.
- Verify that adiabatic path exists: 3 donor device.

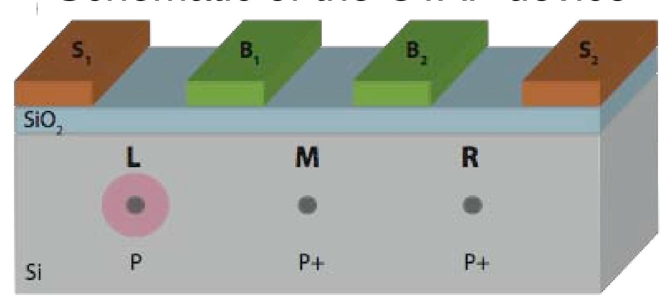
Approach:

- TCAD gates coupled with a 3 donor TB. Hamiltonian to obtain molecular states.
- Simulate "small" 3 M atom device rapidly to demonstrate concept
- Compute time of 4-5 hours on 40 procs.
- Many bias configurations to fine tune gate voltages to explore the CTAP. regime.

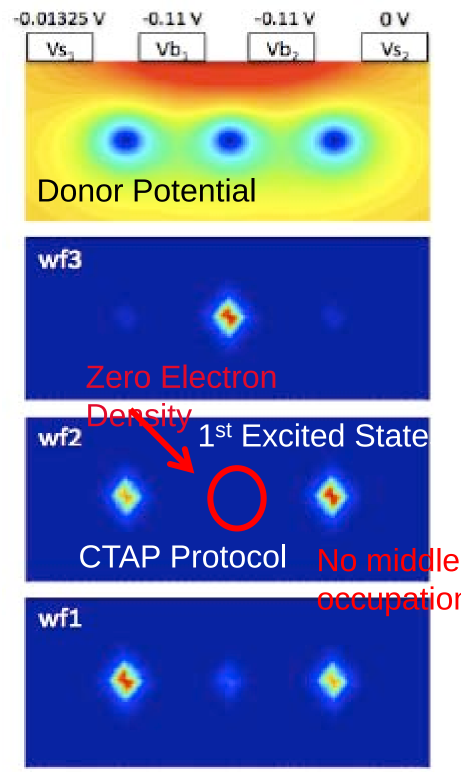
Results / Impact:

- 15nm separated donors to explore rapidly
  => significant gate cross talk
  => Determination of gate bias control tedious
- Demonstrated that the CTAP regime exists for a 3 donor test device.

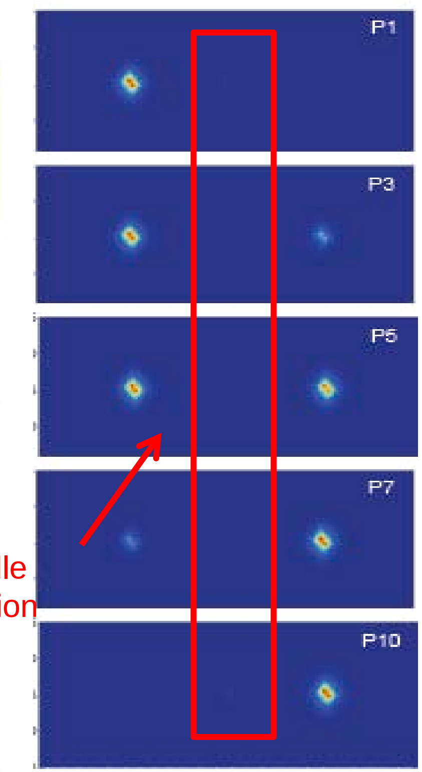
Schematic of the CTAP device



CTAP Protocol



CTAP



Published in Phys. Rev. B. 80, 035302 (2009)

Coherent Transport Adiabatic Passage (CTAP)

Rajib Rahman, Seung Hyun Park, Jared Cole, Andrew Greentree,
Richard P. Muller, Gerhard Klimeck, Lloyd Hollenberg

Atom & Gate Geometry

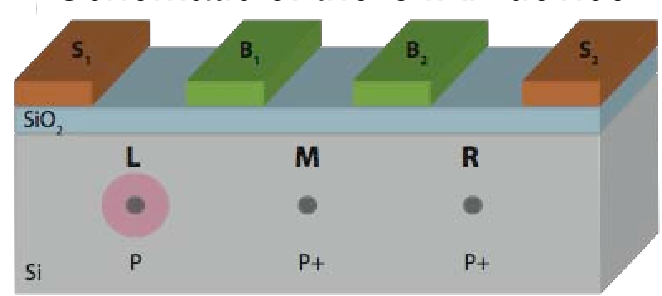
↓

Adaptive Gate Tuning

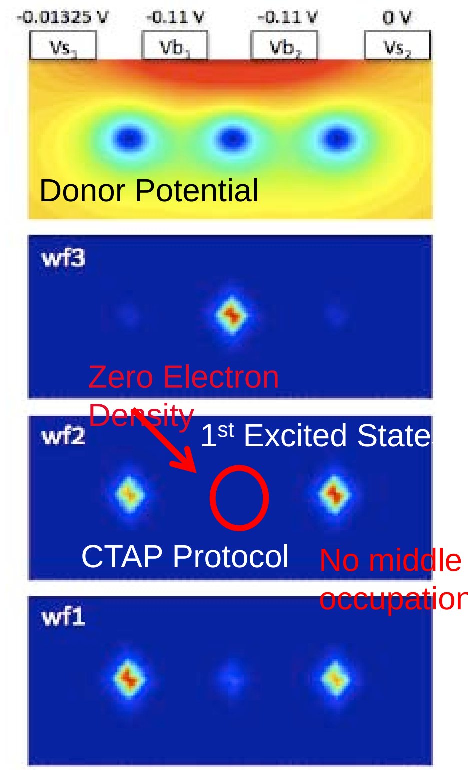
↓

CTAP Operation

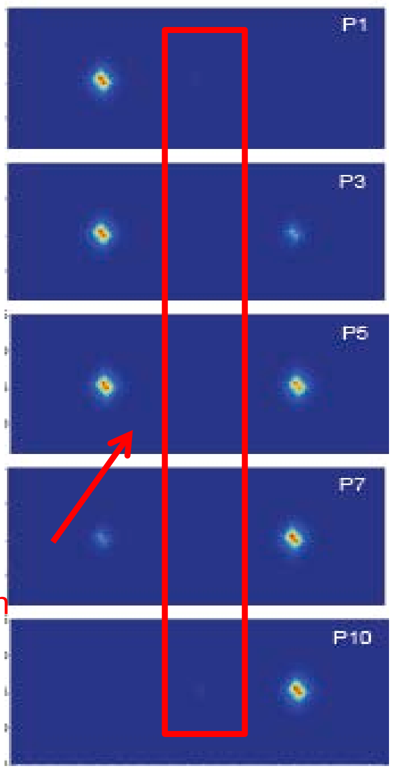
Schematic of the CTAP device



CTAP Protocol



CTAP



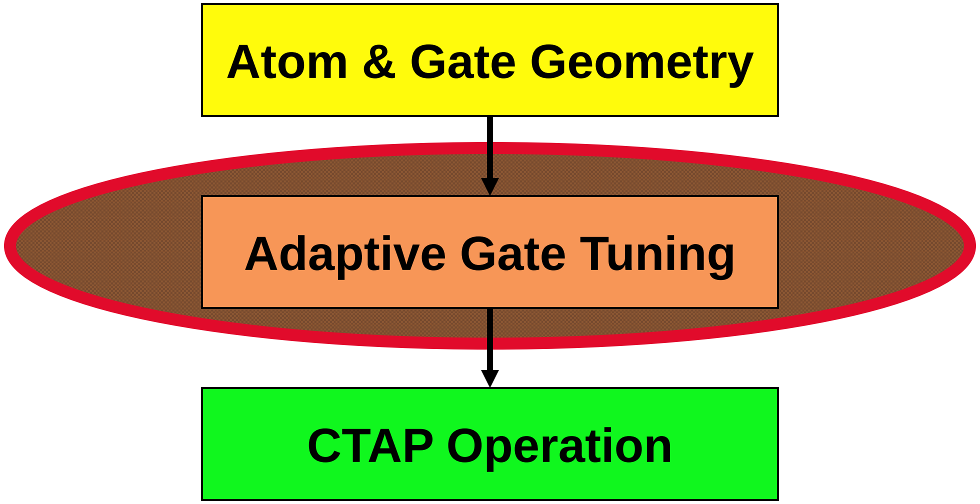
Results / Impact:

- 15nm separated donors to explore rapidly
  => significant gate cross talk
  => Determination of gate bias control tedious
- Demonstrated that the CTAP regime exists for a 3 donor test device.

Published in Phys. Rev. B. 80, 035302 (2009)

Coherent Transport Adiabatic Passage (CTAP)

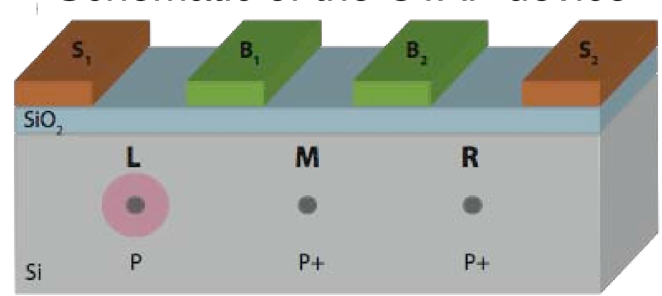
Rajib Rahman, Seung Hyun Park, Jared Cole, Andrew Greentree, Richard P. Muller, Gerhard Klimeck, Lloyd Hollenberg



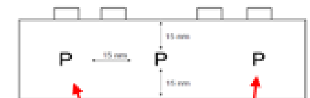
Results / Impact:

- 15nm separated donors to explore rapidly
  => significant gate cross talk
  => Determination of gate bias control tedious
- Demonstrated that the CTAP regime exists for a 3 donor test device.
- Initial straggle case in high cross talk regime indicates a different bias pathway
- Indicative of general need for individual characterization of qubit transport mechanisms
- Simulations enable development of bias control algorithms in actual experiments (e.g. charge sensing)

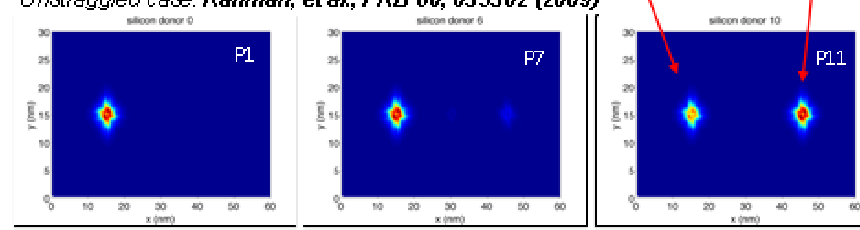
Schematic of the CTAP device



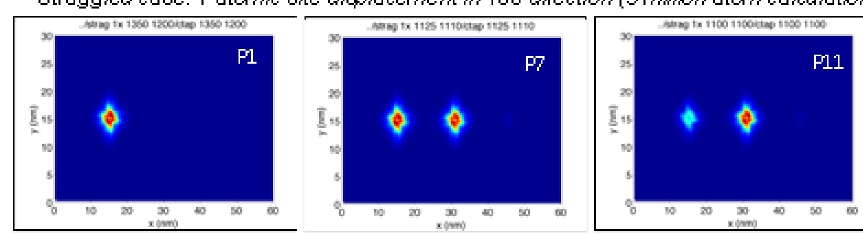
NEMO3D Results



Unstraggled case: ***Rahman, et al., PRB 80, 035302 (2009)***



Straggled case: 1 atomic site displacement in 100 direction (3 million atom calculation)



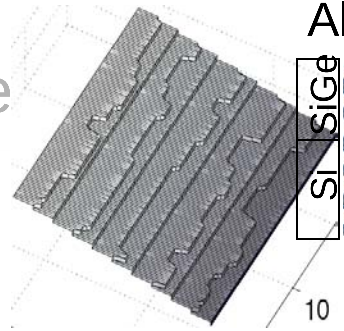
- Next: project NEMO3D results on to 3x3 matrix and get V_{gate} dependence of elements

Sandia / Purdue / Melbourne

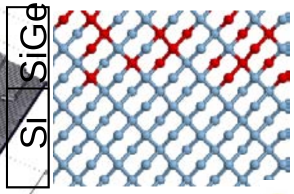
Multi-Million Atom Simulation of Quantum States in Realistically Extended Devices in Silicon

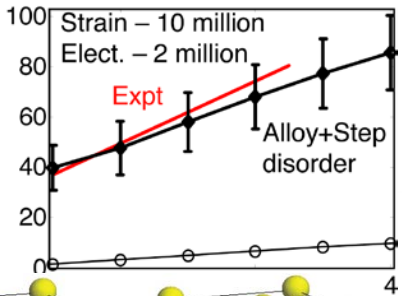
- Motivation
- NEMO Numerical Engine
- Valley splitting
  - »Si quantum wells
  - »Si Quantum Dots
- Single impurities in Si
  - »Metrology – impurity identification
  - »Wavefunction mapping
  - »g-factor engineering
  - »CTAP
- Dense impurities in Si – Si:P
  - »Infinite sheets
  - »Infinite wires
  - »Gating, transport through wires
  - »Impurity-based quantum dots

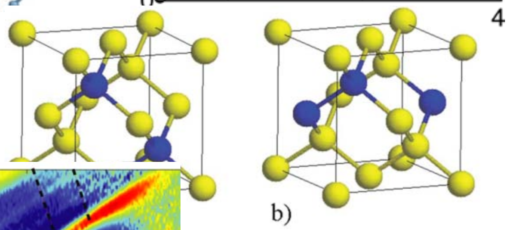
Rough steps

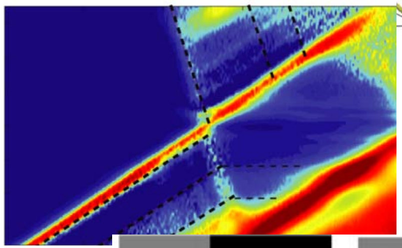


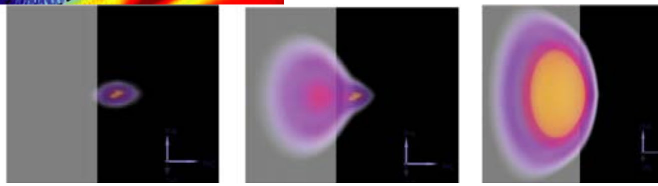
Alloy disorder



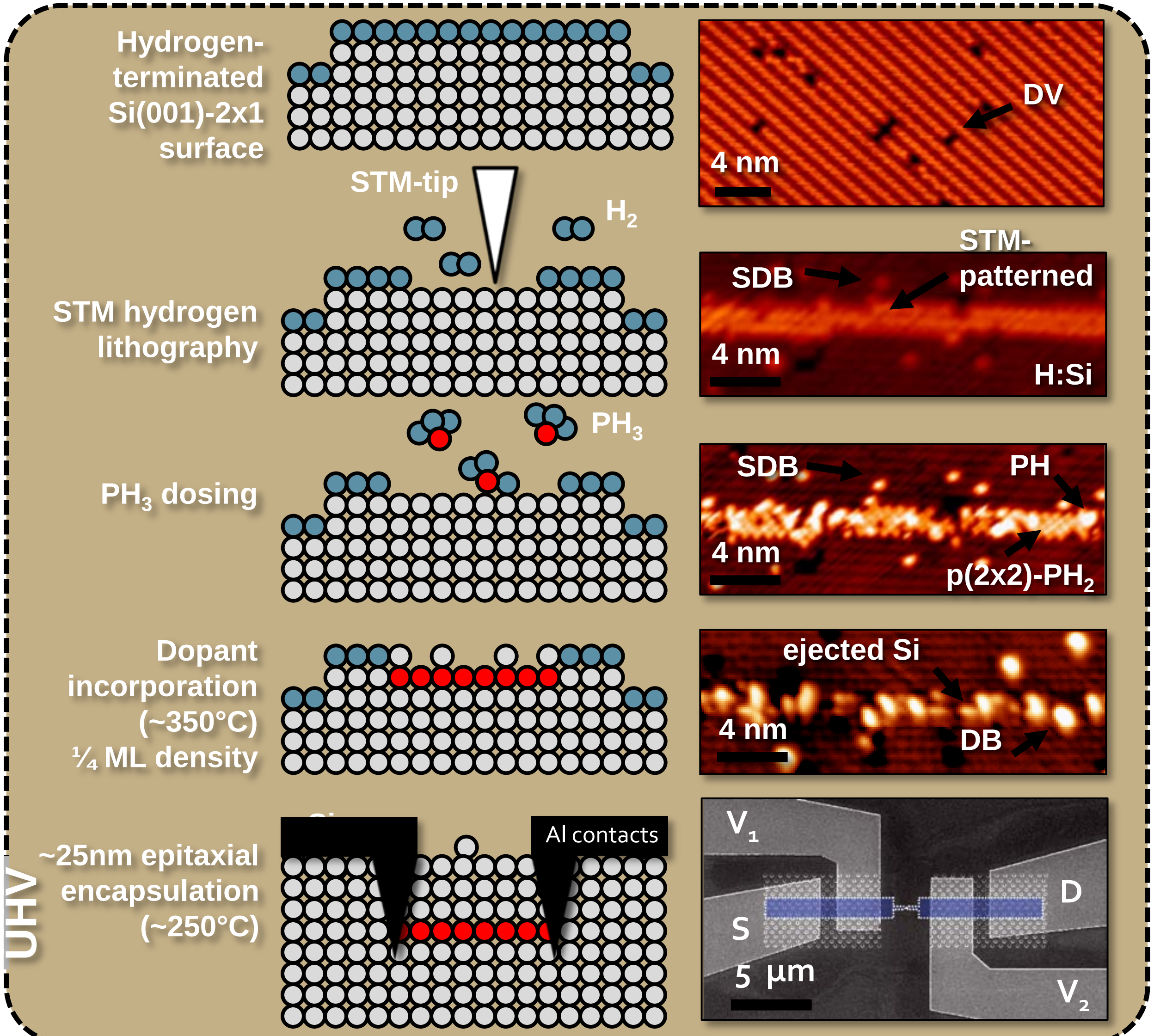








Atomic-Precision Doping by STM



Slide courtesy of Simmons Group

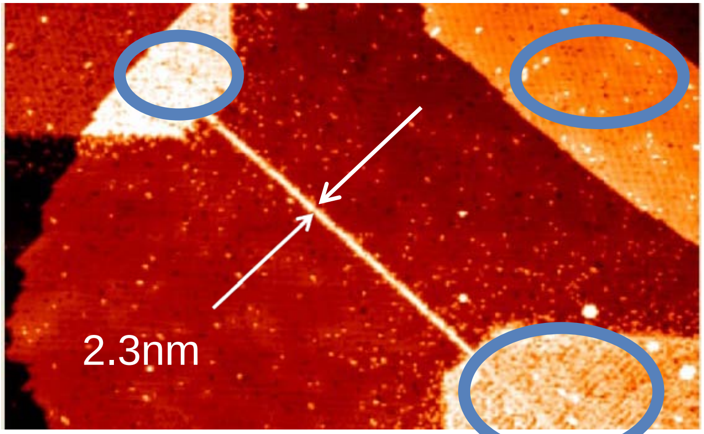
Highly δ-Doped Si Devices

Motivation:
- Understand available experimental data
- Guide experimental set-ups

Problems:
- Validate / confirm our approach to other theories
- Incorporate extended devices
- Understand metallic behavior
- Explain effects of
  - Doping density
  - Wire size / orientation
  - Electrical gating

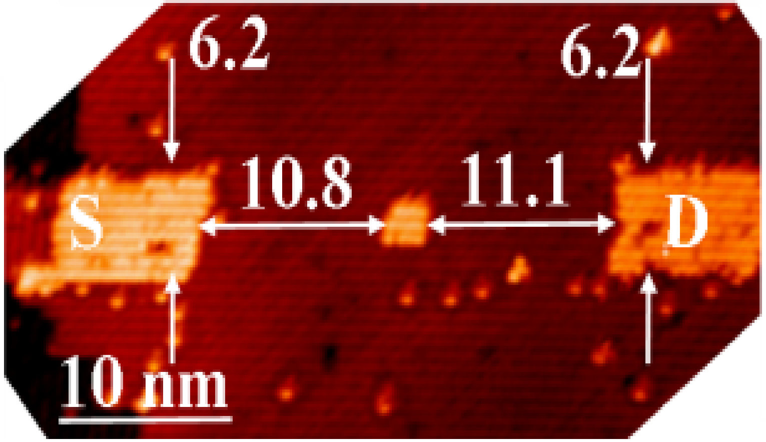
Approach:
- NEMO 3D with tight binding
- Charge-potential self-consistency

- **P δ-doped Si (Si:P) Wire**

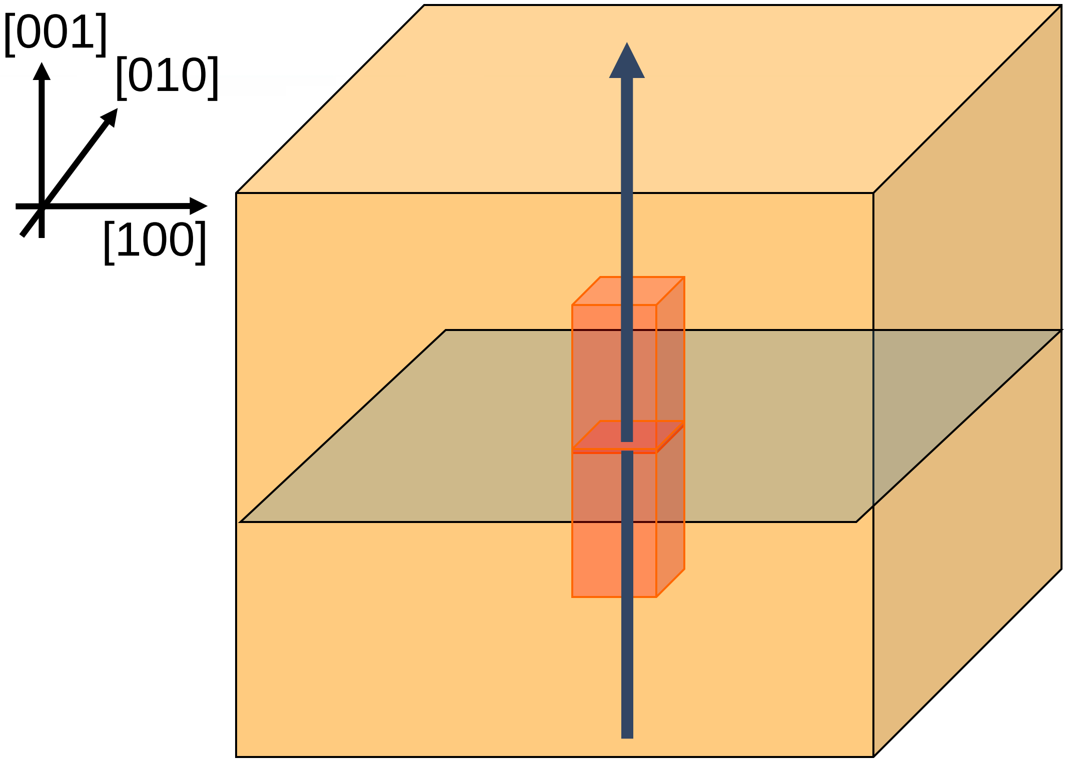


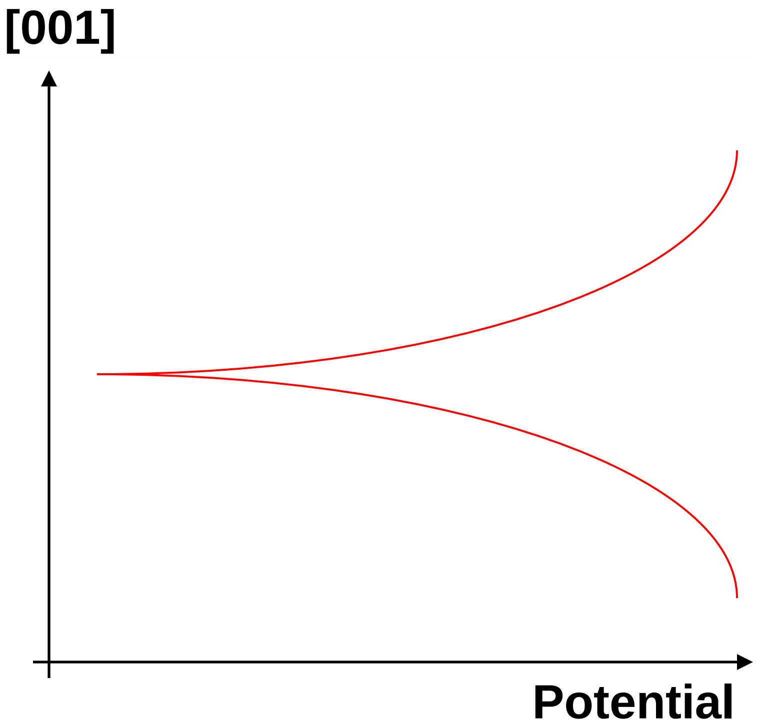
examine large contacts first

- **Si:P Planar quantum Dots**



Contact Regions – Infinite Square Well

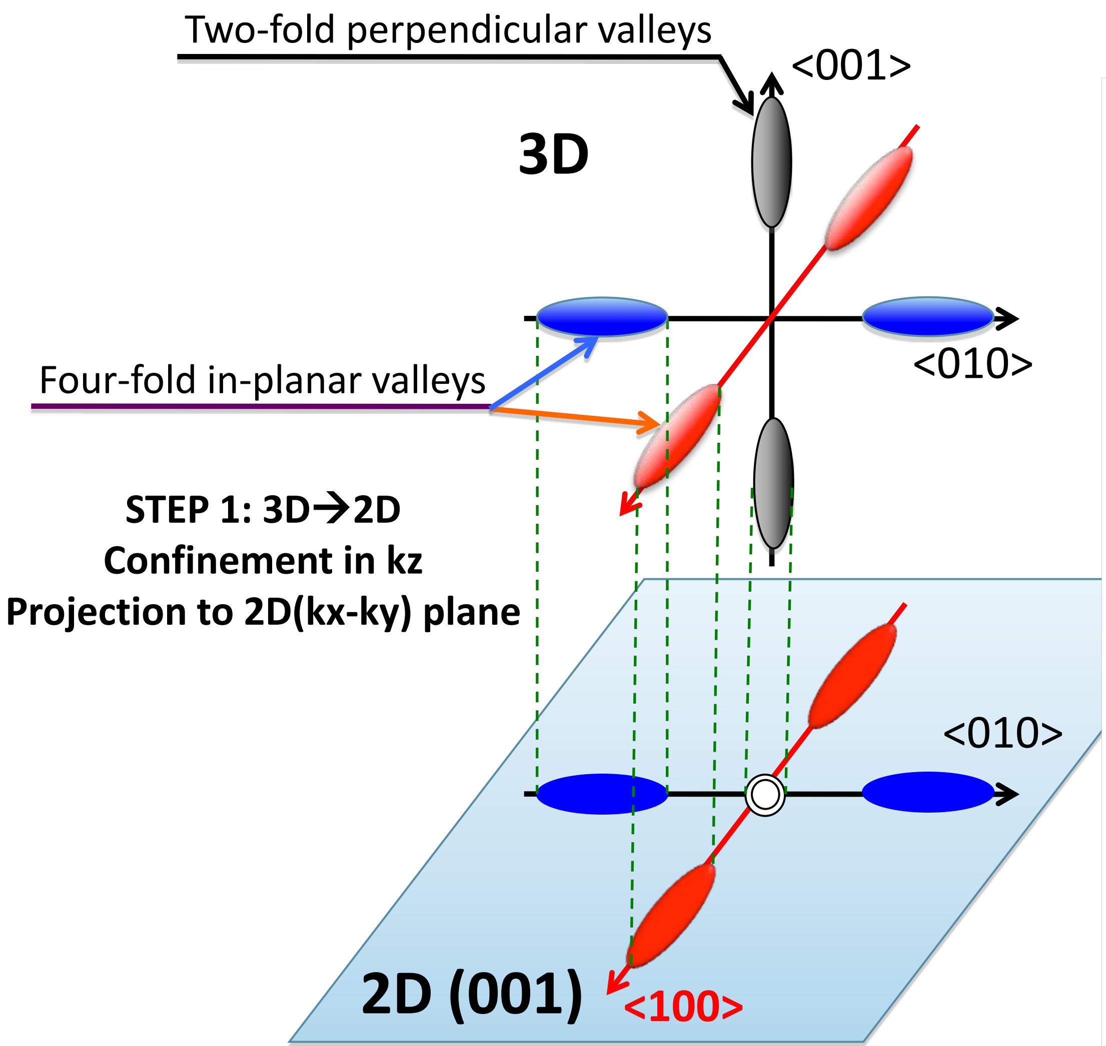


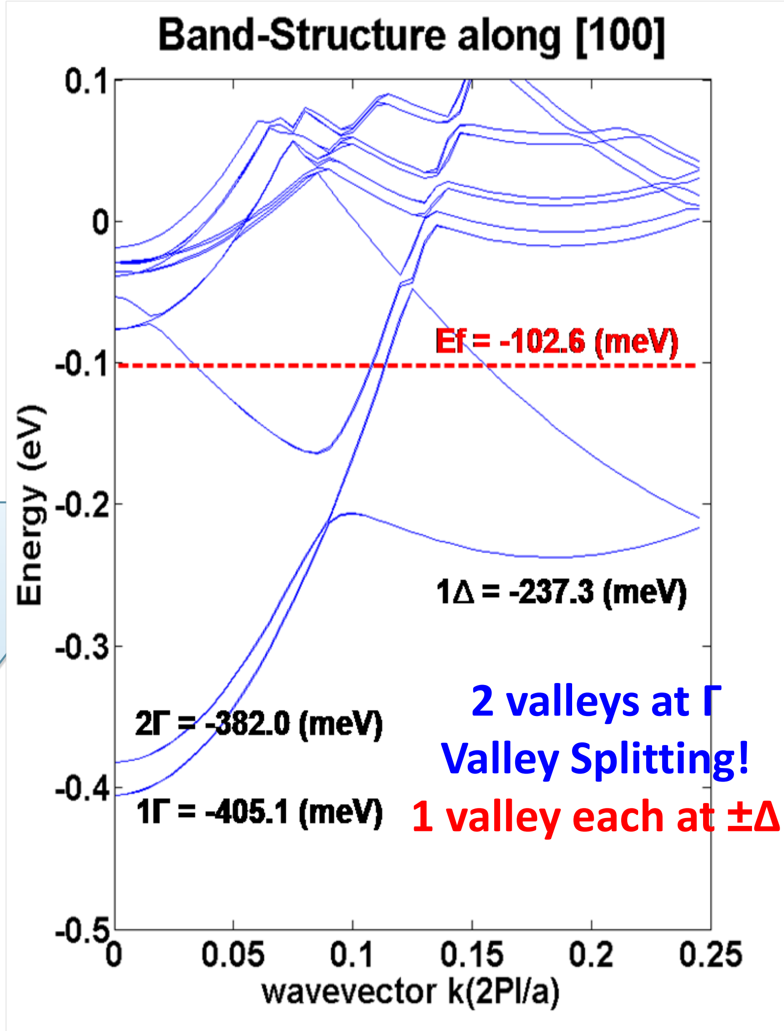


- Extremely thin P-doped layer in Si bulk.
- Confinement happens with impurity potential along [001].
- Need approximation for efficient modeling → Quantum Well Approach.
- Assume periodic boundary condition along [100]/[010]

Band Projection in [100] Si:P Quantum Wells

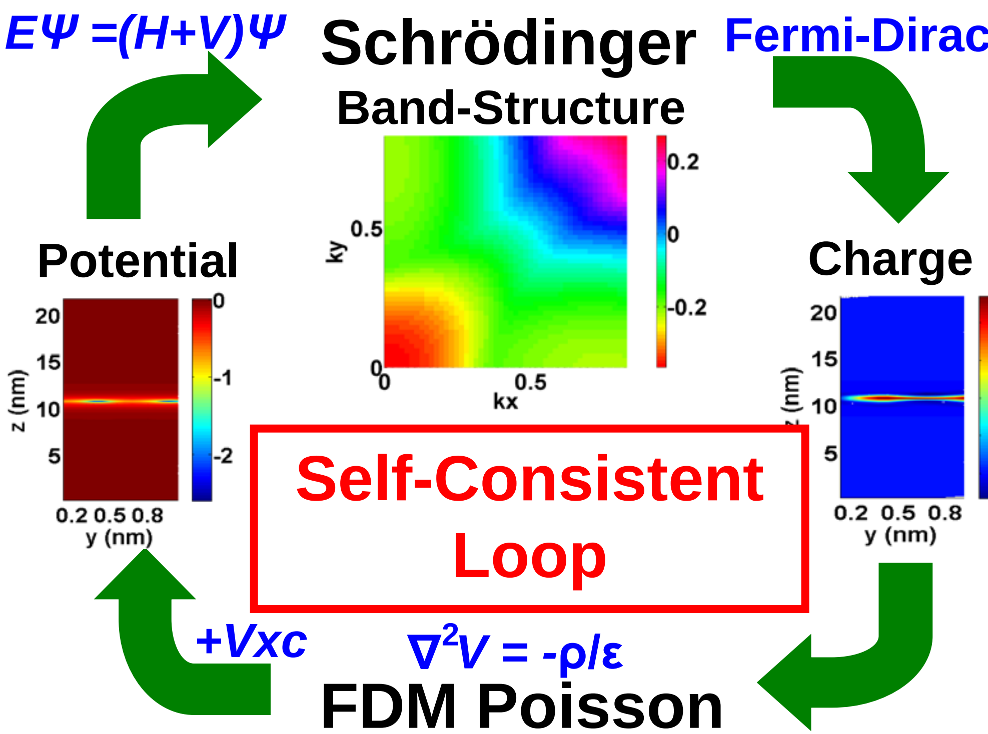
- 3D→2D→1D projection of Si [100] nanowire

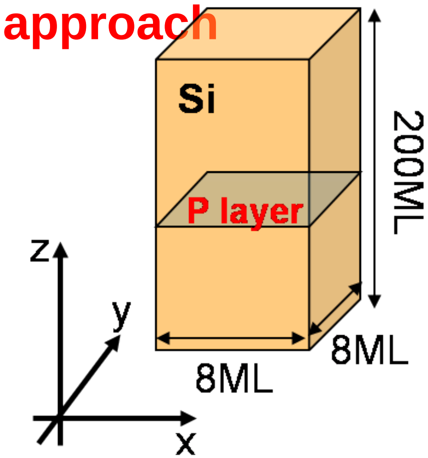




Charge-Potential Self-Consistency

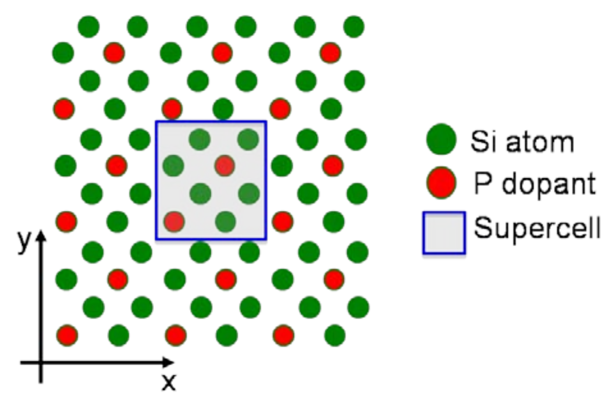
- ¼ ML Doping = 2 impurity ions in the super cell ~ 1.7×10^{14} (cm^2)
- Metal-like system : Charge-Potential Self-consistency
- **Schrödinger-Poisson + Exchange/Correlation with LDA approach**





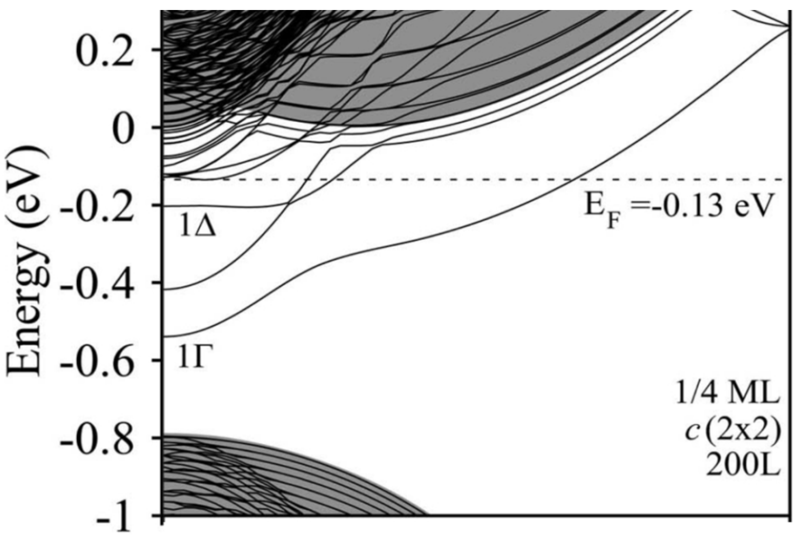
(Periodic along x, y and z)

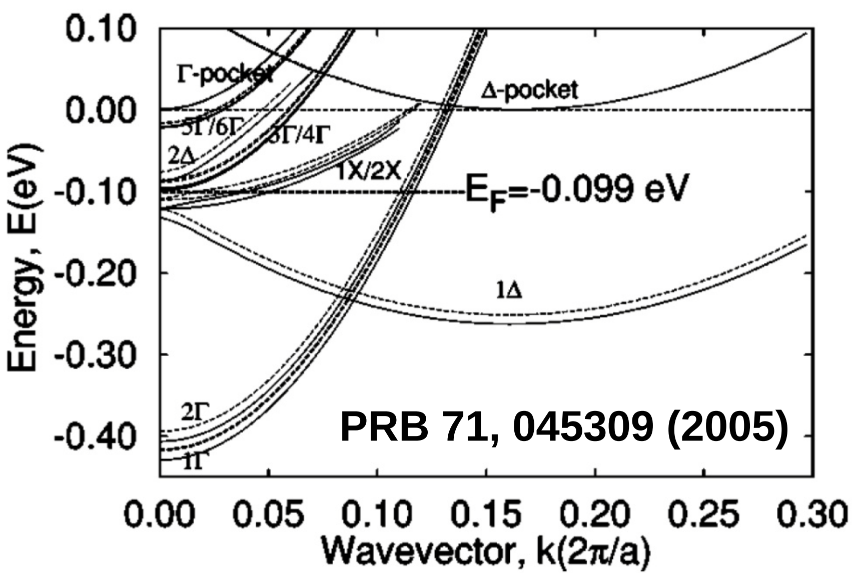
Atomistic Representation of the P δ-layer



Electronic Properties of P δ-doped Si Quantum Well

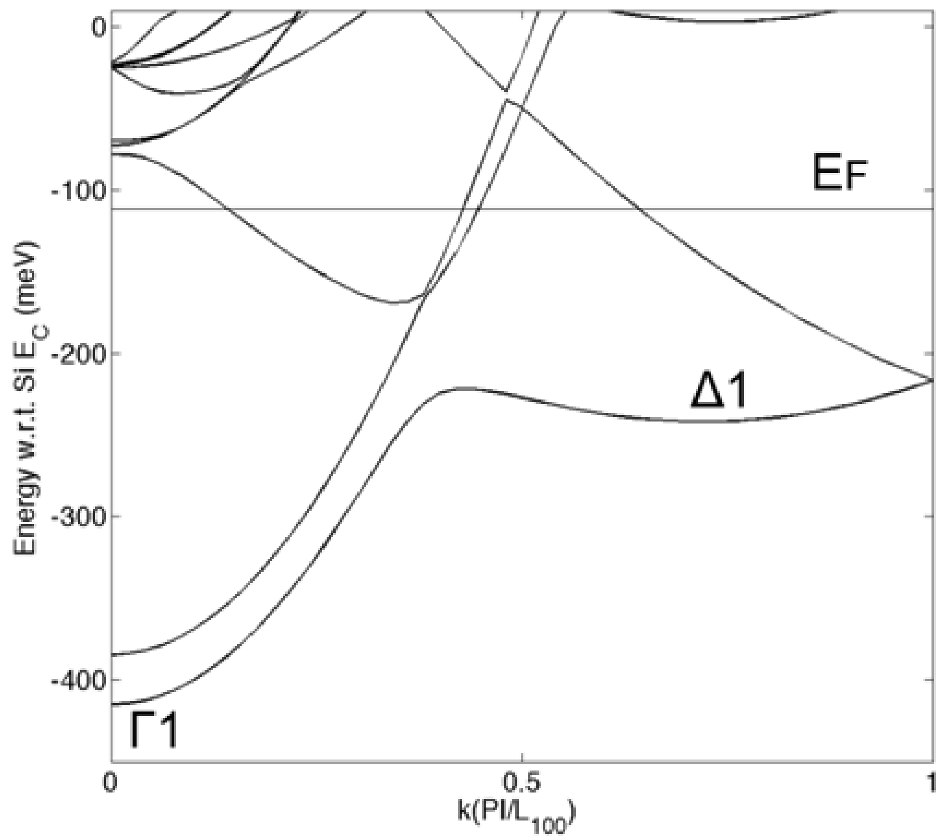
PRB 79, 033204 (2009)



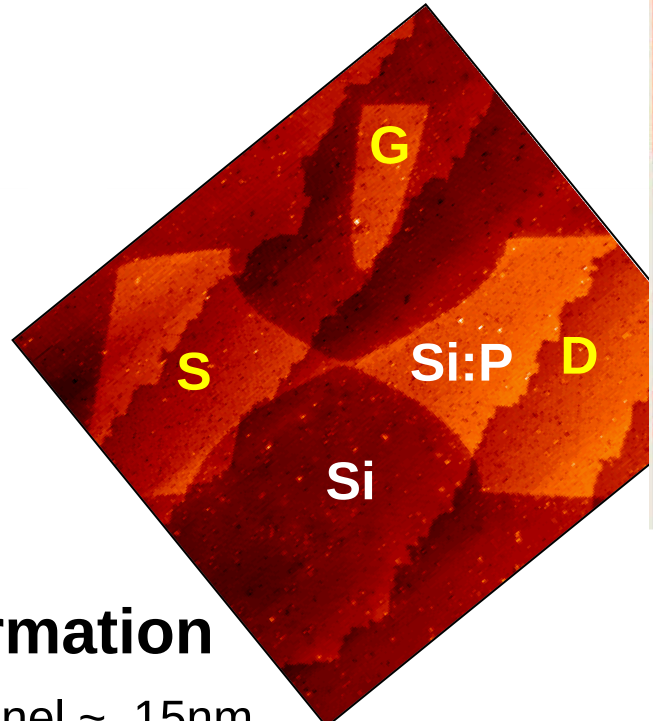


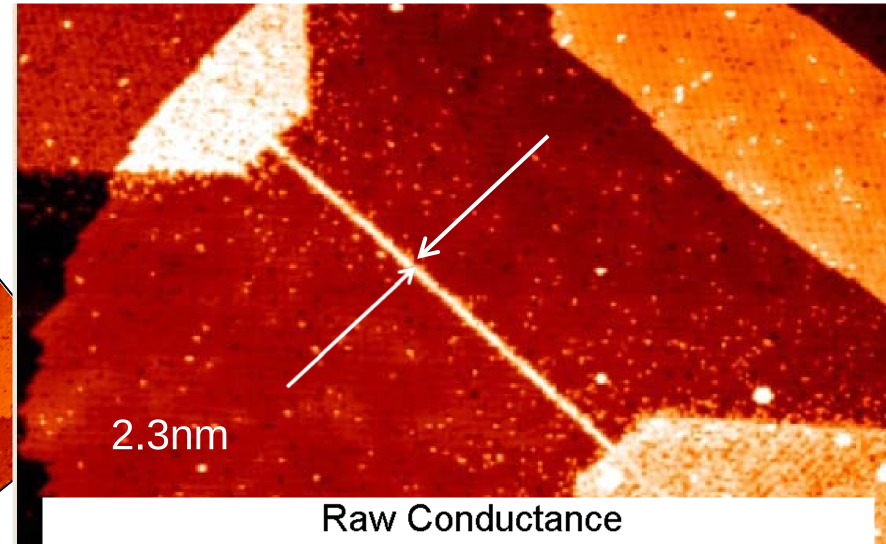
PRB 71, 045309 (2005)

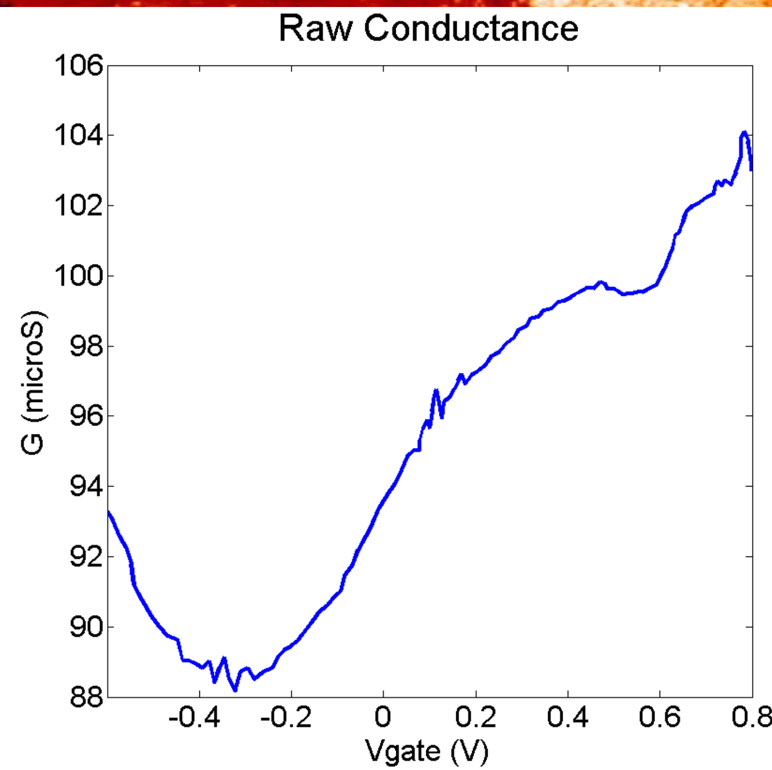
Case	Γ1 (meV)	EF (meV)
Carter *et al*	- 540	- 130
Qian *et al*	- 410	- 99
Ours	- 415	- 111



Si:P Nano-Wires







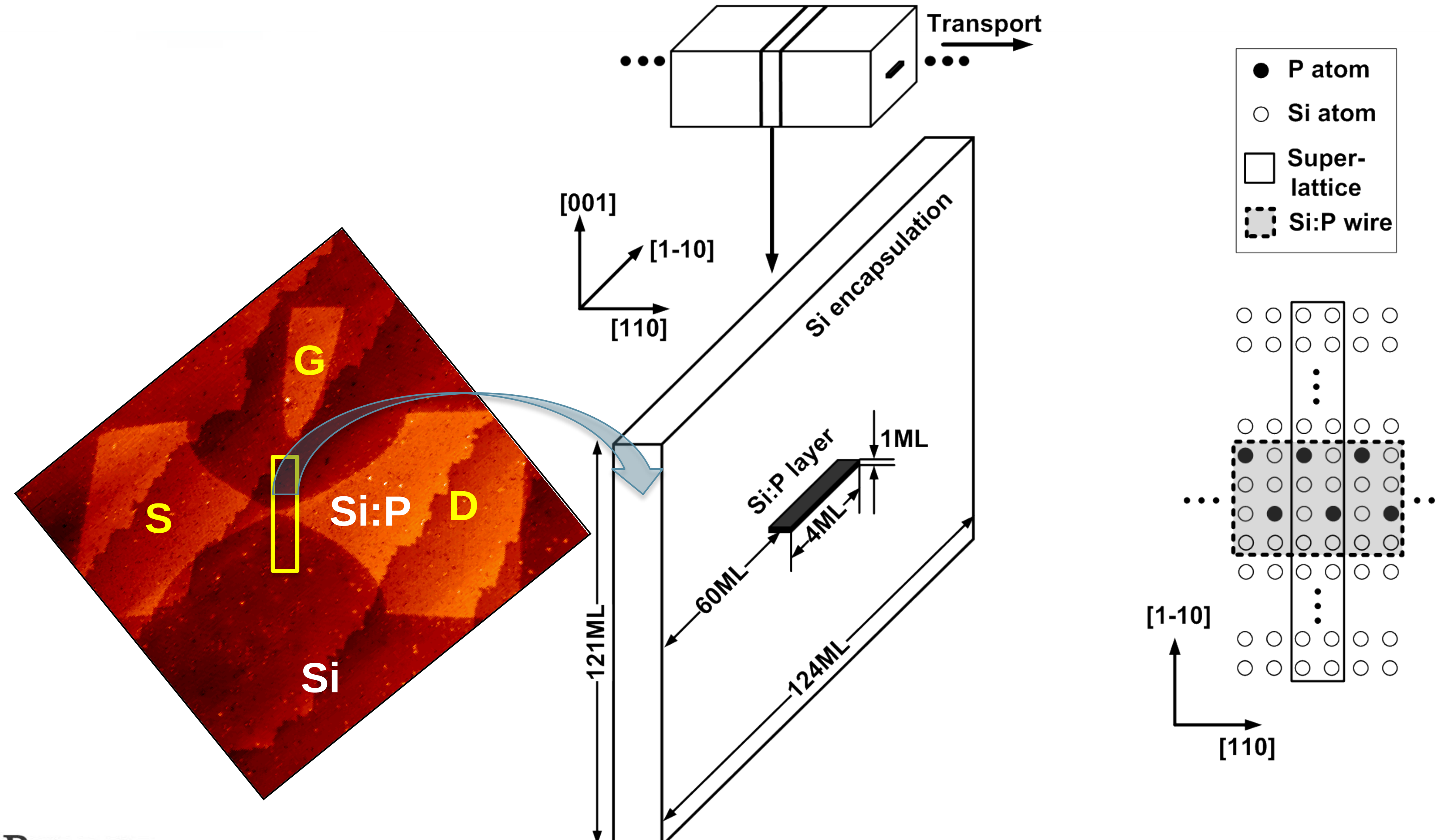
Device Information

- Effective Channel ~ 15nm
- From Gate to Channel ~ 35nm
- T~ 1.2(K). Doping Constant ~ 1/4ML

Problem to be solved

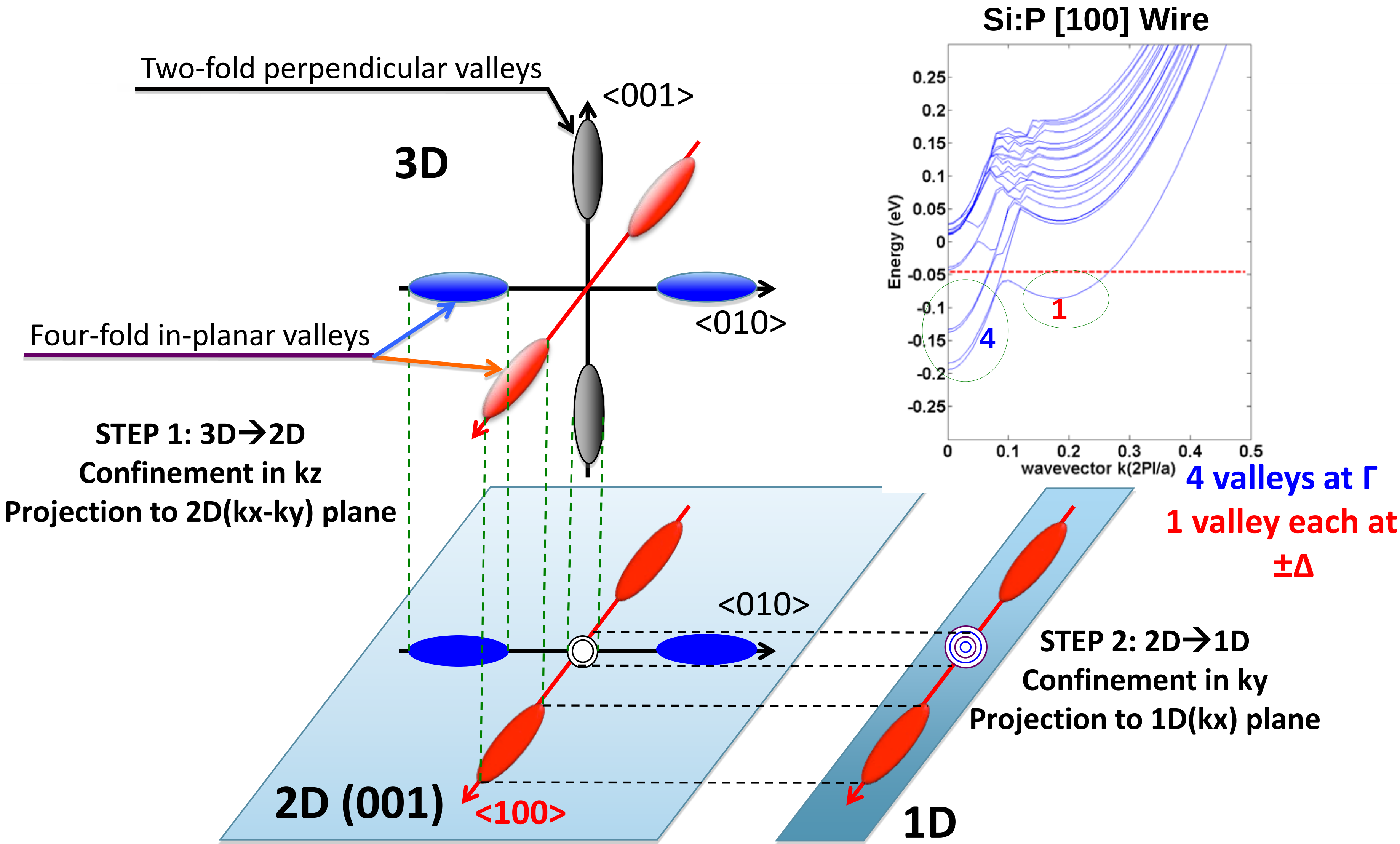
- Gate-dependent S-to-D Conduction Behavior
- Conduction through Donor-bands

Need to reduce computational domain size.



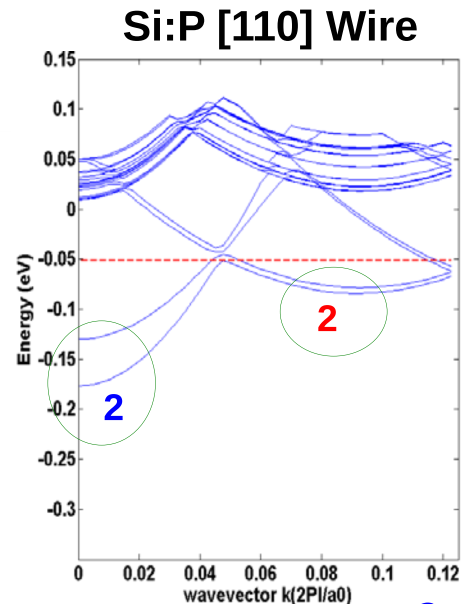
Band projection in [100] Si:P wires

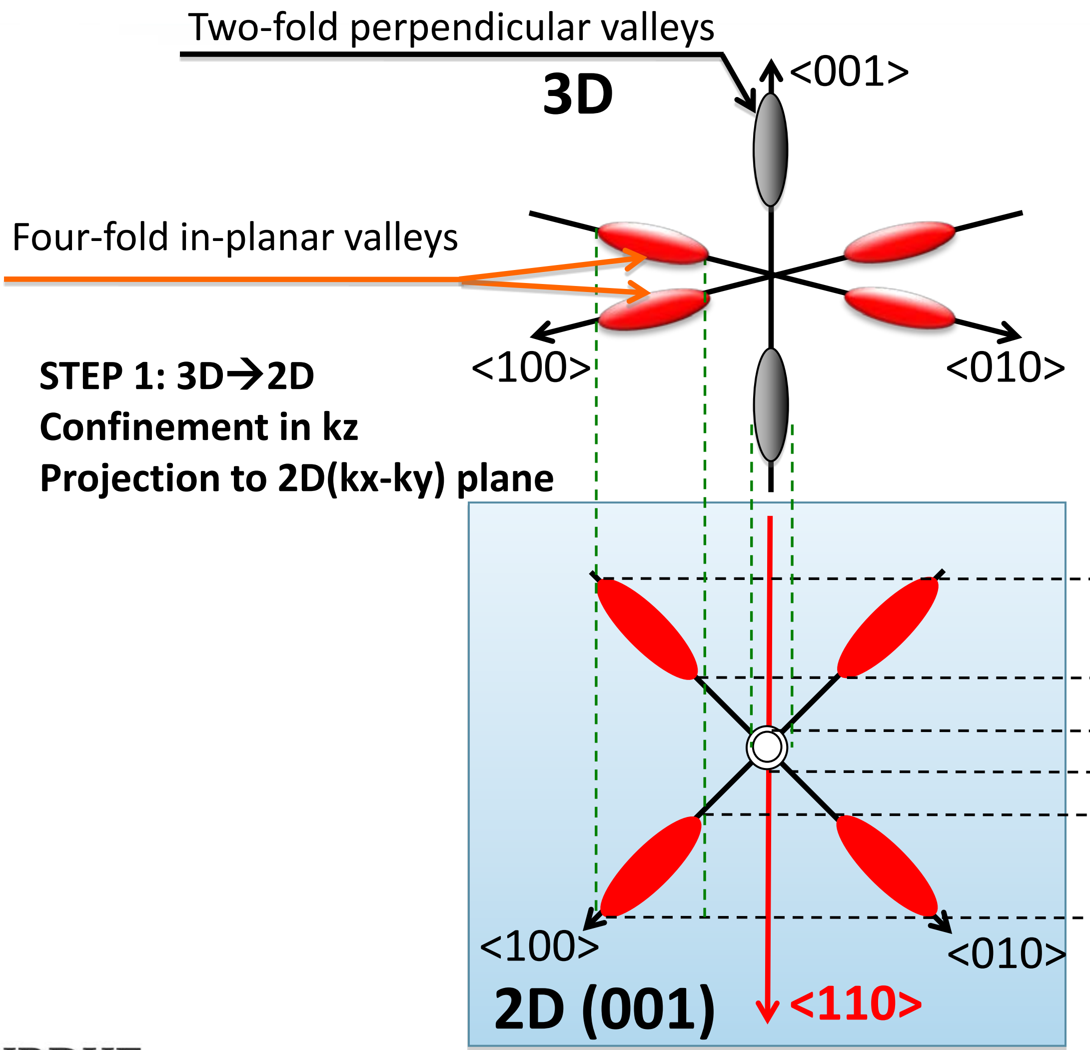
- 3D→2D→1D projection of Si [100] nanowire

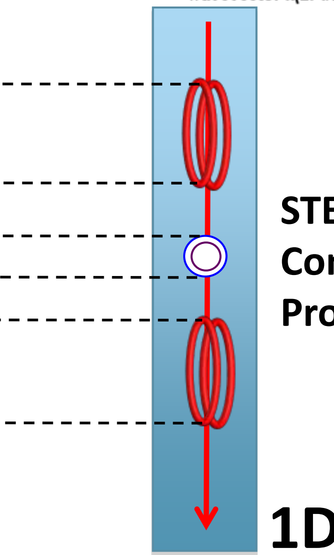


Band projection in [110] Si:P wires

- 3D→2D→1D projection of Si [110] nanowire







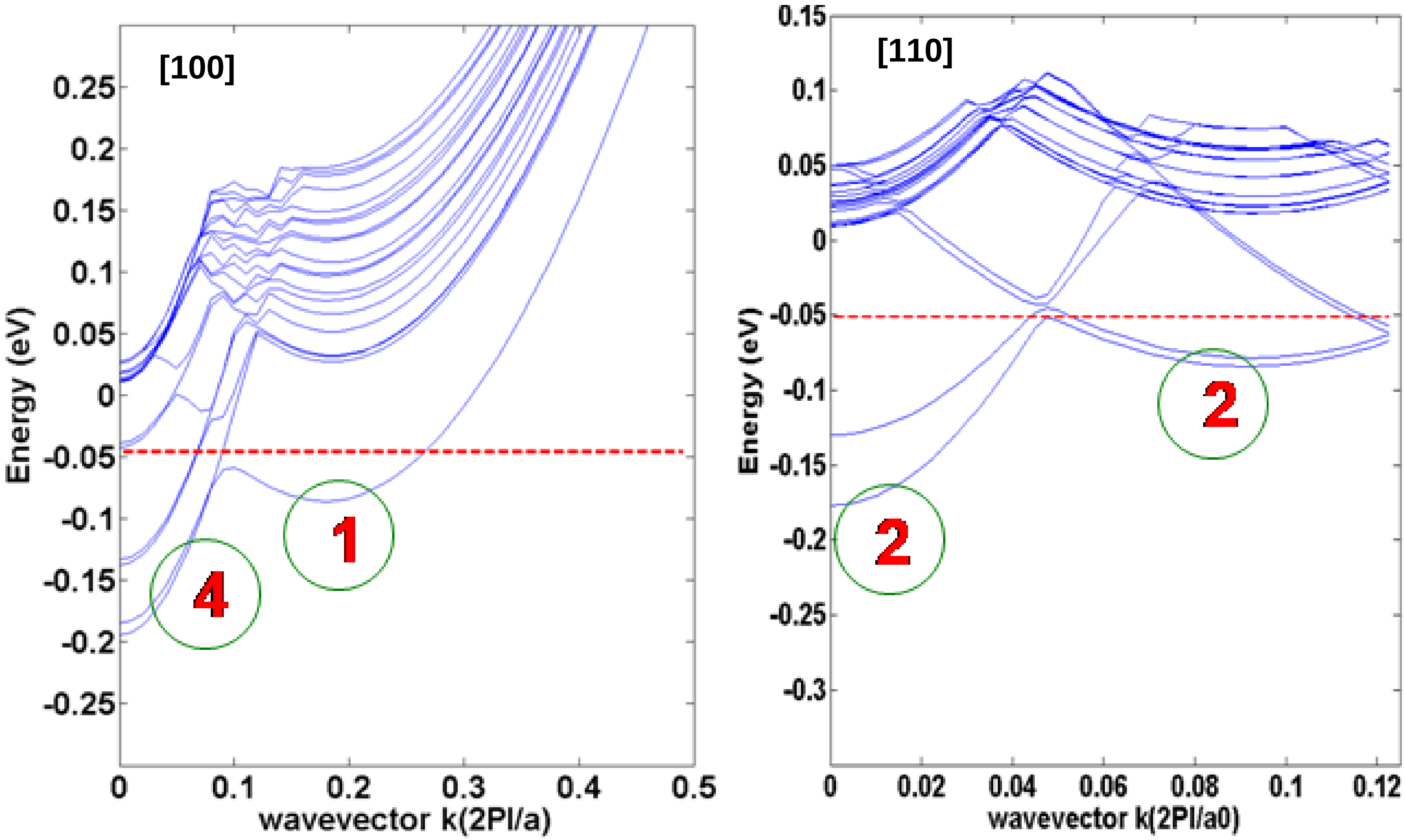
STEP 1: 3D→2D
Confinement in kz
Projection to 2D(kx-ky) plane

2 valleys at Γ

2 valley each at ±Δ

STEP 2: 2D→1D
Confinement in ky
Projection to 1D(kx) plane

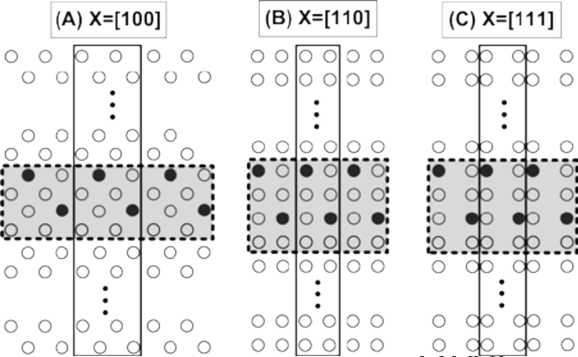
Band Projection in [100]/[110] Si:P Quantum Wire

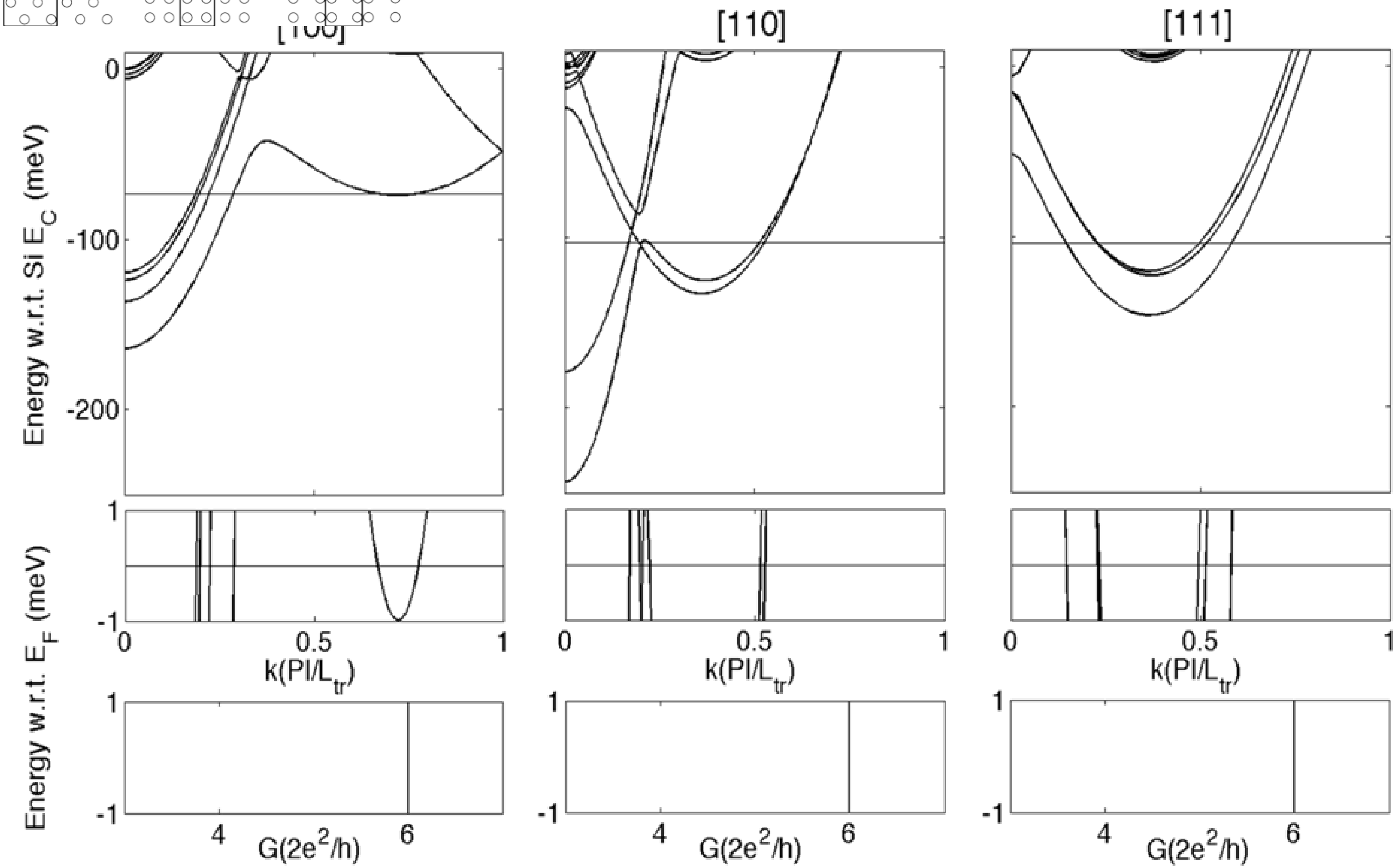


Wires are metllic with:

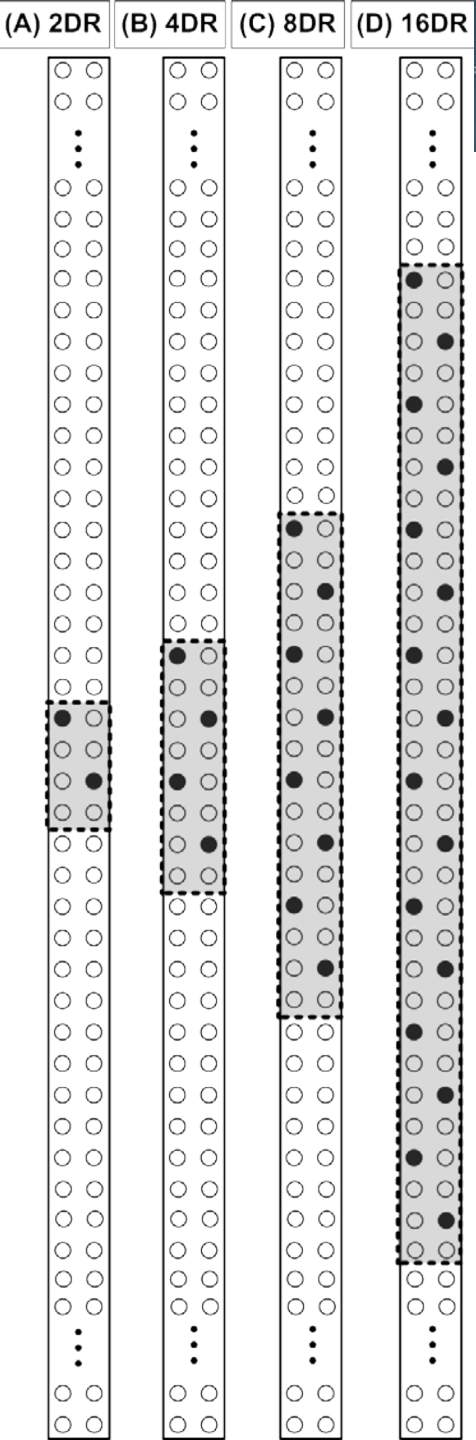
G(Ballistic) ~ $6(2e^2/h)$

Crystal direction Dependence [100],[110],[111]

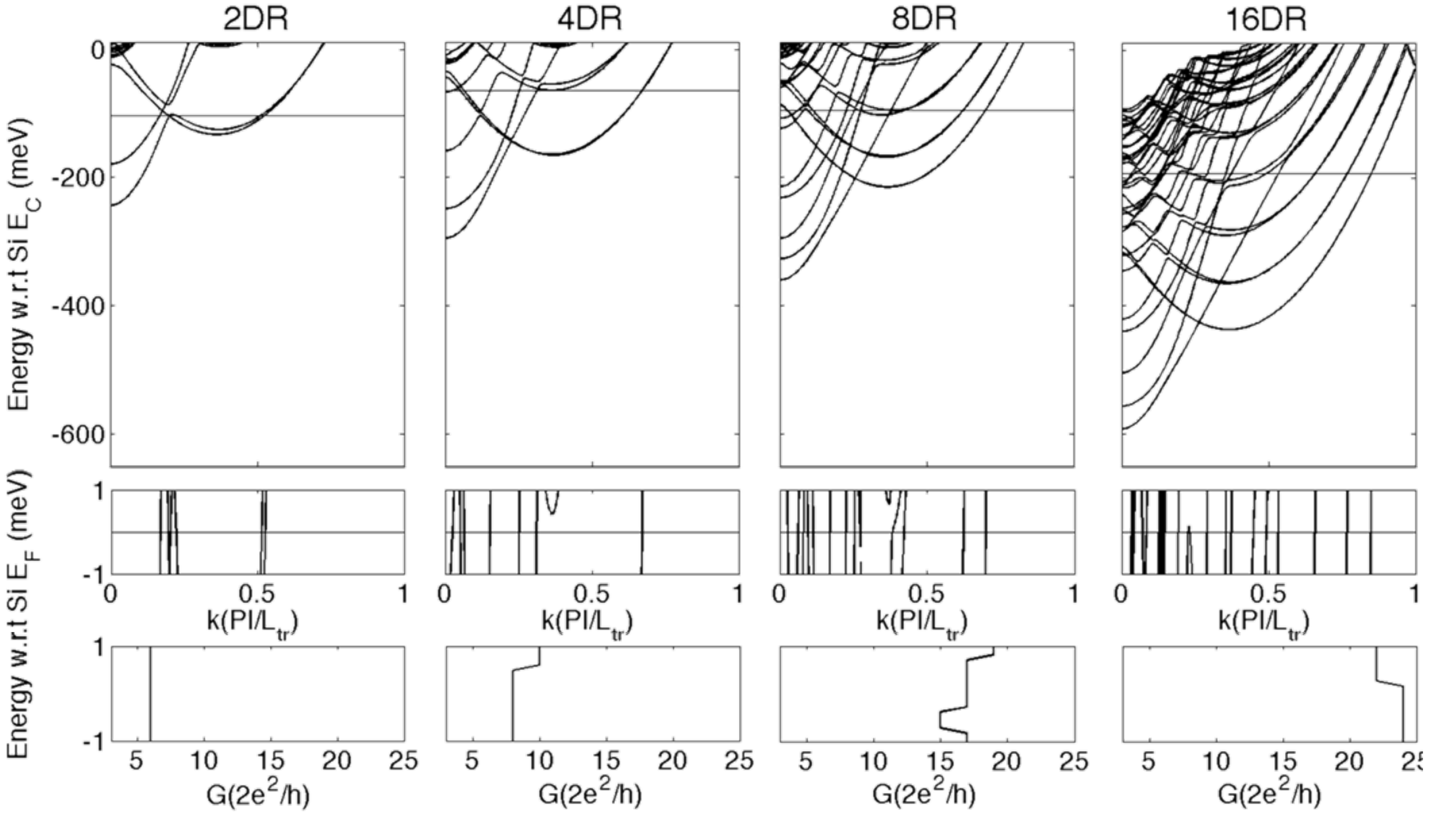




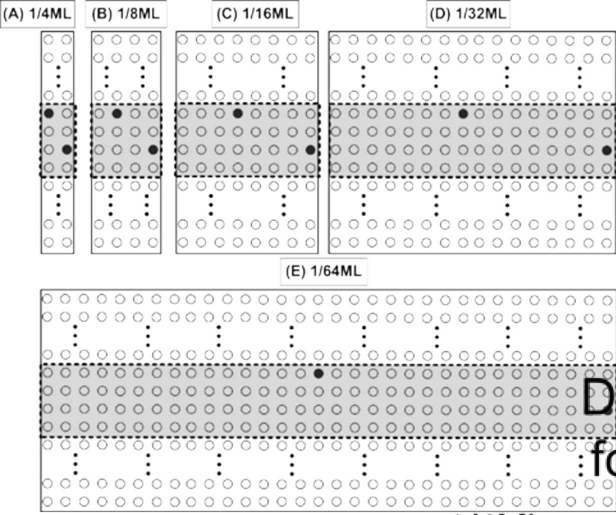
Width Dependence



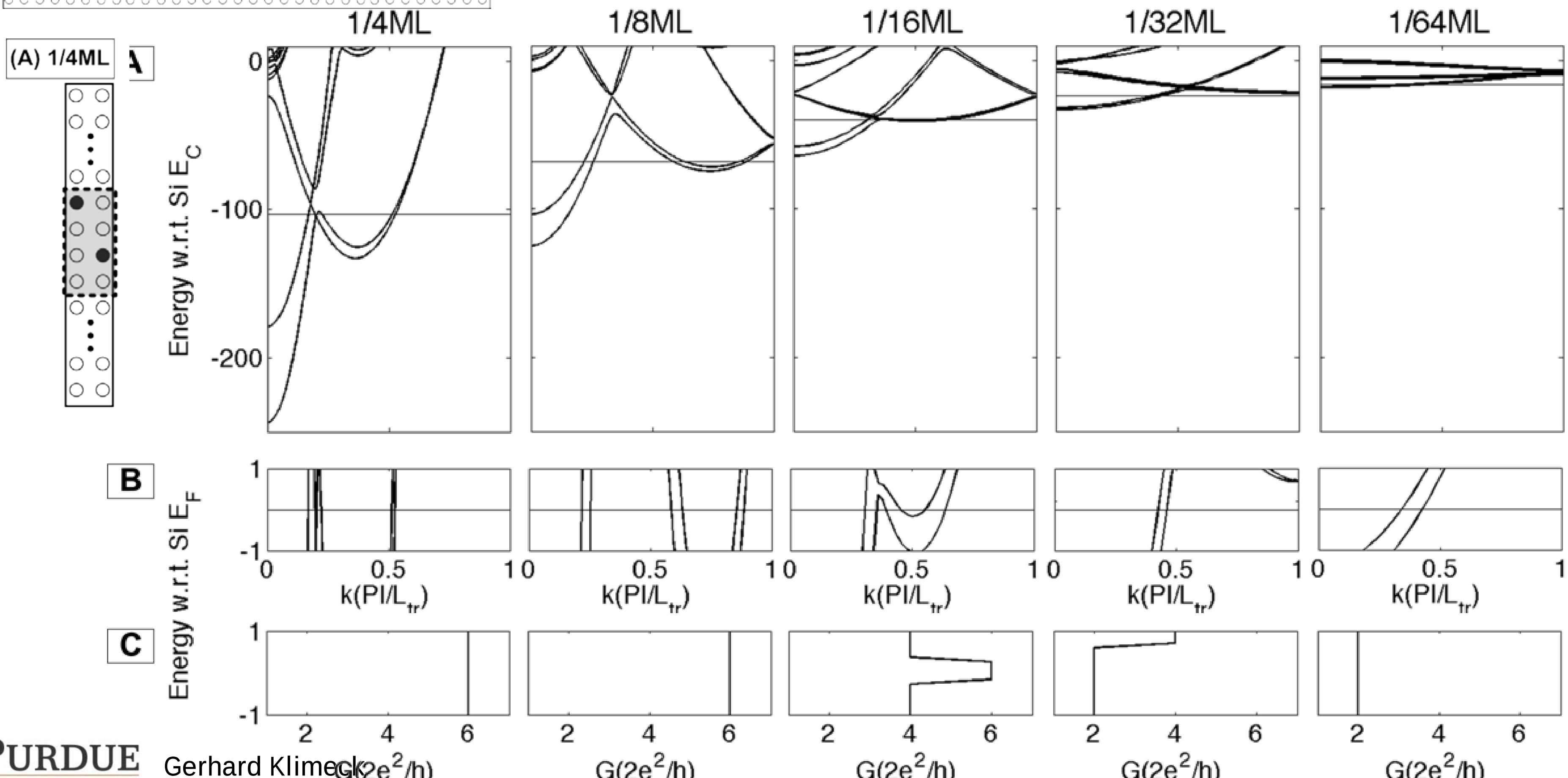
Dependence of bandstructures on width for [110] transport and 1/4ML doping



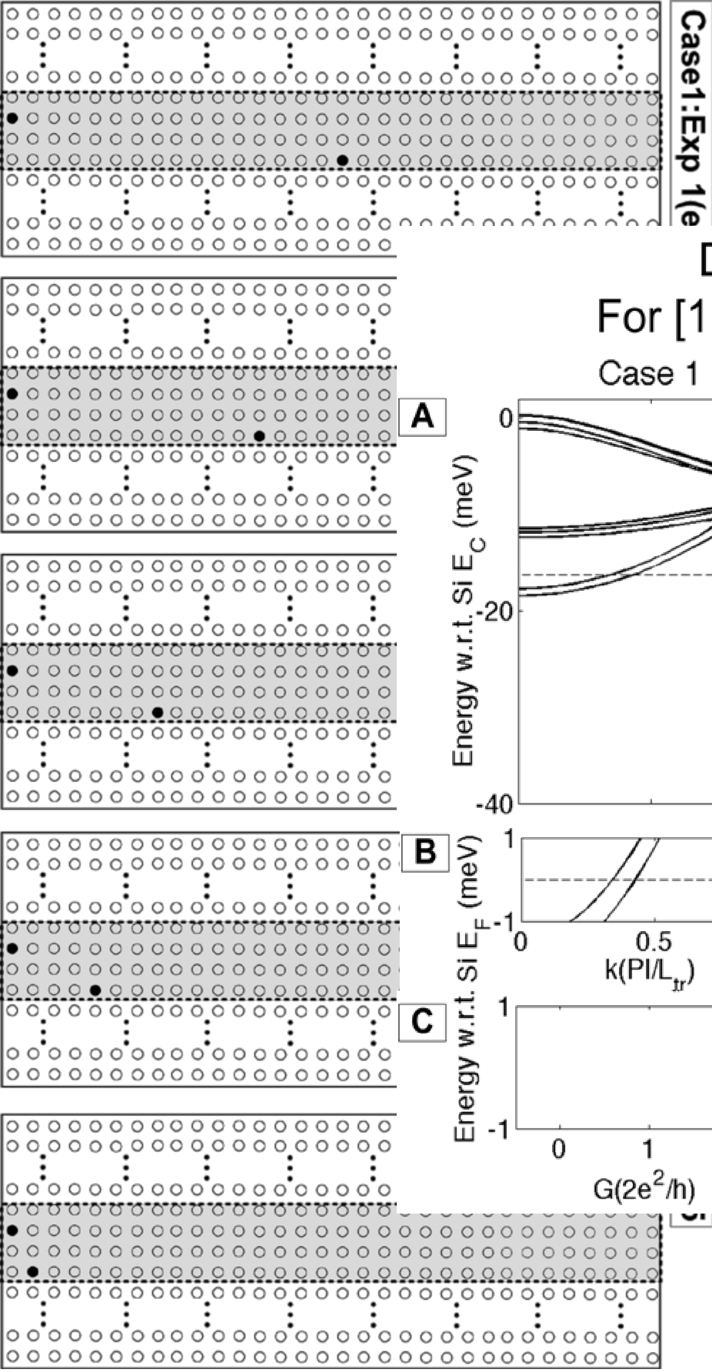
Doping Dependence

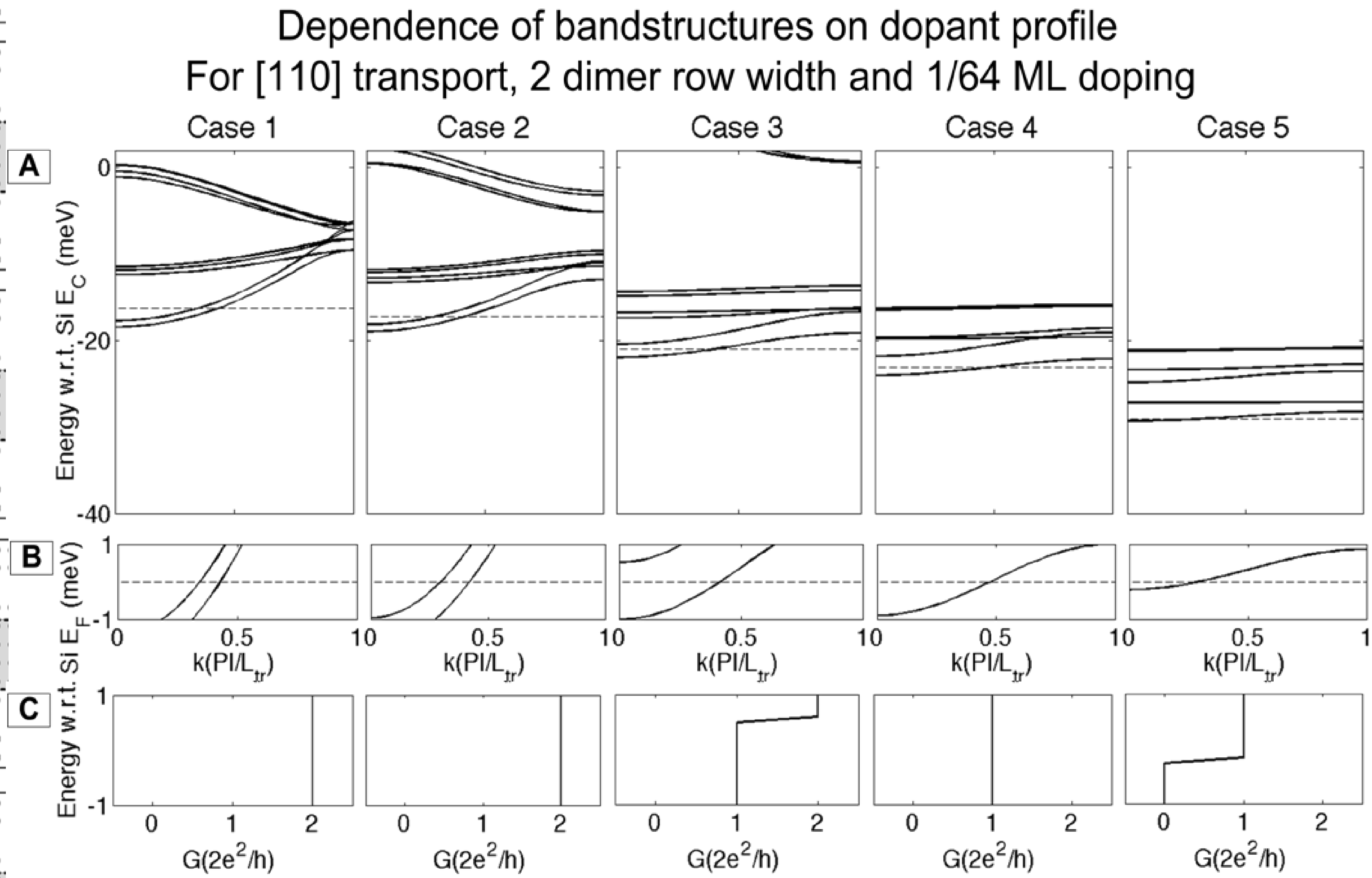


Dependence of bandstructures on doping
for [110] transport and 2 dimer row width

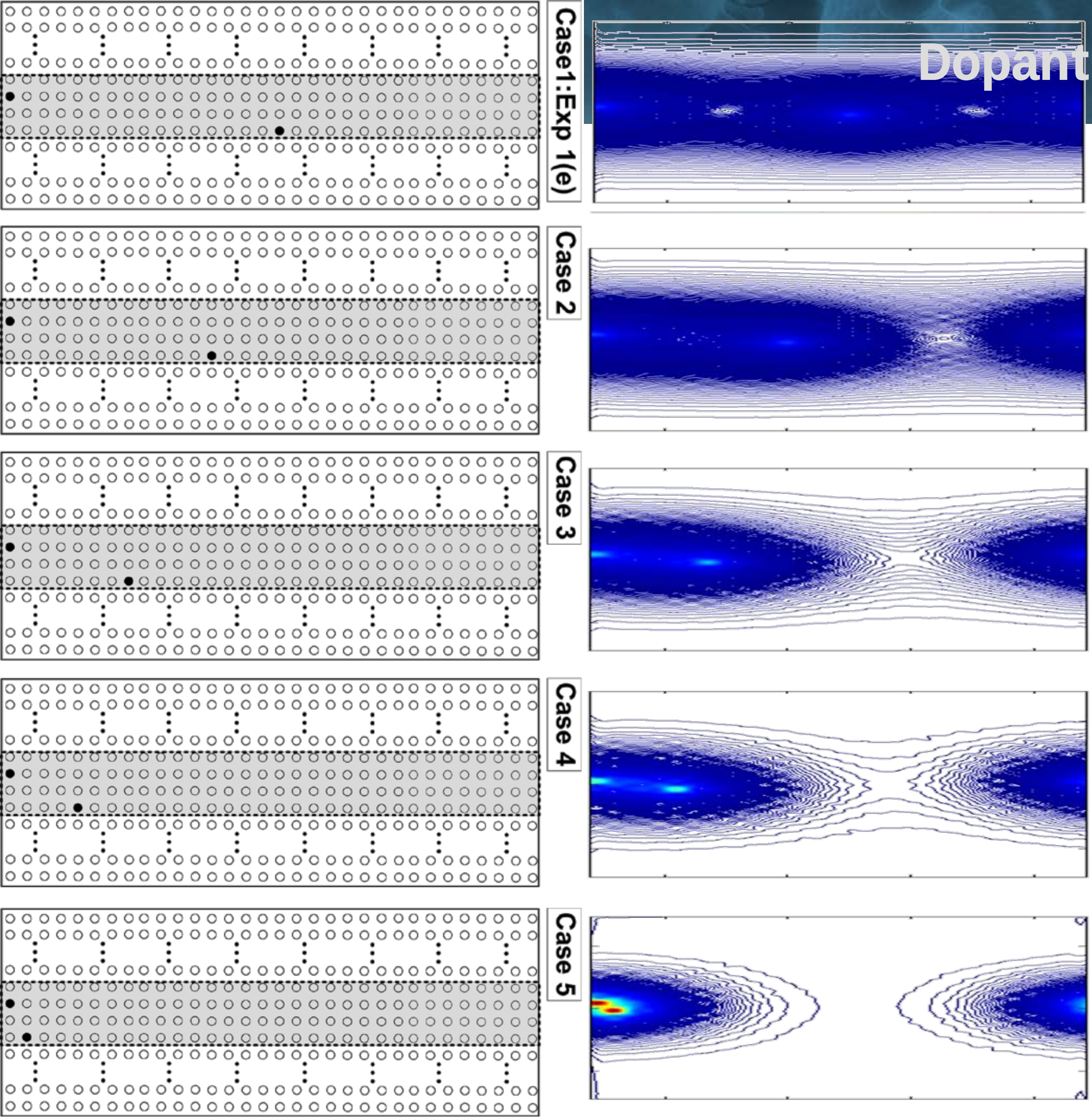


Dopant Placement Details





Dopant Placement Details

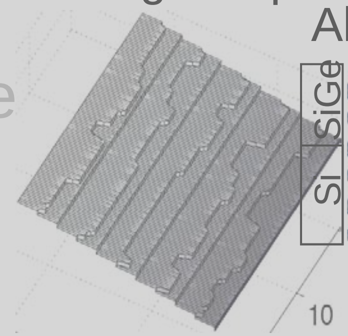


- Charge distribution on δ-doping layer

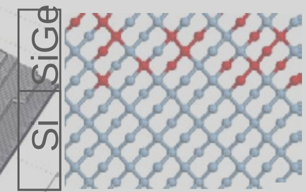
Multi-Million Atom Simulation of Quantum States in Realistically Extended Devices in Silicon

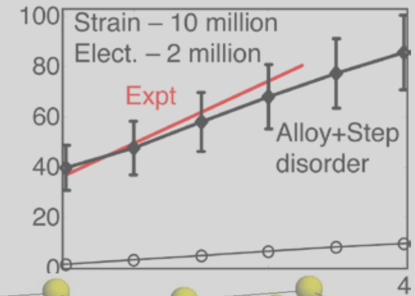
- Motivation
- NEMO Numerical Engine
- Valley splitting
  - »Si quantum wells
  - »Si Quantum Dots
- Single impurities in Si
  - »Metrology – impurity identification
  - »Wavefunction mapping
  - »g-factor engineering
  - »CTAP
- Dense impurities in Si – Si:P
  - »Infinite sheets
  - »Infinite wires
  - »Gating, transport through wires
  - »Impurity-based quantum dots

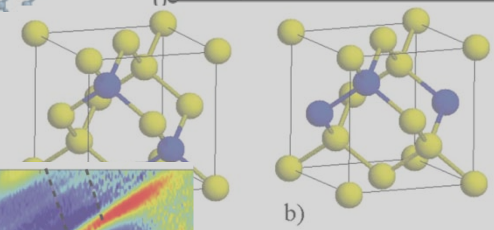
Rough steps

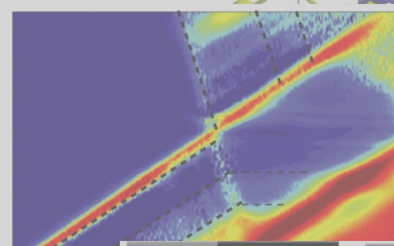


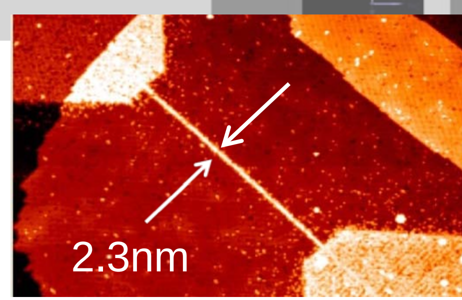
Alloy disorder



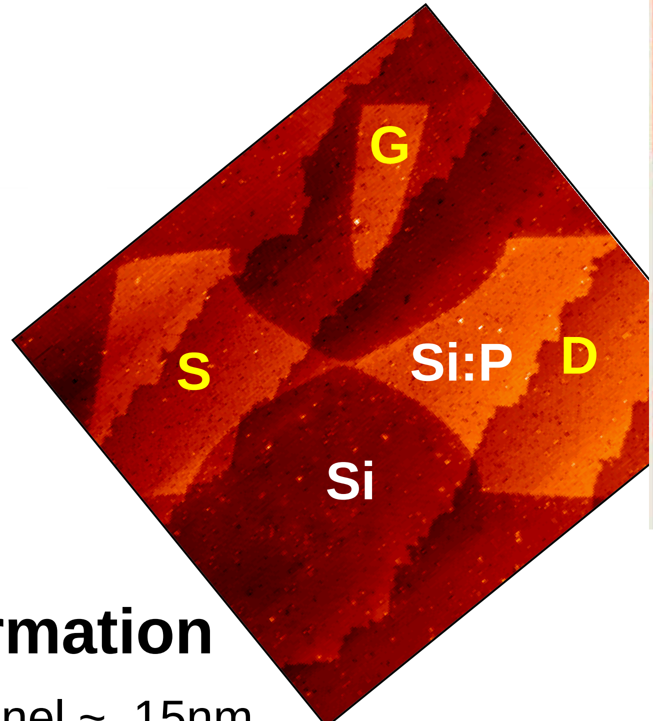


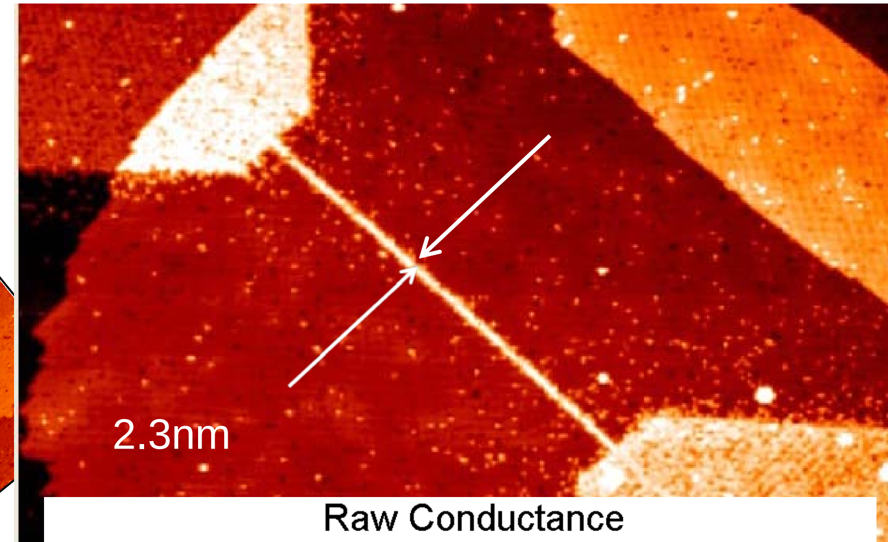


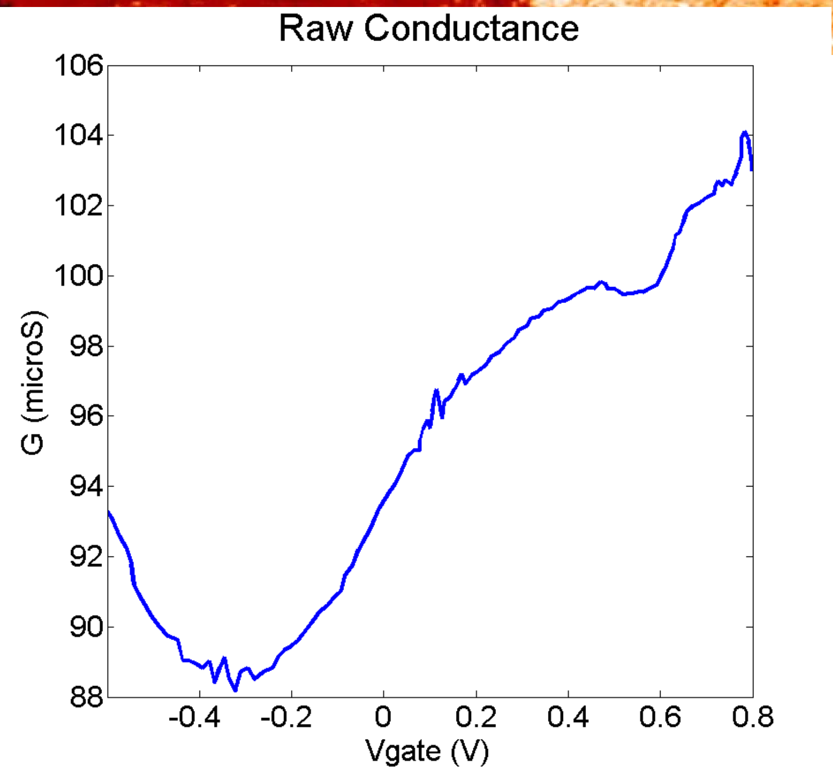




Gating Effects on Si:P Nano-Wires





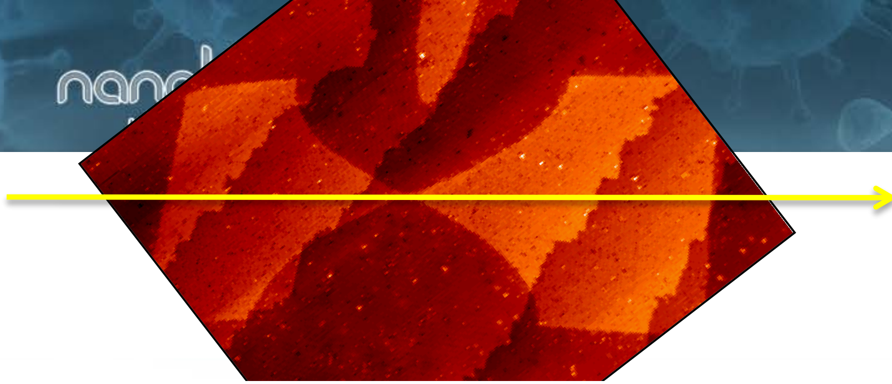


Device Information

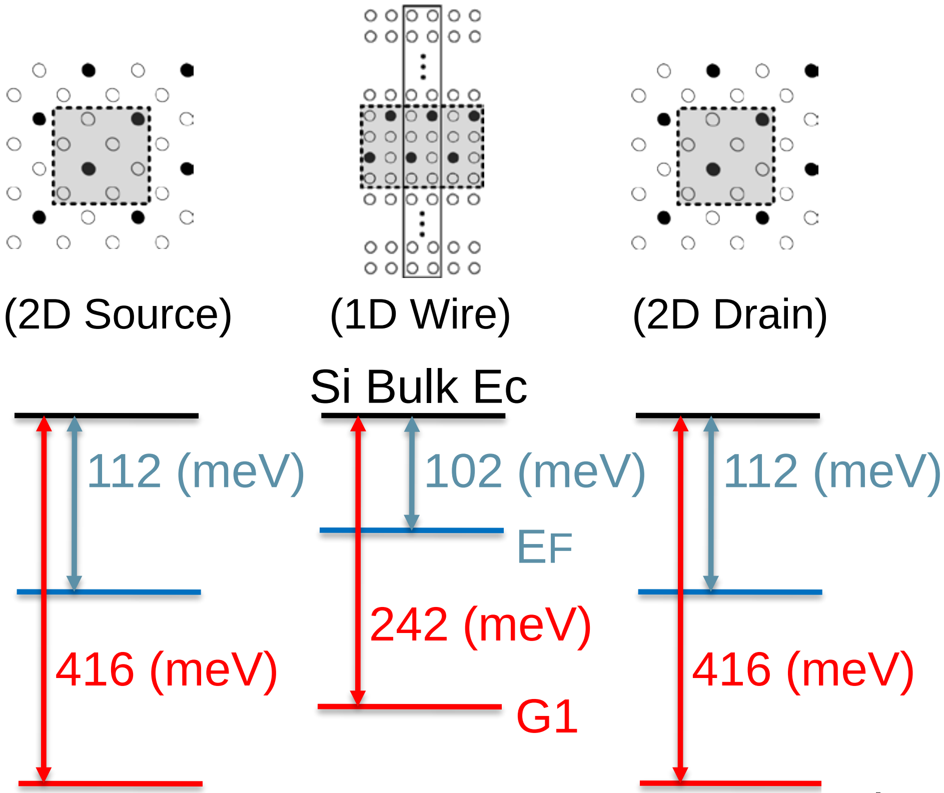
- Effective Channel ~ 15nm
- From Gate to Channel ~ 35nm
- T~ 1.2(K). Doping Constant ~ 1/4ML

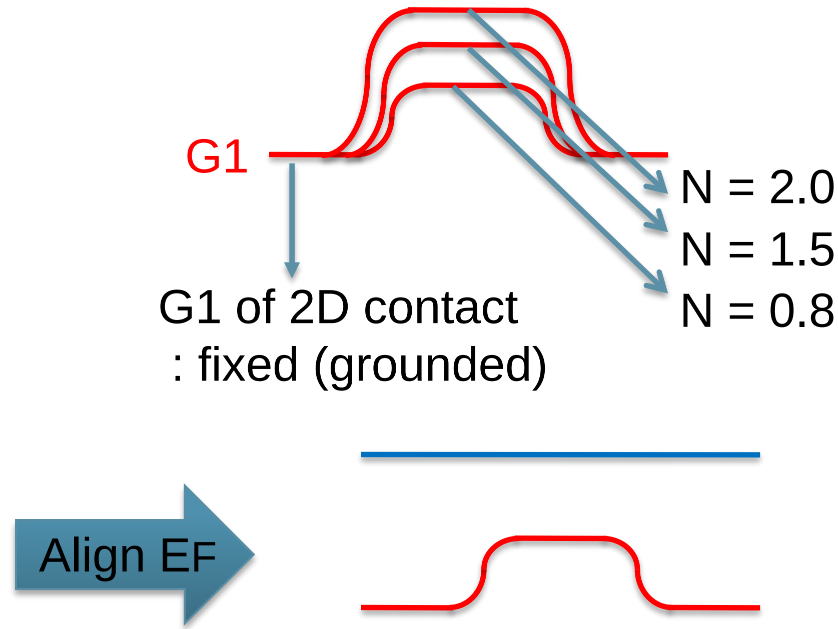
Problem to be solved

- Gate-dependent S-to-D Conduction Behavior
- Conduction through Donor-bands



The Local-bandstructure along transport direction.

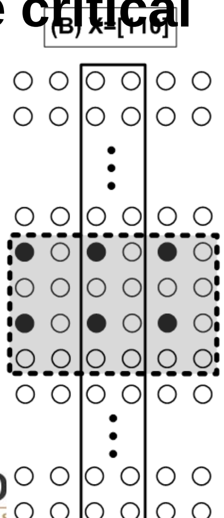


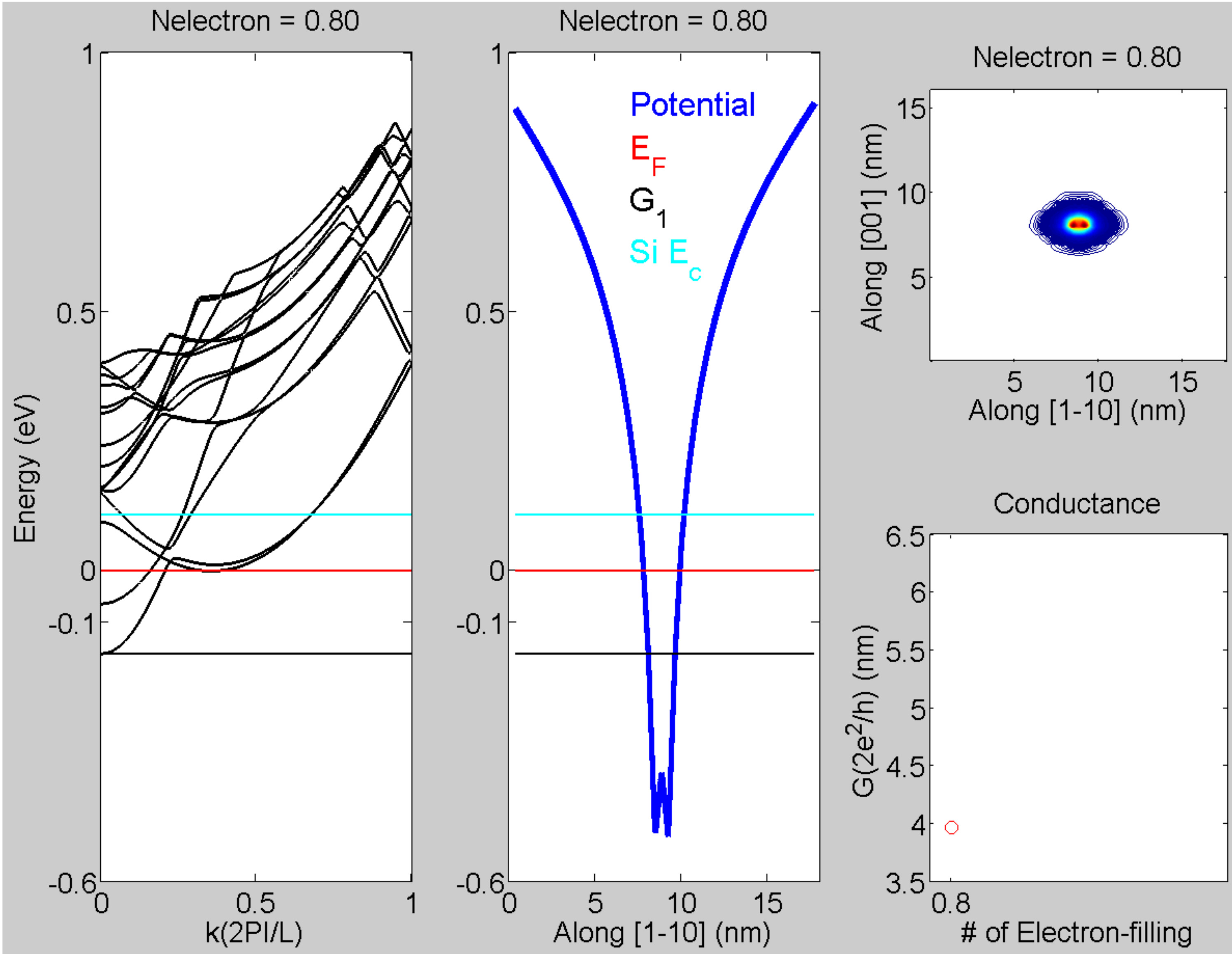


Electrostatic potential is spatially widely reaching
The region is too large (right now) for full self-consistent calculations

Charging Effect on Conduction Property

- We fix # of charge filling => Obtain EF and potential
- Neutral at N=2
- **Dispersion depends on on the electron filling**
- Like usual Si nanowires
- **Electrostatics are critical**



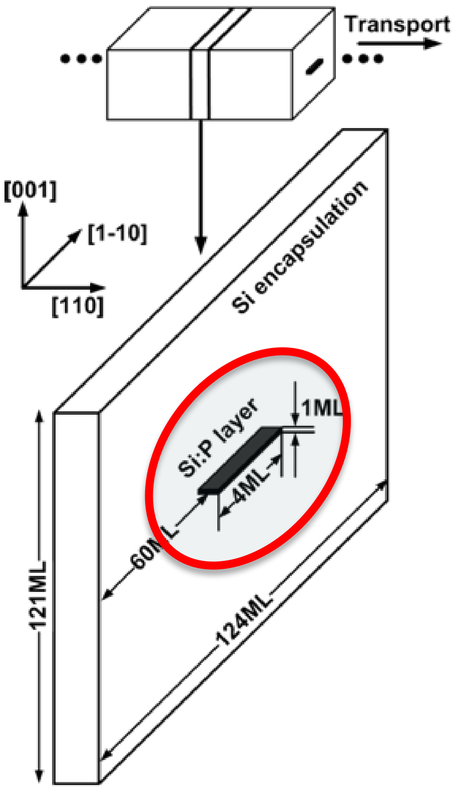


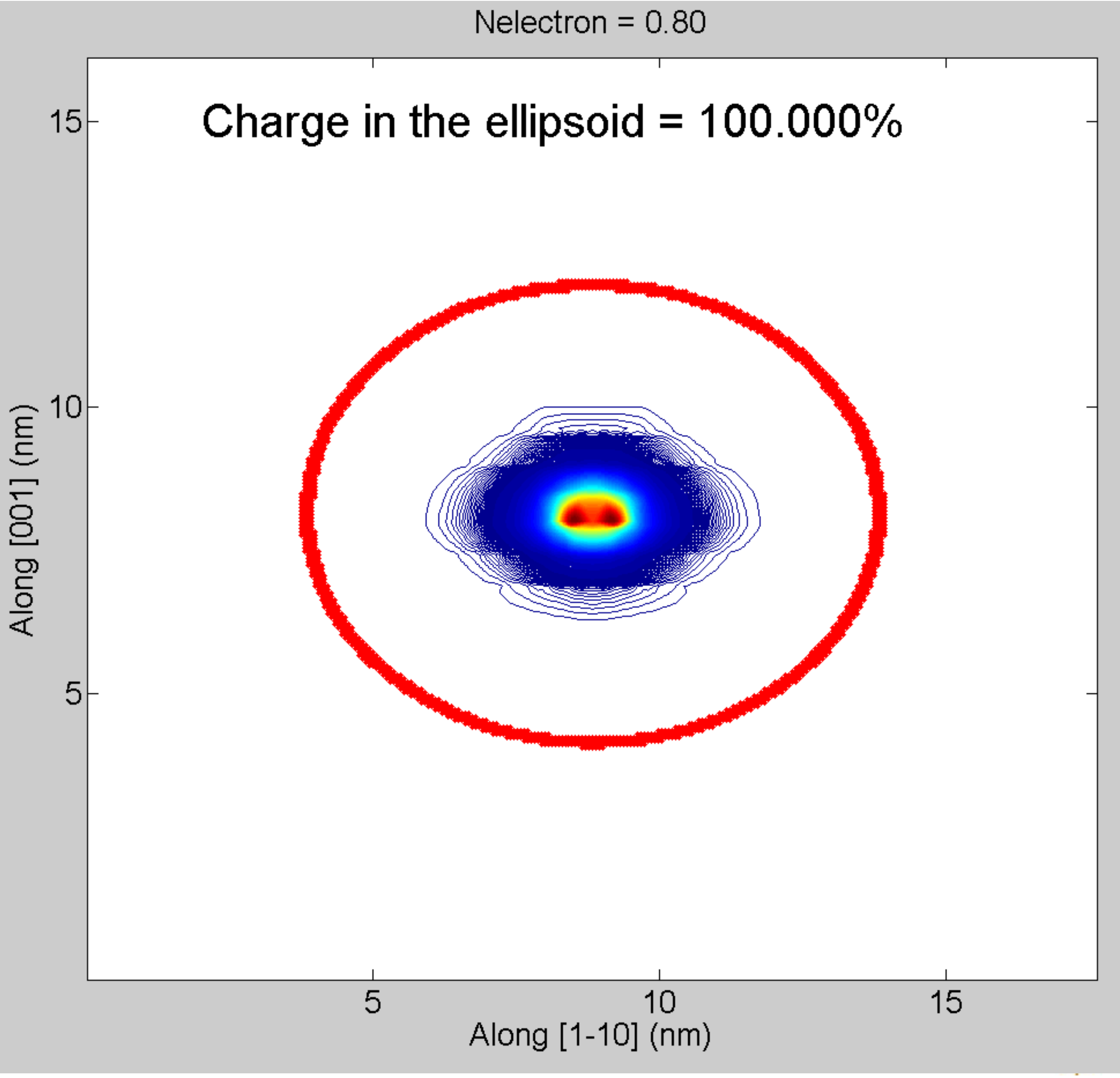
Transport through impurity bands?

- Charge expands in diameter
- Ellipsoid :

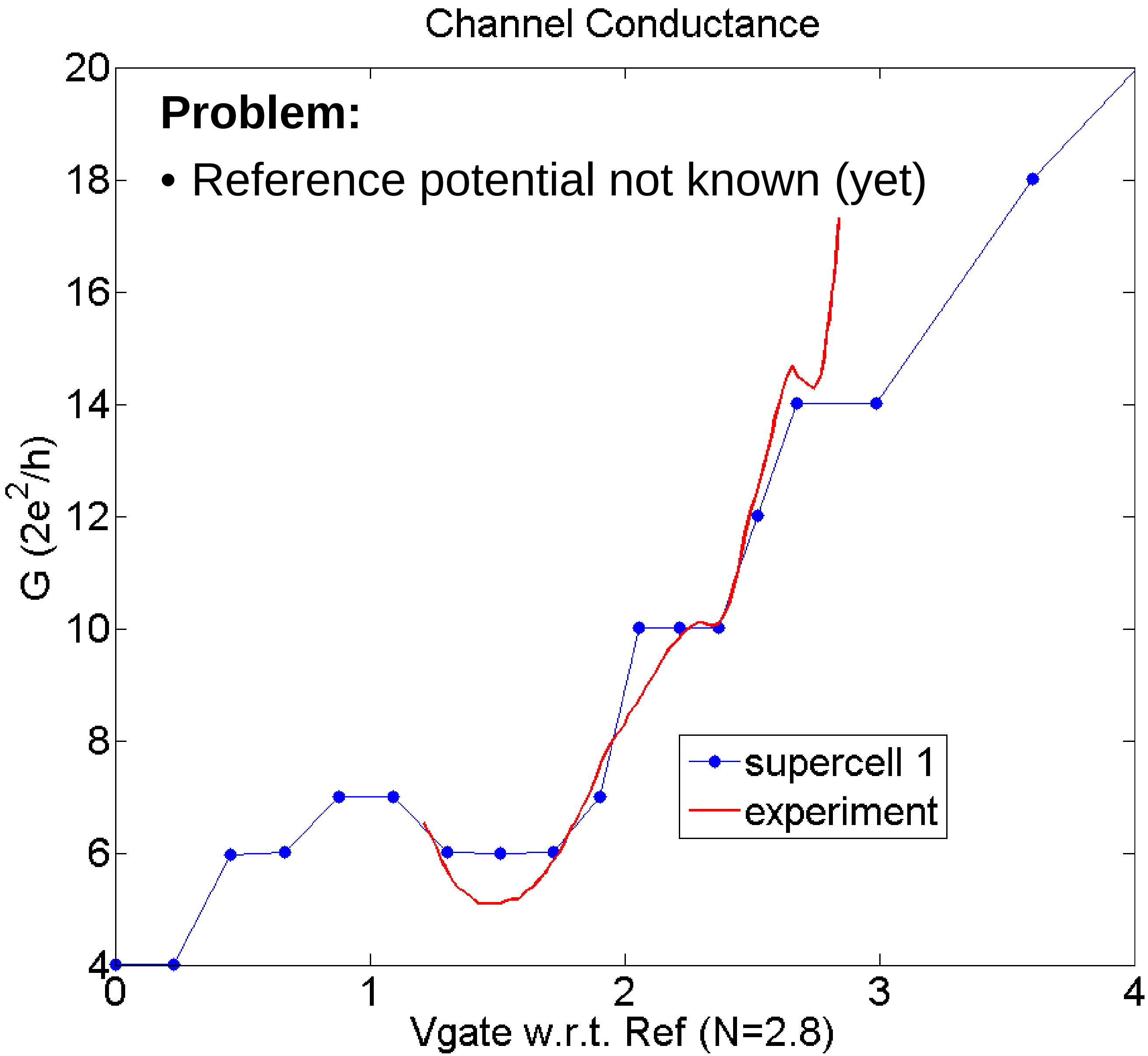
10nm axis along [1-10]

8nm axis along [001]





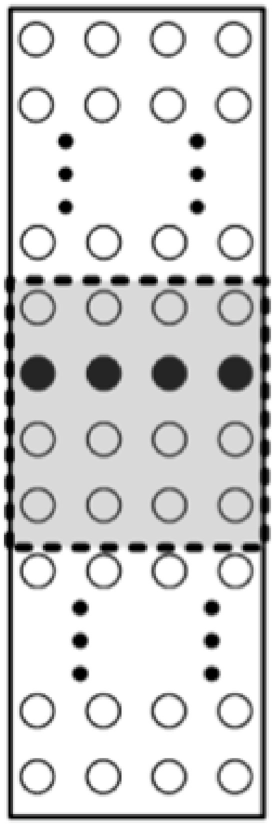
Comparison to experiment - Super Cell 1



Problem:

- Reference potential not known (yet)

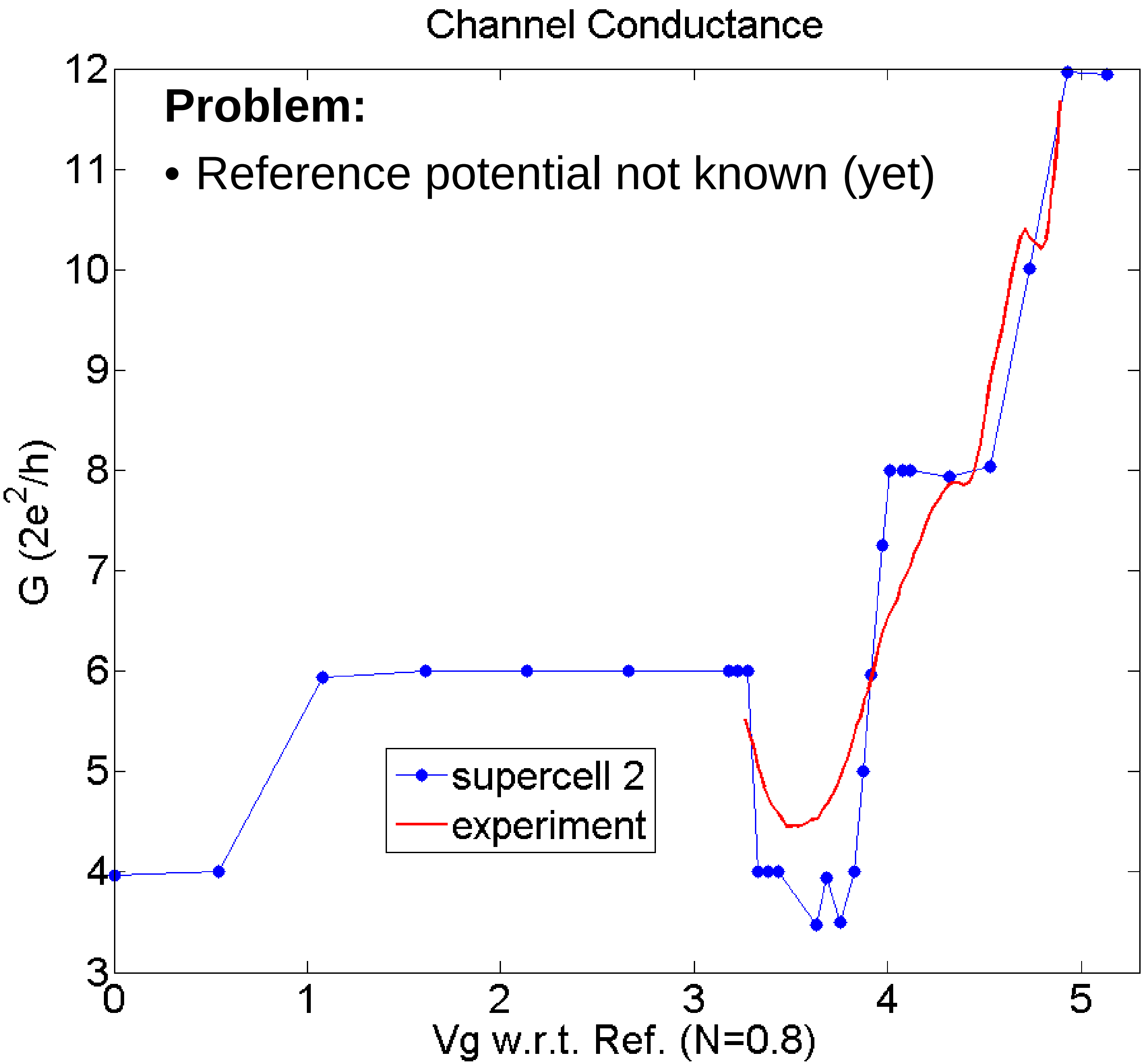
Super-cell configuration



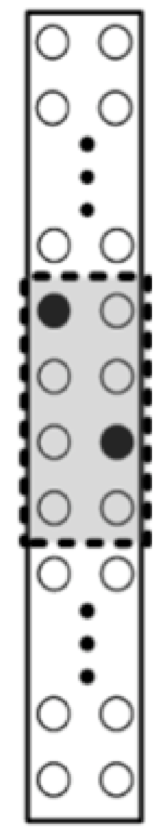
Comparison to Experiment - Super Cell 2

Problem:

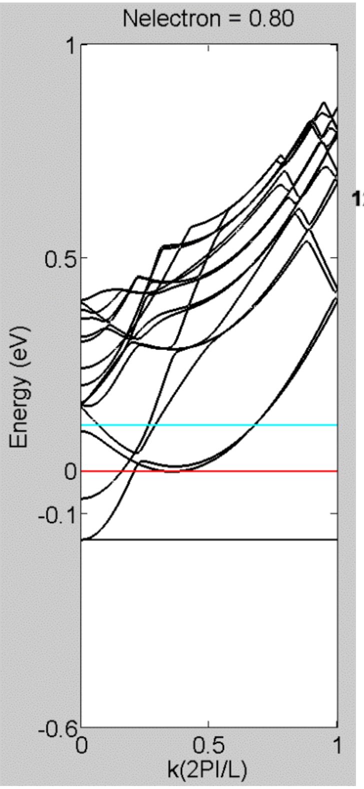
- Reference potential not known (yet)

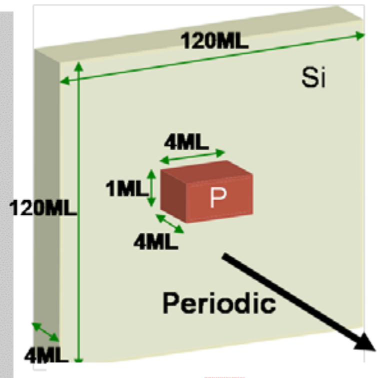


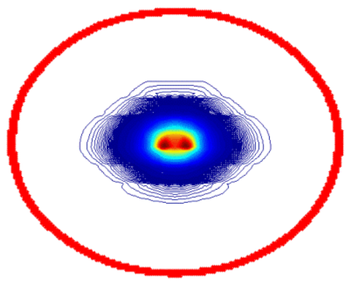
Super-cell configuration



Transport of P δ-doped Si Quantum Wire





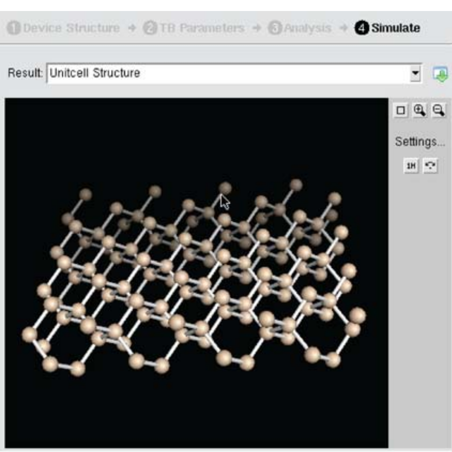


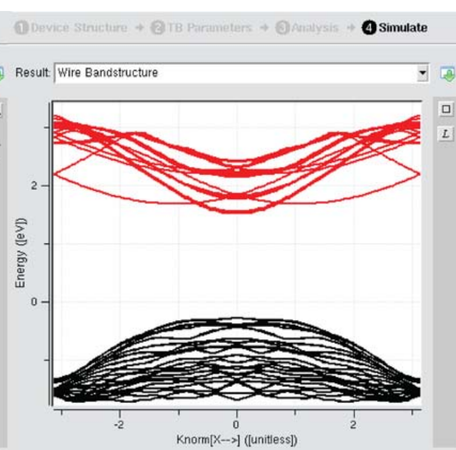
Results – Numerical Experiments :

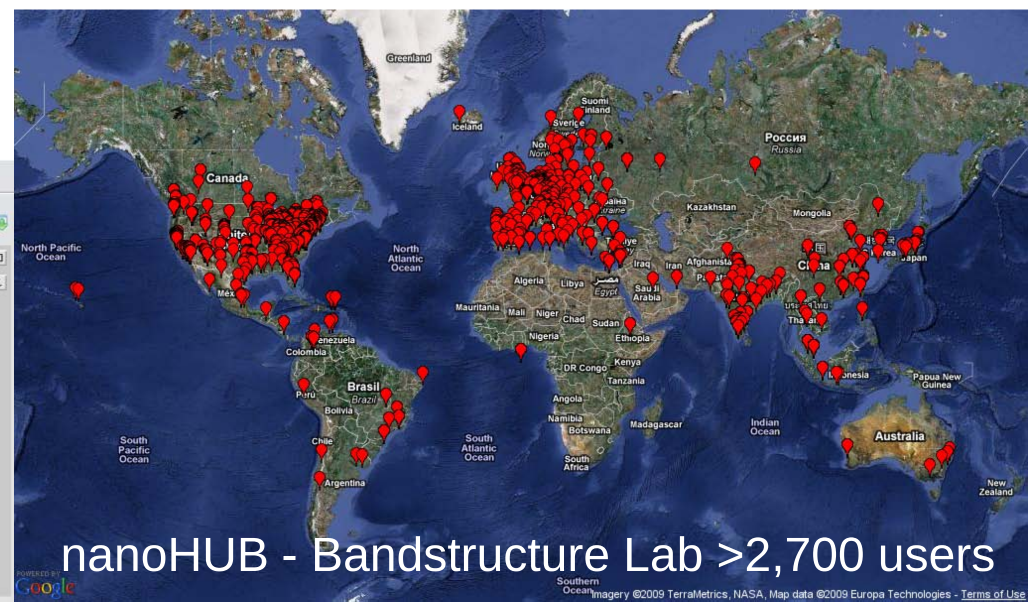
- Direction dependence:
  - Dispersion (strong)
  - Conductance (weak)
- Doping, width, configurations:
  - Dispersion and conductance (strong)
- Strong gate / charge dependence!

Problems:

- Need better control over the spatially extended electrostatic potential



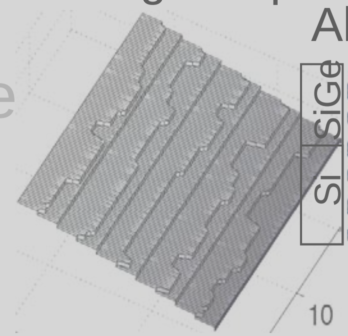




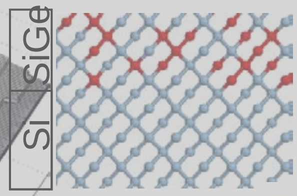
Multi-Million Atom Simulation of Quantum States in Realistically Extended Devices in Silicon

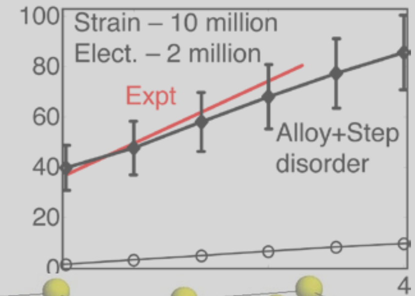
- Motivation
- NEMO Numerical Engine
- Valley splitting
  - »Si quantum wells
  - »Si Quantum Dots
- Single impurities in Si
  - »Metrology – impurity identification
  - »Wavefunction mapping
  - »g-factor engineering
  - »CTAP
- Dense impurities in Si – Si:P
  - »Infinite sheets
  - »Infinite wires
  - »Gating, transport through wires
  - »Impurity-based quantum dots

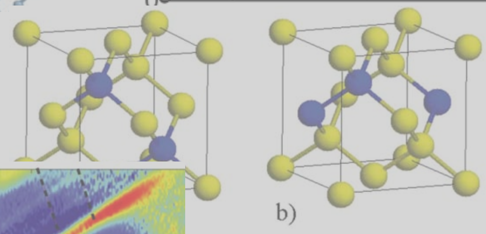
Rough steps

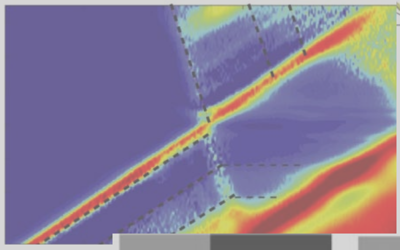


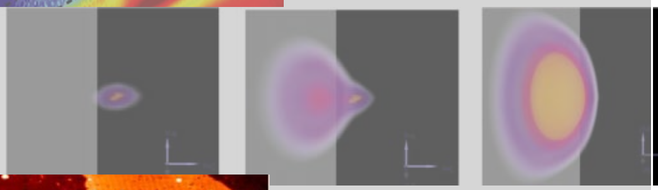
Alloy disorder

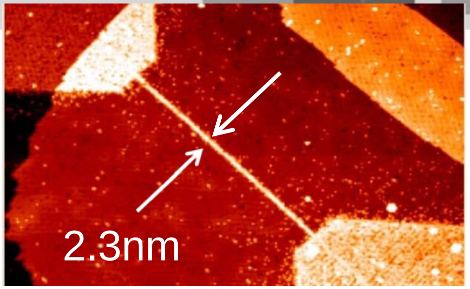


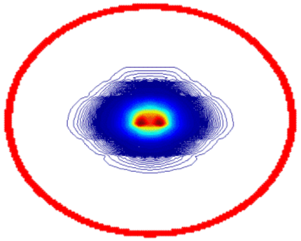




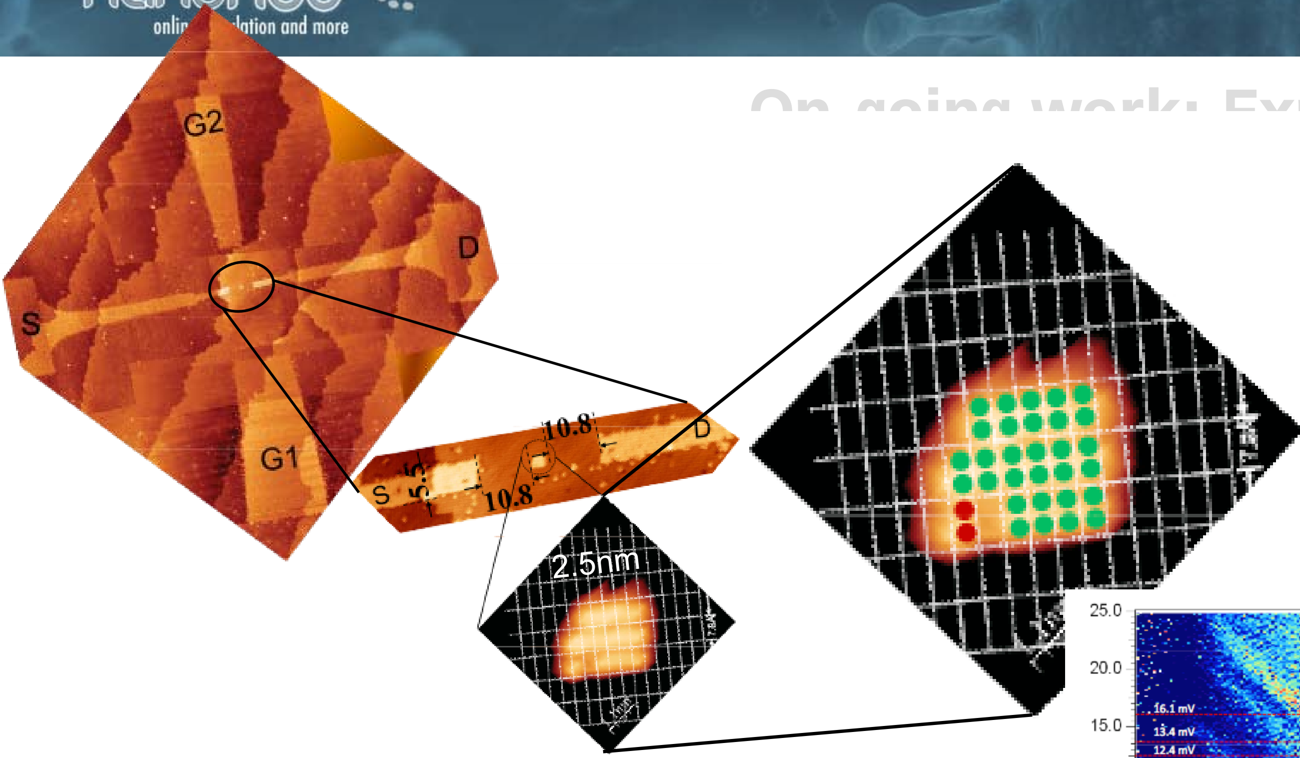


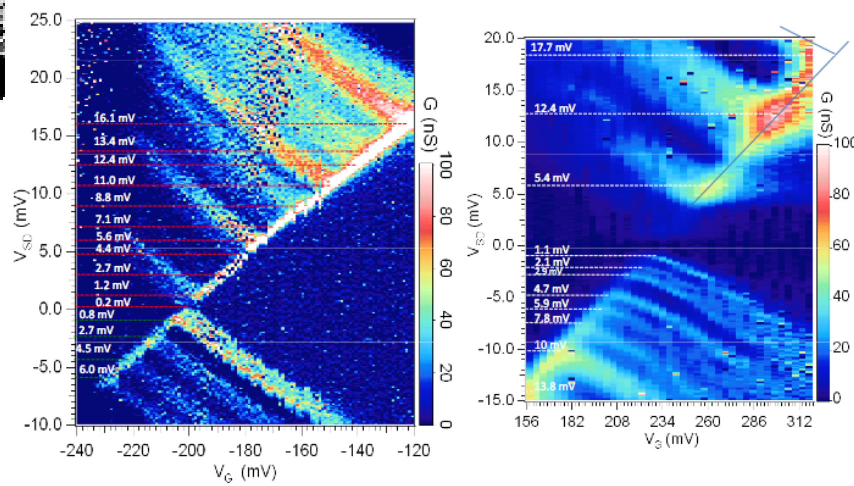






On-going work: Exploring Si:P QD, D85



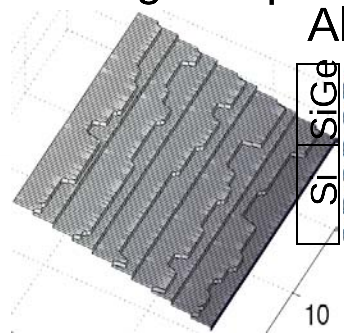


- Identify the correct state of the system
  - » Number of donors (#P) in the dot
  - » Number of filled electrons (#e) in the dot
  - » Correct estimate of the excited spectrum from the Coulomb diamond.

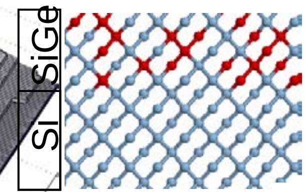
Multi-Million Atom Simulation of Quantum States in Realistically Extended Devices in Silicon

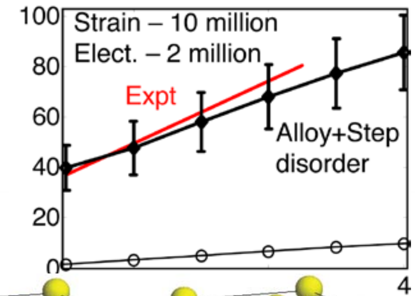
- Enable:
  - » Numerical experiments – one could not do otherwise
    - ✓ Experimentally
    - ✓ Analytically
  - » **Realistically extended** devices
  - » Quantitative explanation of experiments
    - ✓ Valley splitting in quantum wells
    - ✓ Single impurities
    - - Not yet …. Dense impurity channels
- Strain and electrostatics are far-reaching into the crystal
- Disorder at the interface is critical
- Valley splitting is interface dominated - sensitive to the details of the interface!
- Scattered Impurity placement in dense Si:P systems does not affect performance radically

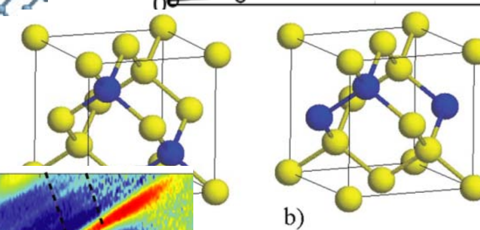
Rough steps

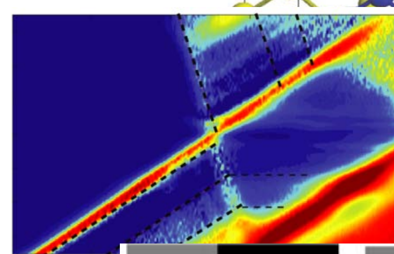


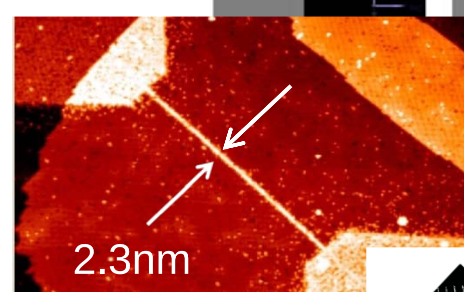
Alloy disorder

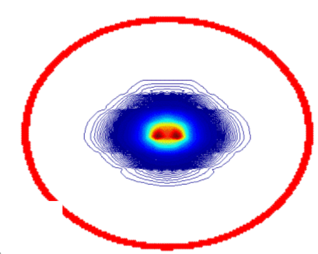


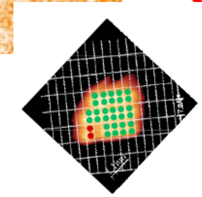












Thanks to

NRI

Nanoelectronics • Architectures
MIND
MIDWEST INSTITUTE FOR NANOELECTRONICS DISCOVERY

SRC

FCRP

SCIENCE TO SHAPE THE FUTURE OF THE ARMY
ARMY RESEARCH OFFICE
1951

NSF