PACS-CSにおける物性物理学研究

ExaFLOPS 201x -

K 2011 -

T2K 2008 -

PACS-CS 2005 - 2007

CP-PACS 1996 -

QCDPAX 1989

Lattice QCD

SX9 2007

SX8 2004

SX6 2001

SX5 1998

(ES)

SX4 1994

SX3 1989

SX2 1983

NEC

2007 - U Tokyo

1995 – 2007 U Tsukuba

CNT, Si,,,

Days of vectorization and computations

1985 – 1995 NEC

1983 – 1984 IBM

myself

PACS-CSにおける物性物理学研究

ExaFLOPS 201x -

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Real-Space Density-Functional-Theory (RSDFT) Code for Unprecedentedly Large-Scale Calculations

CNT, Si,,,

Days of vectorization and computations

Lattice QCD

QCDPAX 1989

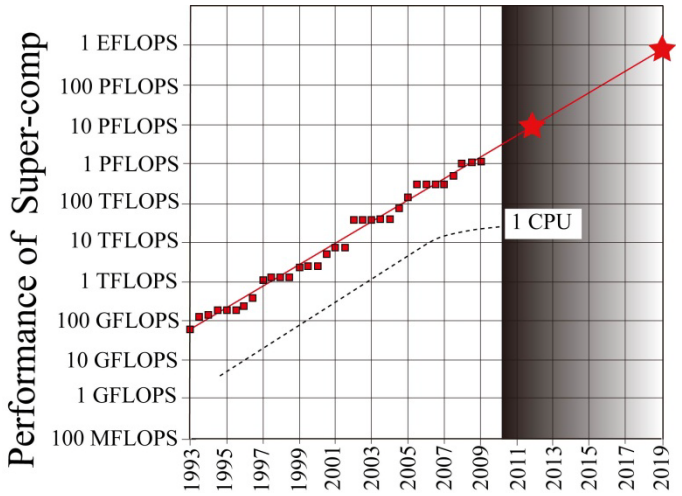
1985 – 1995 NEC

1983 – 1984 IBM

myself

Computics: Fusion of Materials Science and Computer Science

Computers that are changing rapidly



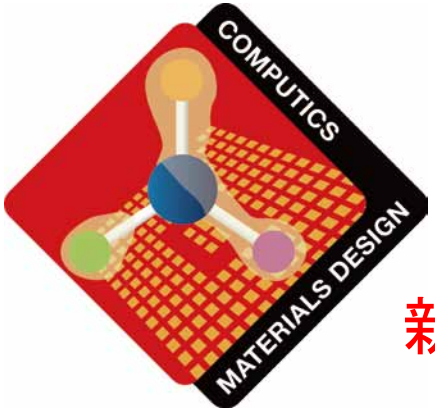
- ✓ Saturation of performance of a single computation processor
  Breakdown of Moore's Scaling Law
- ✓ Multi-core massively parallel architecture in the next generation
  Kobe-K : 80,000CPU x 8 cores
- ✓ Accelerator introduced in the next next generation
  Supercomputer that is a monster

Collaboration between Computational Materials Science and Computer Science is Imperative

- Developments of Mathematical Methodology and Algorithms Suitable to Current Hard wares
- Tuning of High Performance Computation codes based on deep knowledge of hard wares

Computics: Fusion of Materials Science and Computer Science

Computics,
A New Approach to
Materials Science in 21st Century,
in addition to *Mathematics*
that plays an important role from
Newton's Principia



新学術領域研究：http://computics-material.jp/

Development and Status of Computational Materials Science

80s ~ **Success of Computaional Science Approach**

Density Functional Theory(DFT) *(W. Kohn: Novel Prize 1998)*

Car-Parrinello Molecular Dynamics (CPMD) (1985)

Various Developments in Quality and Quantity

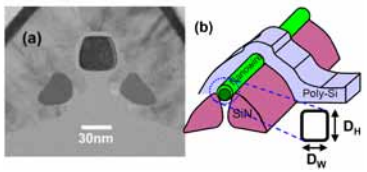
Clarification and Prediction of Material Properties and their Dynamics based on First Principles of Quantum Theory

90s ~ **Limitation of DFT** (Strongly Correlated System, Excitation Spectrum)

From Now On!

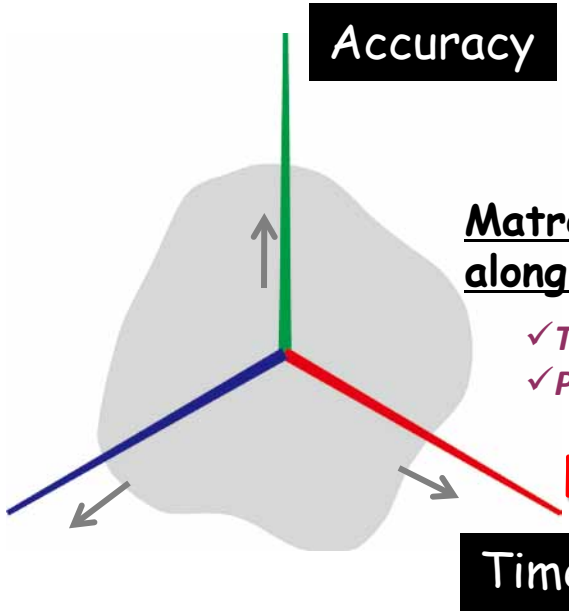
Future in nano devices

Next-Generation NWFET



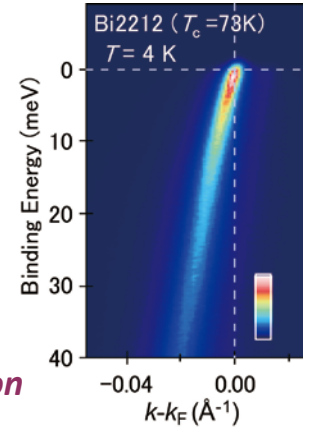
Quantum effects at room temp

Larger scale:
Nano world =
100,000-atom world



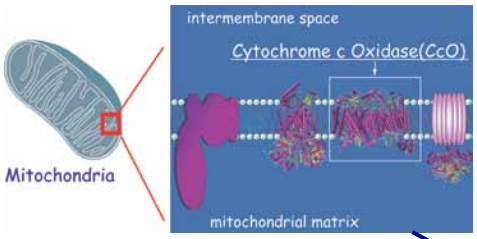
Matreials design along time axes

✓*Time-resolved ARPES*
✓*Photo-induced function*

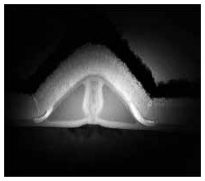


From sub-Femto sec with electrons to Nano sec with ions

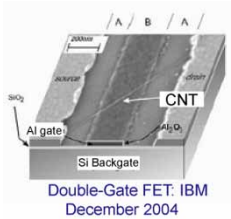
Why Large-Scale Density Functional (DFT) Calculations?



Cytochrome c Oxidase
X-ray dtermined structure
more than 10,000 atoms involved



CMOS
gate length = 5 nm
NEC 2003



FET with CNT
IBM 2004

0.1 nm 1 nm 10 nm sub μm

Theory Experiment

100 atoms

10,000 atoms

100,000 atoms

Quantum-theory-based large-scale DFT calculations and experiments meet together in Nano World !

Density Functional Theory (DFT)

Total energy of a material is a functional of electron density:

$$E[n(\mathbf{r})] = \langle \Psi | H | \Psi \rangle = \langle \Psi | T + V_{nucl} + V_{ee} | \Psi \rangle$$
$$= T_s[n(\mathbf{r})] + \int v_{nucl}(\mathbf{r}) n(\mathbf{r}) d\mathbf{r} + \frac{1}{2} \iint \frac{n(\mathbf{r}) n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r} d\mathbf{r}' + E_{XC}[n(\mathbf{r})]$$

When the electron density is written as $n(\mathbf{r}) = \sum_{i:\ \text{occupied}} |\varphi_i(\mathbf{r})|^2$

we obtain Euler equation (Kohn-Sham) equation,

$$\left[-\frac{1}{2}\nabla^2 + v_{eff}(\mathbf{r}; n(\mathbf{r})) \right] \varphi_i(\mathbf{r}) = \varepsilon_i \varphi_i(\mathbf{r}) \qquad v_{eff}(\mathbf{r}) = v_{nucl}(\mathbf{r}) + \int \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' + \frac{\delta E_{XC}[n]}{\delta n(\mathbf{r})}$$

Forces acting on nuclei ***R*** are calculated as

$$F_u = -\frac{d}{dR_u}\left(E[n] + E_{nucl-nucl}\right) = \left[\frac{\partial E}{\partial R_u}\right]_{\varphi} + \sum_i \int \left(\frac{\delta E}{\delta \varphi_i} \frac{d\varphi_i}{dR_u} + \frac{\delta E}{\delta \varphi_i^*} \frac{d\varphi_i^*}{dR_u} \right) d\mathbf{r}$$

Helmann-Feynman Force　　Pulay Correction

Solving Kohn-Sham Equation

Introducing complete basis set $\chi_n(r)$ to expand Kohn-Sham wave function:

$$\varphi_j(\vec{r}) = \sum_n c_{jn}\, \chi_n(\vec{r})$$

to convert the differential equation to a matrix equation, and then solve it by iterative techniques. Most convenient basis set has been plane wave basis set:

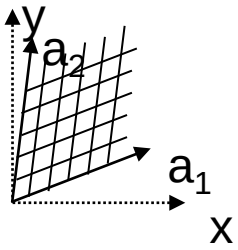
$$\chi_n(\vec{r}) = e^{\,i\,(\vec{k}+\vec{G}_n)\cdot\vec{r}}$$

In the plane-wave scheme, several quantities such as n(r), v(r) etc is Fourier-transformed and Inverse-Fourier-transformed frequently.

FFT: a heavy communication burden on parallel-architecture computers

Solving Kohn-Sham Equation Using Real-Space Finite-Difference Scheme

Introducing mesh points with spacing H in real space,

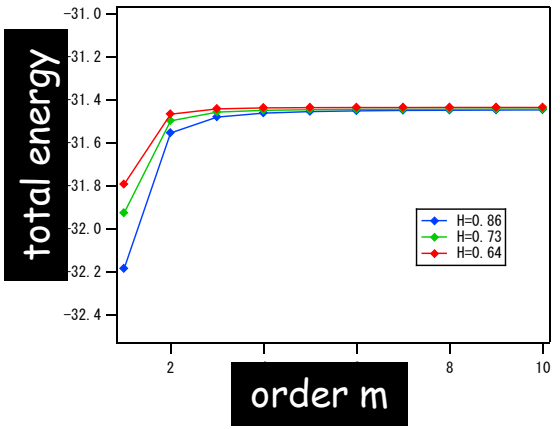


Kohn-Sham differential equation is converted to a m-th order finite-difference equation:

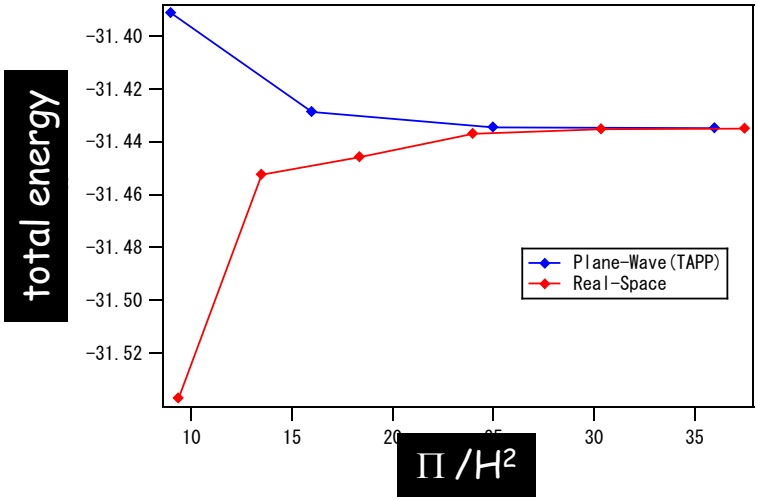
$$\frac{\partial^2}{\partial x^2}\varphi_j(x,y,z) = \sum_{m=-M}^{M} c_m \, \varphi_j(x+mH,y,z)$$

All the quantities computed at each mesh point, KS Hamiltonian expressed as a matrix.

Check of finite difference



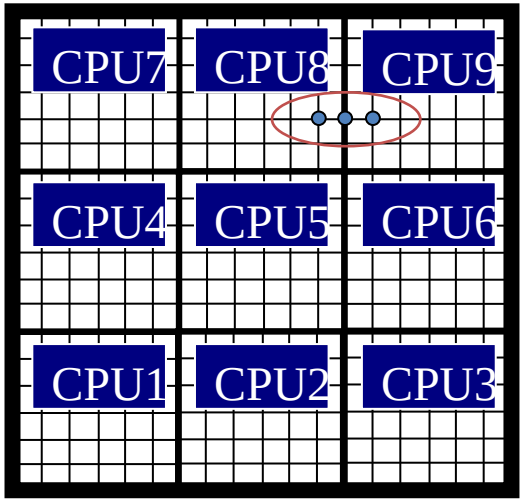
Check of mesh spacing
⇒ systematic accuracy improvement



Advantages of Real-Space DFT (RSDFT) in Parallel Computing

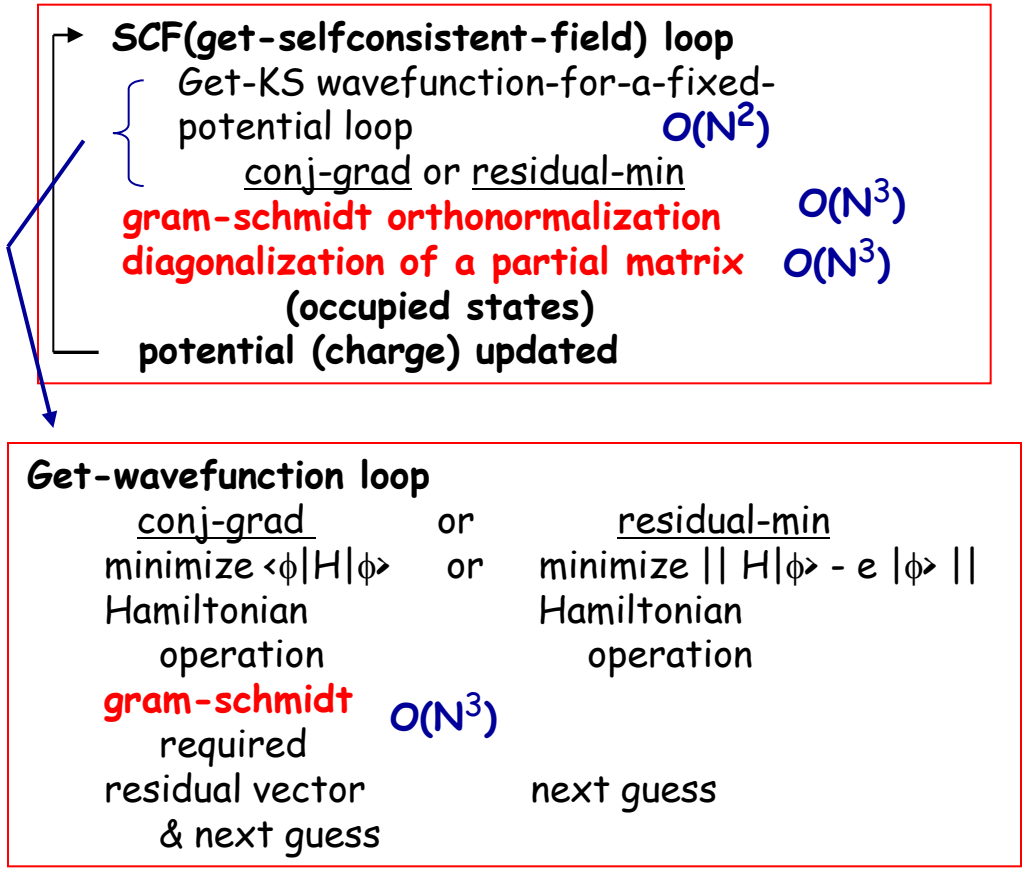
- Almost free from FFT, reducing communication burden
  ⇒ high efficiency
- Flexible boundary condition to wave-functions
  ⇒ targets expanded including charged objects
- Utilize inherent locality of the system
  ⇒ prospect to efficient O(N) scheme

On multi-core parallel machines:
- Huge number of 3D mesh points divided into moderate-size cells
- Each cell treated by a single CPU
- Also, electron states are grouped and each group is treated by a single CPU or a core : Hybrid parallelization
- MPI for CPU and OpenMP for core



Some Details and Their Optimization

- Residual minimization as well as conjugate-gradient minimization to solve KS equation
- Change of algorithm for Gram-Schmidt to utilize BLAS*-level3 matrix-matrix operations
- Divide-and-Conquer algorithm to solve secular equation in subspace



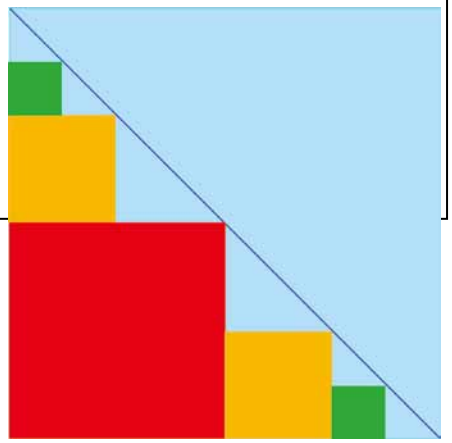
Order N^3 Calculations, but the N^3 part is highly optimized!

* BLAS = Basic Linear Algebra Subprograms

Gram-Schmidt Orthonormalization: Active use of Level 3 BLAS in O(N³) Computation

$$\psi_1' = \psi_1$$
$$\psi_2' = \psi_2 - \psi_1' \langle \psi_1' | \psi_2 \rangle$$
$$\psi_3' = \psi_3 - \psi_1' \langle \psi_1' | \psi_3 \rangle - \psi_2' \langle \psi_2' | \psi_3 \rangle$$
$$\psi_4' = \psi_4 - \psi_1' \langle \psi_1' | \psi_4 \rangle - \psi_2' \langle \psi_2' | \psi_4 \rangle - \psi_3' \langle \psi_3' | \psi_4 \rangle$$
$$\psi_5' = \psi_5 - \psi_1' \langle \psi_1' | \psi_5 \rangle - \psi_2' \langle \psi_2' | \psi_5 \rangle - \psi_3' \langle \psi_3' | \psi_5 \rangle - \psi_4' \langle \psi_4' | \psi_5 \rangle$$
$$\psi_6' = \psi_6 - \psi_1' \langle \psi_1' | \psi_6 \rangle - \psi_2' \langle \psi_2' | \psi_6 \rangle - \psi_3' \langle \psi_3' | \psi_6 \rangle - \psi_4' \langle \psi_4' | \psi_6 \rangle - \psi_5' \langle \psi_5' | \psi_6 \rangle$$

Part of the calculations can be performed as Matrix x Matrix operations!



Performance of Gram-Schmidt Routine (on 1000 CPUs of Tsukuba PACS-CS)

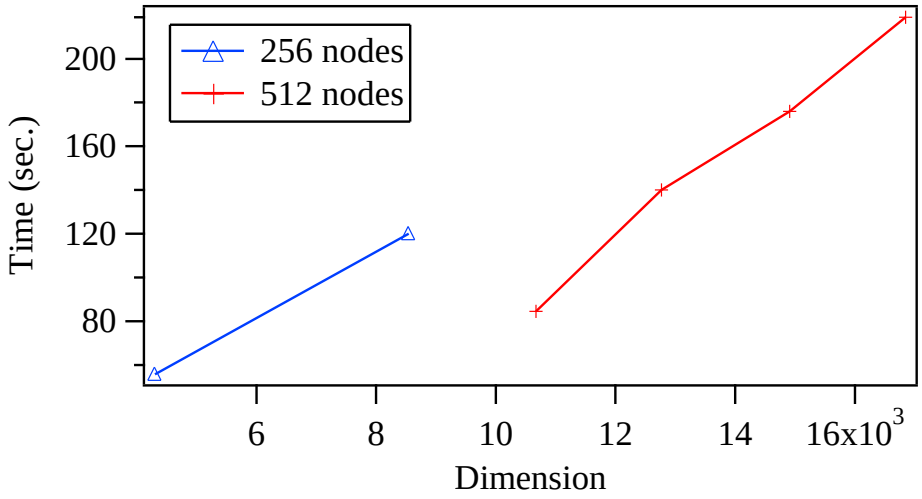
Theoretical Peak Performance	Our RSDFT (Operation)	Our RSDFT (Operation & Communication)
5.6 GFLOPS/cpu	4.3 GFLOPS/cpu	3.5 GFLOPS/cpu

O(N³) part computed at 80% of the theoretical peak performance!

* BLAS = Basic Linear Algebra Subprograms

Divide and Conquer for Subspace Diagonalization

1. Calculation of Matrix Elements
   BLAS-3
2. Diagonalization



PDSYEVD
(Solver in SCALAPACK)
using Divide & Conquer

3. Vector (Wavefunction) Rotation
   BLAS-3

Now, Imamura Algorithm
In future,
Sakurai-Sugiura Algorithm

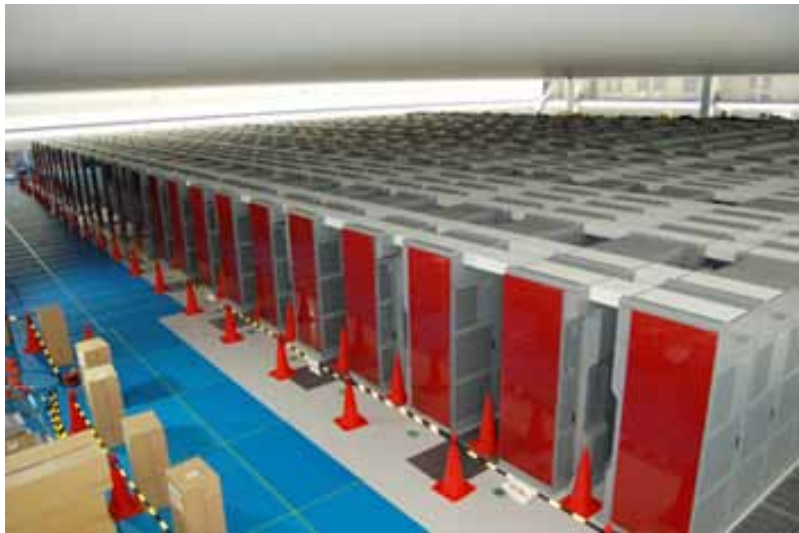
RSDFT on K(京) at Kobe

- ✓ 100,000-atom DFT calculations using hundreds of thousands cores with unprecedentedly efficient performance have been done
- ✓ 10,000-atom DFT calculations have become just an overnight task

In collaboration with,

Jun-ichi Iwata (Univ Tokyo)
Yukihiro Hasegawa (Riken)
Miwako Tsushi (Univ Tsukuba)
Daisuke Takahashi (Univ Tsukuba)
Kazuo Minami (Riken)
Taisuke Boku (Univ Tsukuba)
Shinnosuke Furuya (Univ Tokyo)
Mitsuo Yokokawa '(Riken)
,,,

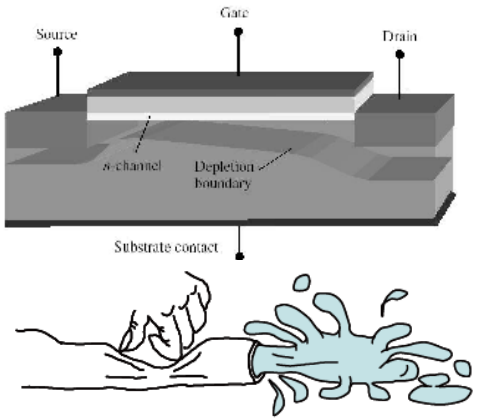
who are in the fields of materials science & computer science.

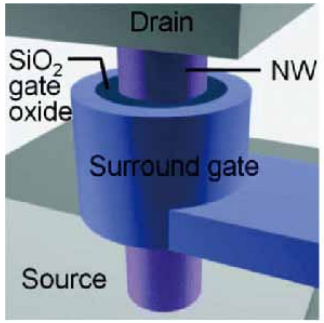


Prediction of Electron States of Si Nanowires

Si Nanowire, a Booster
in the next-generation seiconductor technology
More Moore → More than Moore

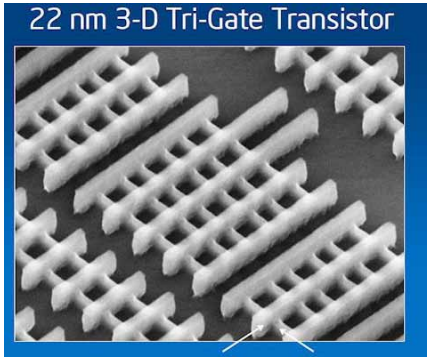
planar transistor





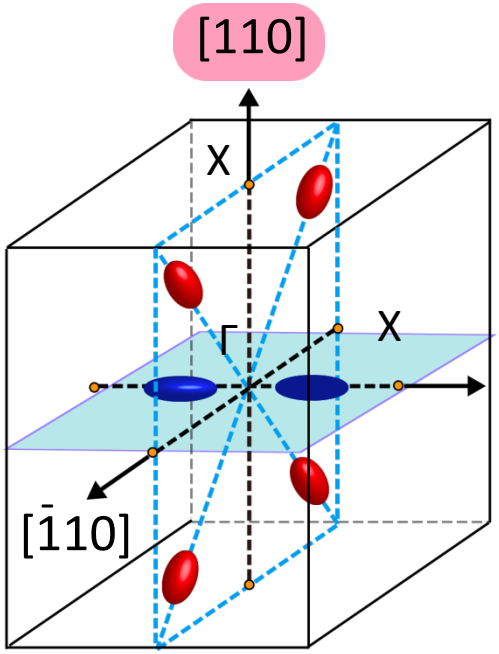
Surrounding gate transistor

Gate Controllability
→ Suppress short-channel effects
Suppress leaks at off state
→ save energy



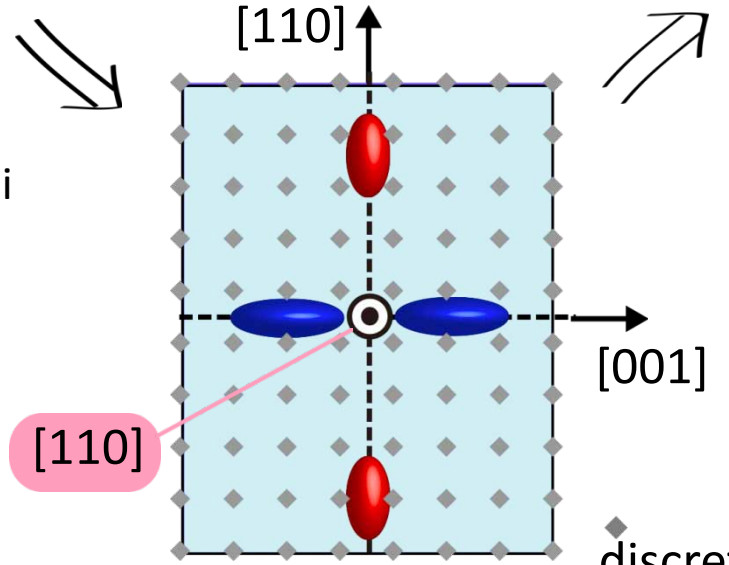
Actually tri-gate by Intel in 2011

Effects of quantum confinement of [110]-SiNWs



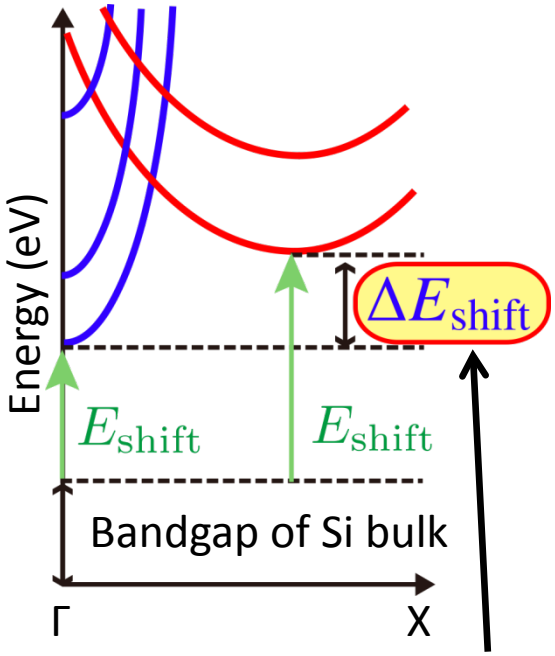
Brillouin Zone (BZ) of bulk Si
and
six conduction band valleys

Quantum confinement effects



discrete k

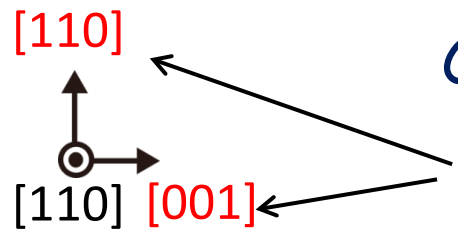
Conduction band structure
of [110]-SiNW



This quantity is
decisive in
the number of the
conduction channels.

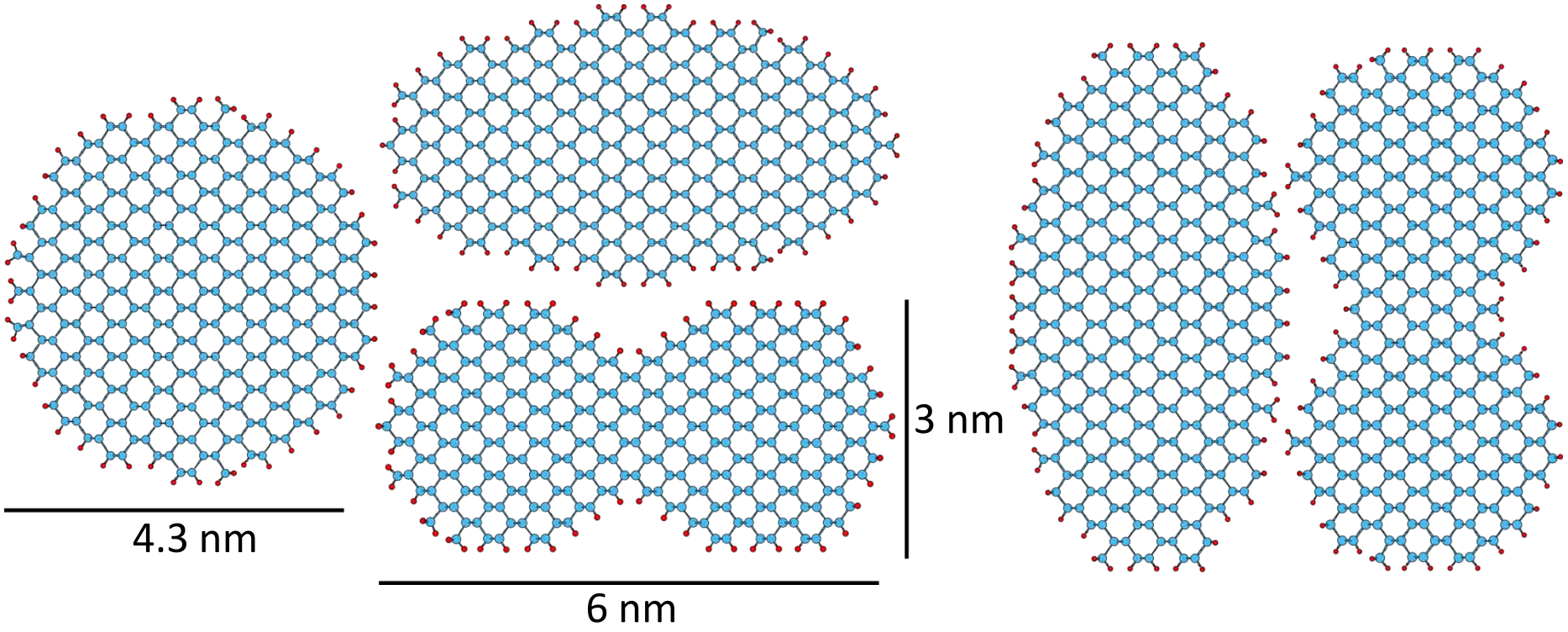
Positions of allowed wave numbers
depend on cross-sectional morphology

Cross Sectional Shapes, Diametes, Directions,,, What is the best Choice?



Considering Si (110) Nano Wire,

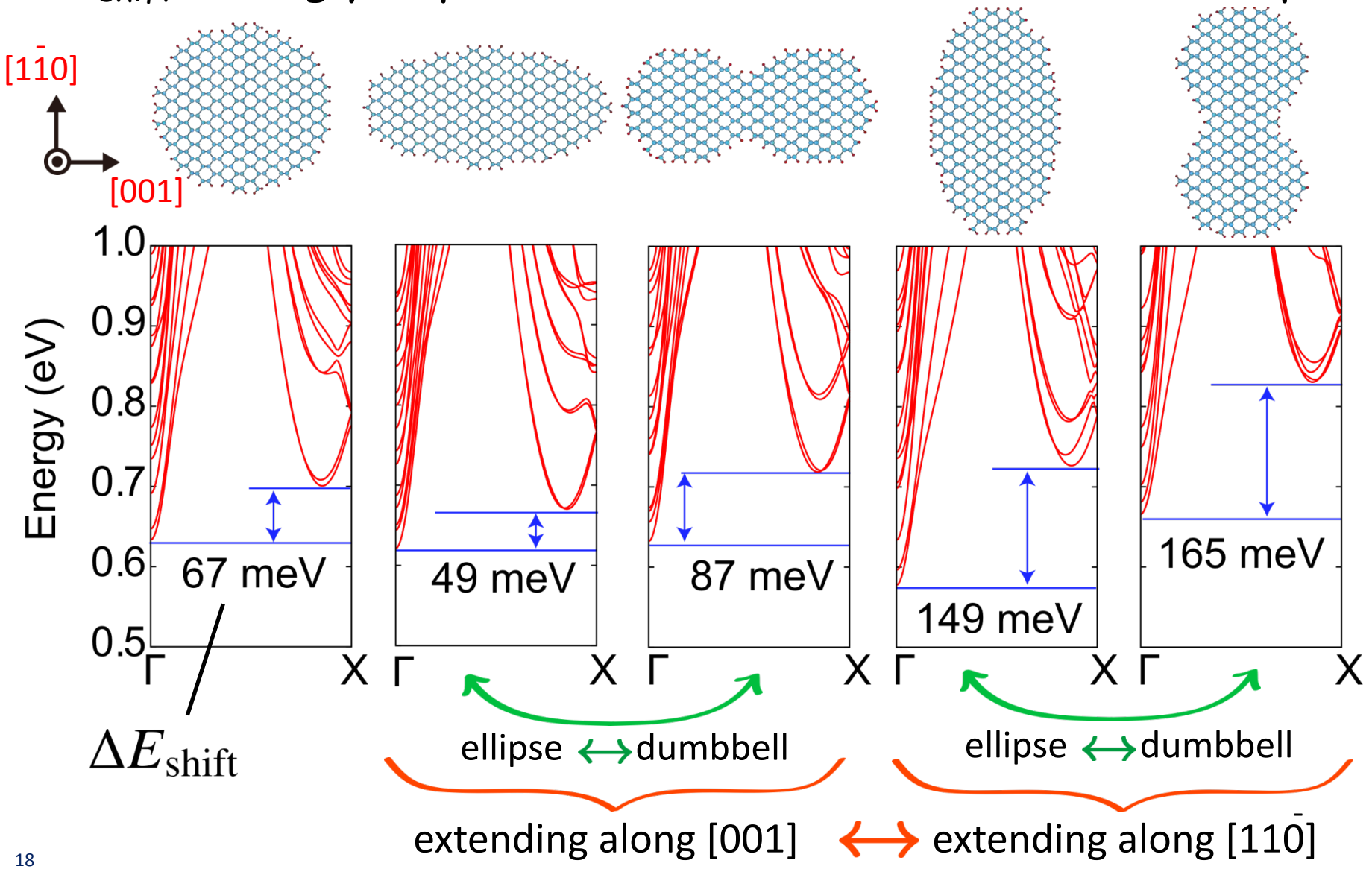
Directions inequivalent to each other



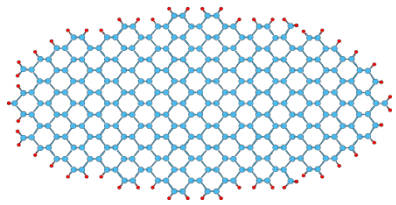
DFT could Give the Answer

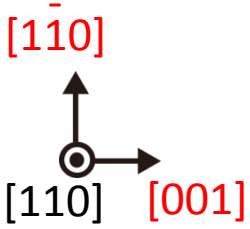
Conduction Band Structures of Various Si(110) NWs

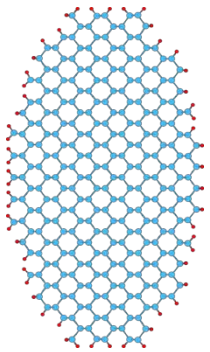
ΔE_{shift} strongly depends on the cross-sectional nano-shapes

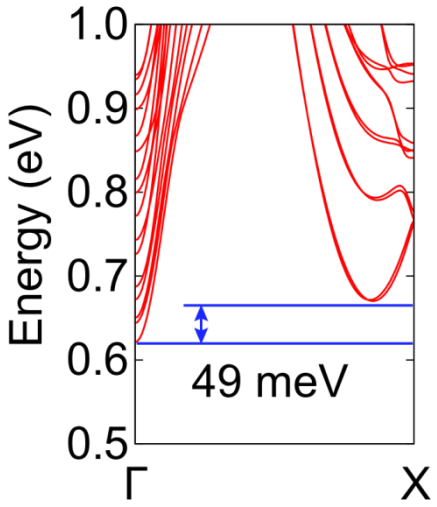


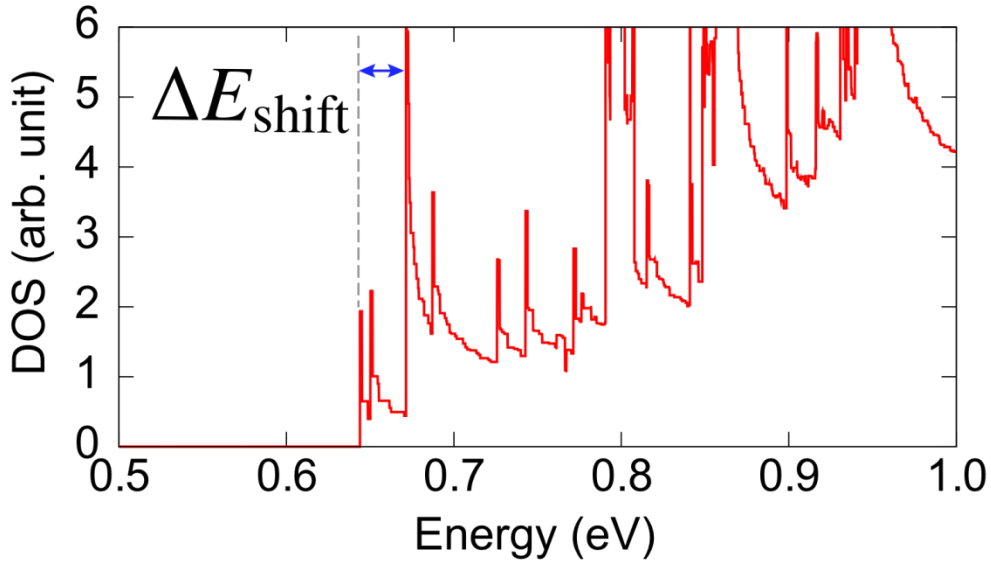
Density of states of SiNWs

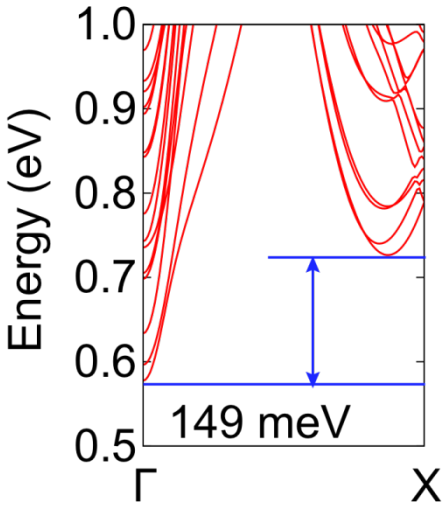


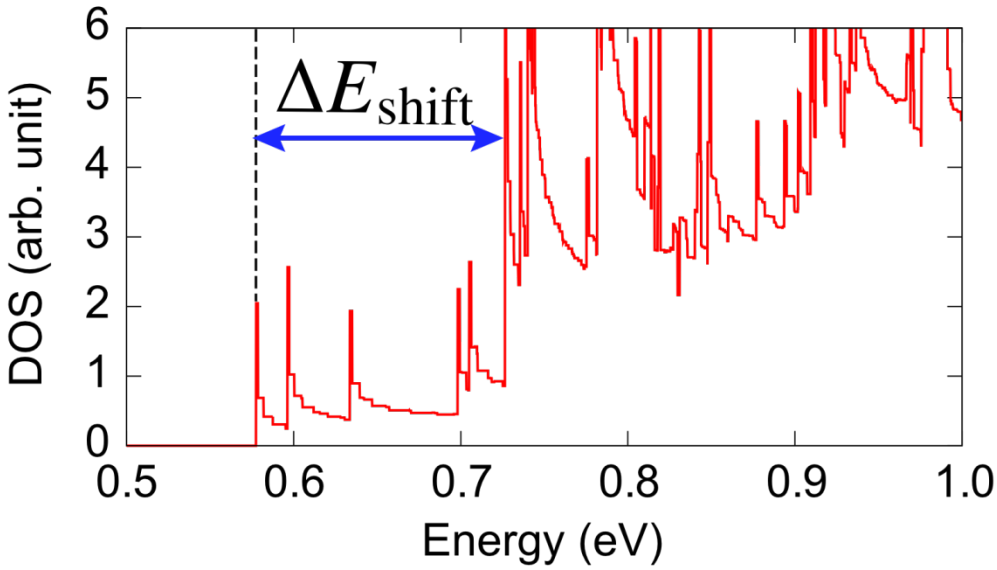








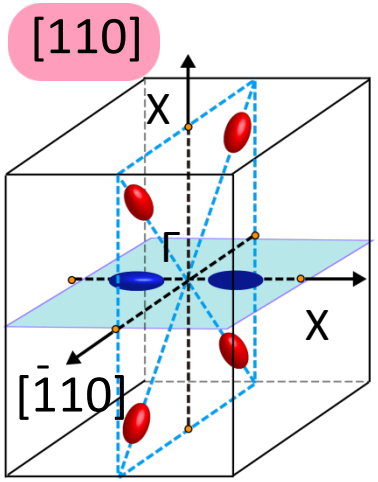


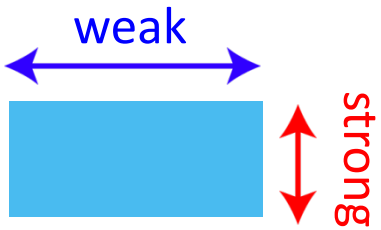


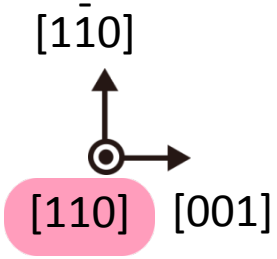
The number of channels near the CBM is strongly related to ΔE_{shift}

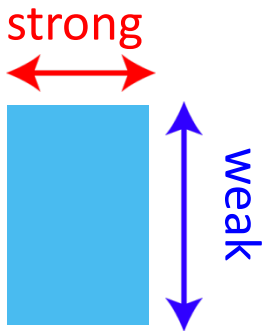
Interpretation of calculated results

discrete k
CBM
Second minimum

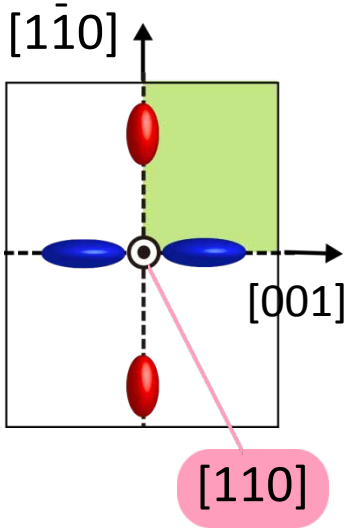


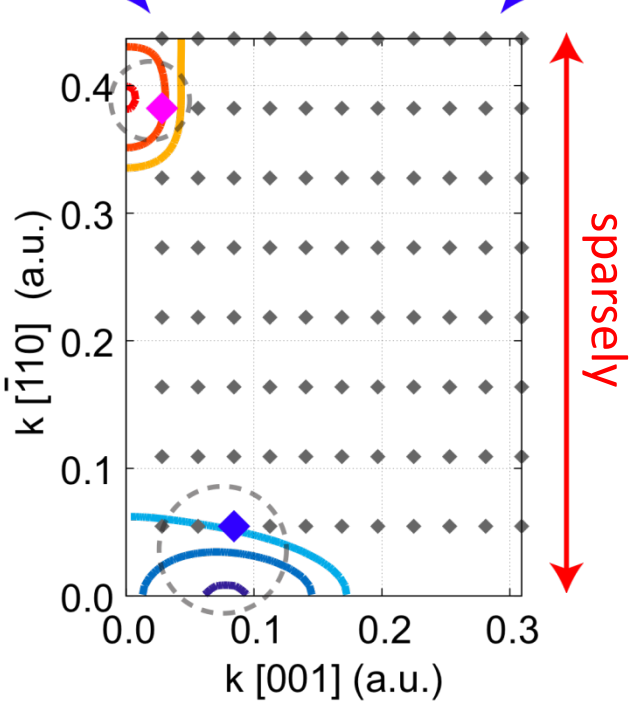






densely



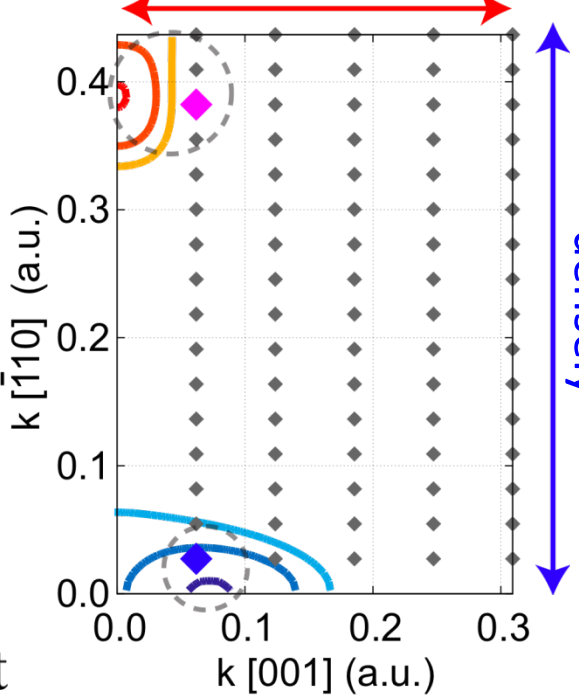


CBM

Second minimum

ΔE_{shift}

sparsely



Correspond to the results from our first-principle calculations

SiNWs with sidewall roughness

Roughness makes the radius of NWs vary along circumference and wire axis.

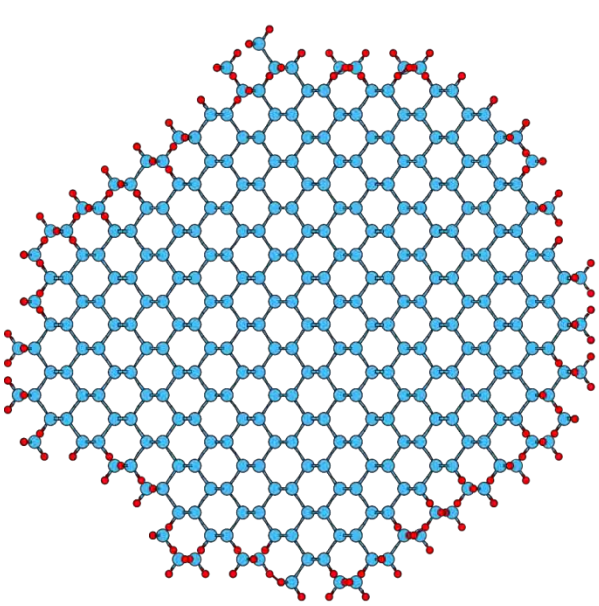
⇨ Lorentzian autocorrelation function

$$< \delta R(\boldsymbol{r}')\delta R(\boldsymbol{r}' - \boldsymbol{r}) >= \Delta^2 e^{-\frac{r}{L_r}}$$ ← correlation length : $L_r = 0.54\,nm$

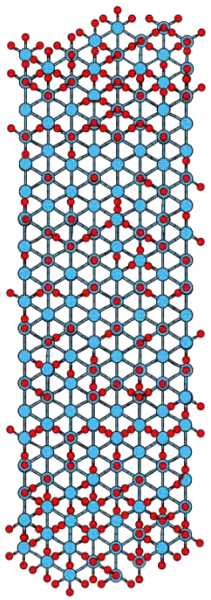
$$(\delta R(\boldsymbol{r}) = R(\boldsymbol{r}) - R_0,\ R_0 = 2.2nm)$$

This model is obtained by experimental data of Si(100)-SiO interface.

$\Delta = 0.2\ nm$

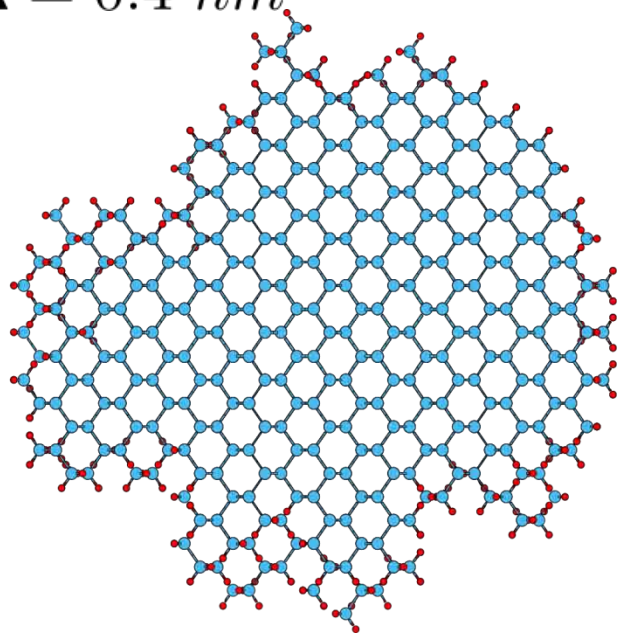


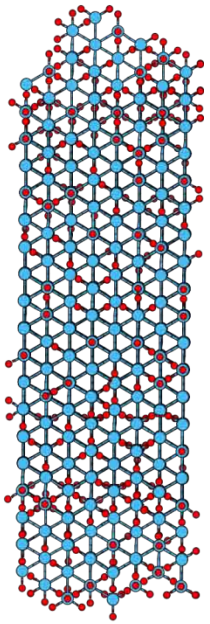
cross-sectional view



side view

$\Delta = 0.4\ nm$



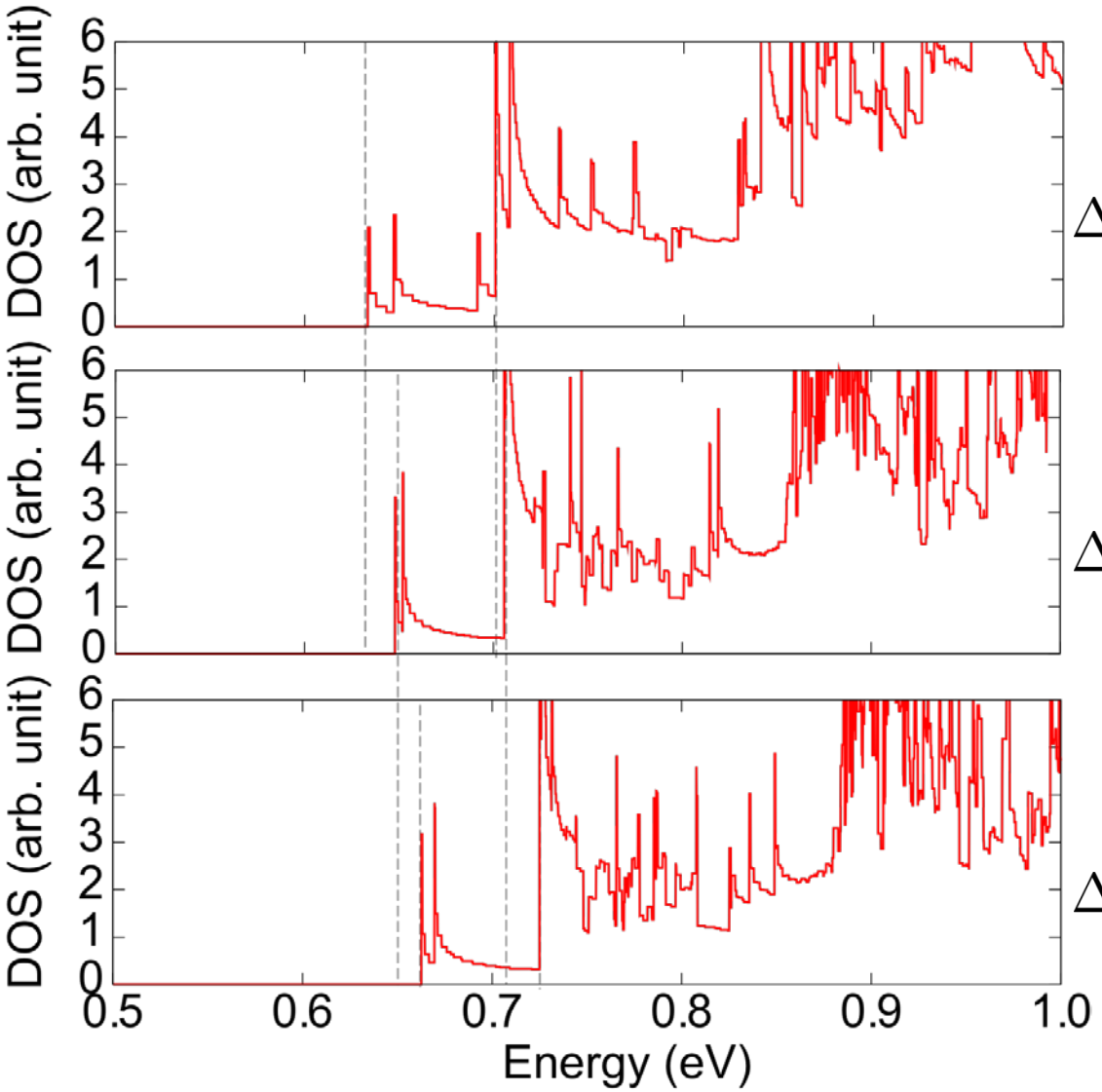


Effects of DOS on surface roughness

without roughness

Δ = 0.2 nm

Δ = 0.4 nm



$E_g = 0.63$ eV
$\Delta E_{\mathrm{shift}} = 67$ meV

$E_g = 0.65$ eV
$\Delta E_{\mathrm{shift}} = 58$ meV

$E_g = 0.66$ eV
$\Delta E_{\mathrm{shift}} = 62$ meV

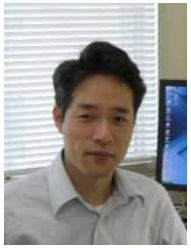
Effects of roughness are minor when Δ is smaller than 0.4 nm

PACS-CSにおける物性物理学研究

ーRSDFTを中心にー

- 物質科学と計算機科学の共同での、RSDFTコードの開発：超並列マルチコア・アーキテクチャ上でのHigh Performance
- 10,000 – 100,000原子系の電子状態、構造決定が可能に





新学術領域研究：http://computics-material.jp/