Physical Properties of Nanostructures: Theory and Simulations

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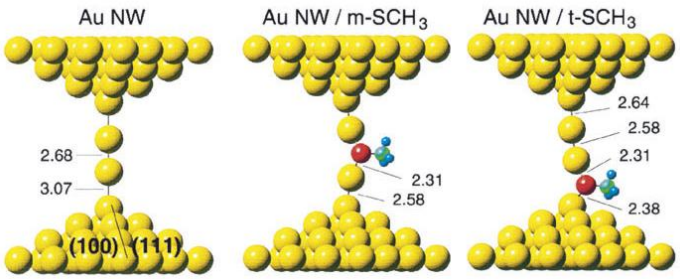
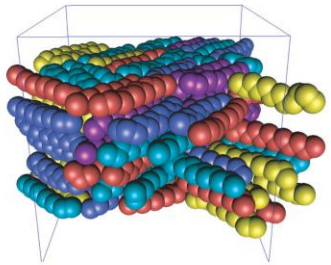
Outline

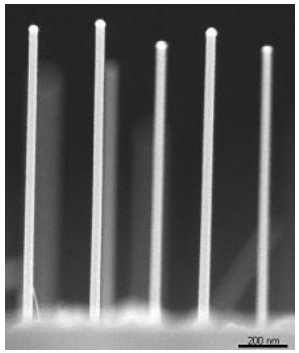
- Introduction on nanoscience
- Ab initio simulations: Density Functional Theory (DFT)
- Quantum confinement in Si nanowires (Si NWs)
  - Electronic structure
  - Transport properties
  - Doping effects
- Physical properties of SiGe nanowires (SiGe NWs)
  - Reduced quantum confinement effect
  - A good thermoelectric material
  - Efficient p- and n-type doping
- Conclusions

I. Introduction on nanoscience

Nanoscience



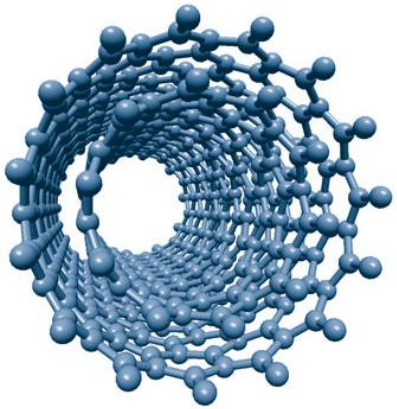


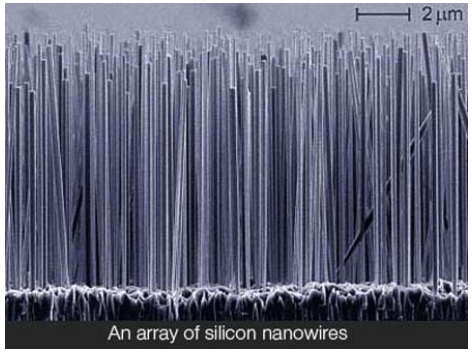


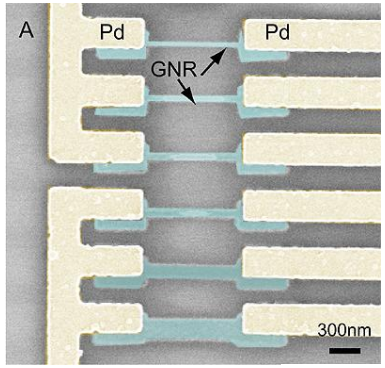
The study of structures, dynamics, and properties of systems in which one or more of the spatial dimensions is nanoscopic (1-100 nm)

Dynamics and properties that are distinctly different (often in an extraordinary way) from both small-molecule systems and systems macroscopic in all dimensions

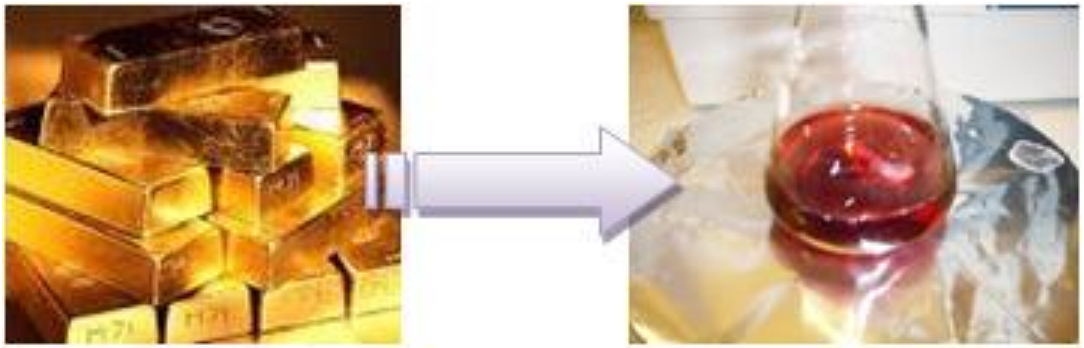
U.S. National Nanotechnology Initiative, nano.gov







The importance of the size



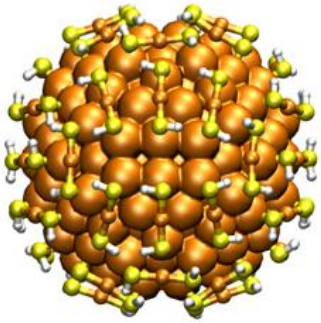
Dependence of color on gold size

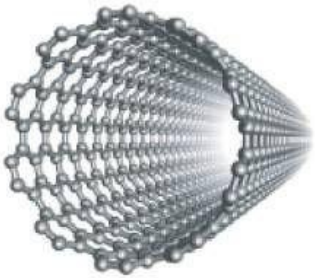
As the size of the material is reduced, and the nanoscale regime is reached, it is possible that the same material will display totally different properties

Nano building blocks

What are the nano building blocks that would play an analogous role to macro building blocks ?

Clusters and molecular nanostructures

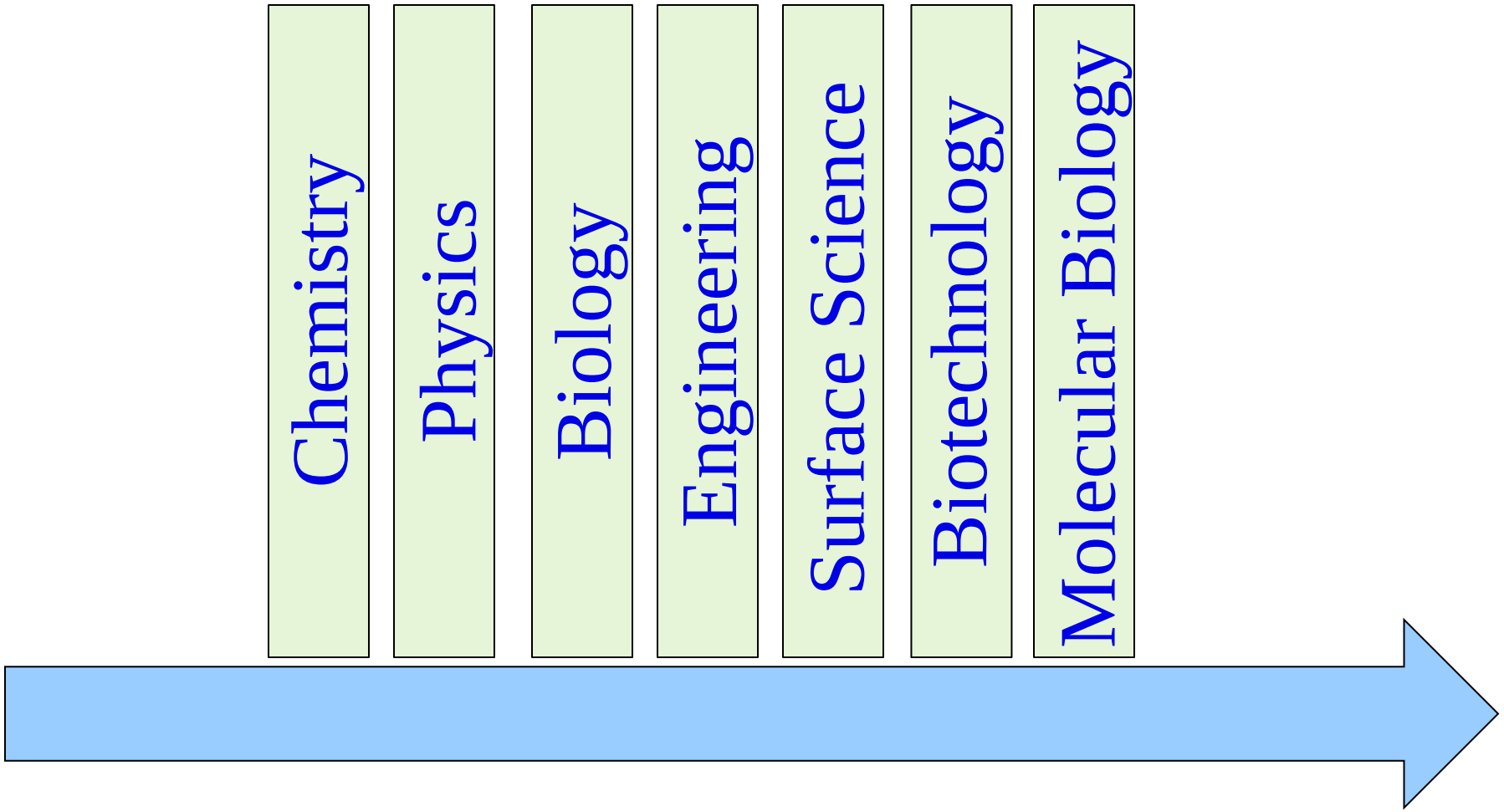




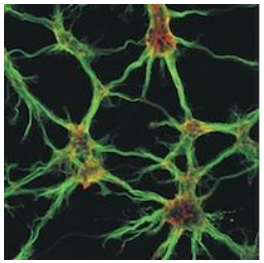
Nanotubes and related systems

Quantum wells, wires, films and dots

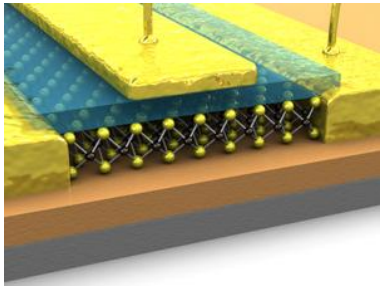
From nanoscience to ...



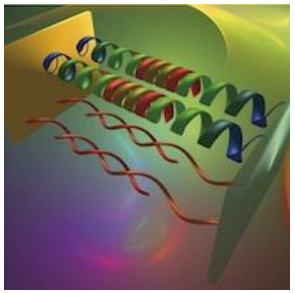
... nanotechnology



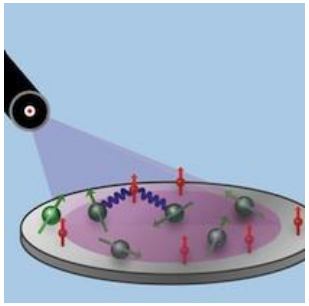
Biomedicine



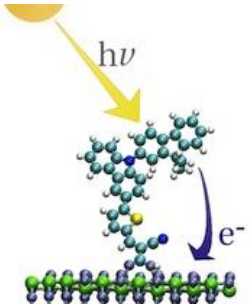
Nanoelectronics



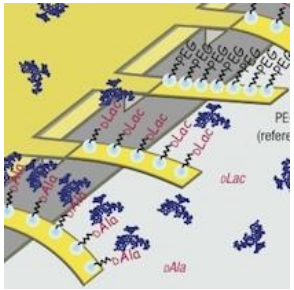
Biomaterials



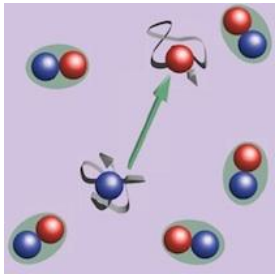
Quantum information



Optoelectronics



Sensors



Spintronics

The future of nanoscience

• The application of new extraordinary experimental tools has created an urgent **need for a quantitative understanding** of matter at nanoscale

• The **absence of quantitative models** that describe newly observed phenomena increasingly limits progress in the field

• The absence of such tools would also **seriously inhibit wide-spread applications** ranging from molecular electronics to biomolecular materials

The case of thermal conductivity

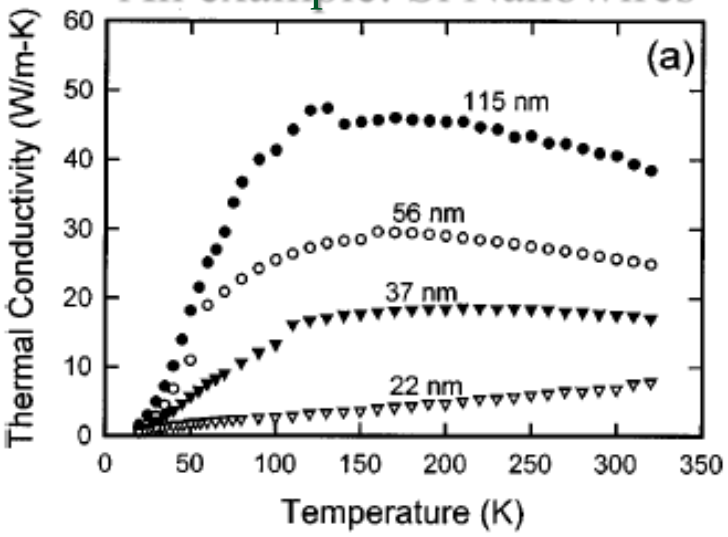
$$J = -k\nabla T$$

Is the Fourier's law applicable to nanostructures?

How size effects can affect thermal conductivity?

Can present theories interpret satisfactorily experiments?

An example: Si Nanowires



Li et al. Appl. Phys. Lett. 83, 2934 (2003)

Measured thermal conductivity lower than bulk and diameter dependent

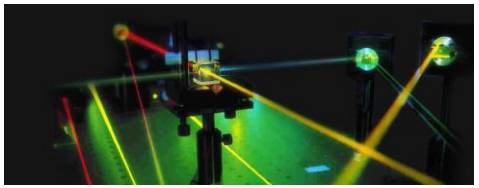
Quantum effects not negligible

Breakdown of Fourier's law

Where do we need a theoretical effort?

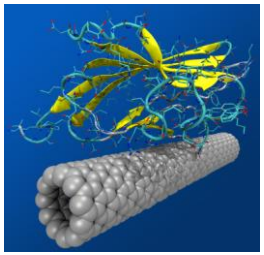
Transport in nanostructures

Electronic and optical properties



Coherence and decoherence tunneling

Soft/hard matter interfaces



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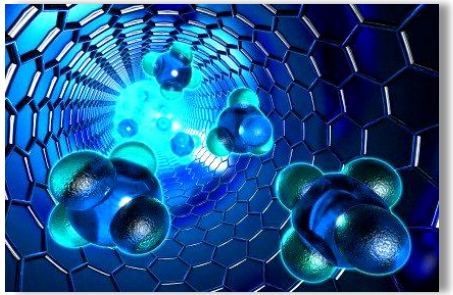
II. Ab initio simulations: Density Functional Theory (DFT)

Ab initio calculations

- Fundamental laws of physics (quantum mechanics)
- Set of “accepted” approximations to solve the corresponding equations on a computer
- No empirical input (the only input is the atomic number)
- Very accurate for most materials (errors typically less than few %)

What do we want to calculate?

Atomistic computational modelling of materials



Ab-initio quantum mechanical theory and codes

Atomically understand and design new properties of materials

ELECTRONIC STRUCTURE

Electron Density, Dipole moments, Band structure, Wave Function, Density of States, …

M.Amato et al. Nano Lett. 594, 11 (2011)

TRANSPORT PROPERTIES

Transmission, Conductance, Scattering rates

M. Amato et al. Nano Lett. 2717, 12 (2012)

OPTICAL PROPERTIES

Optical absorption, Exciton localization, Band gap, EELS

S. M. Falke et al. Science 1001, 344 (2014)

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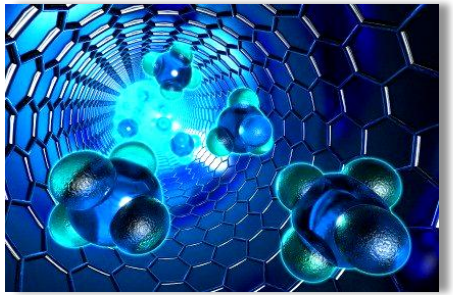

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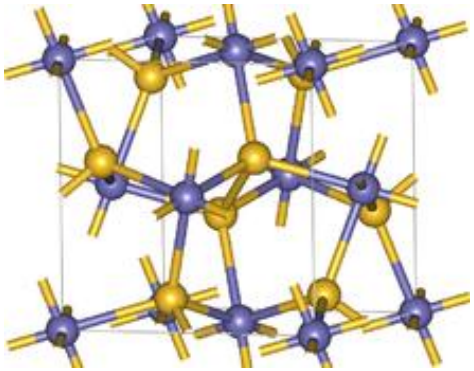
The many body electronic structure problem



N_e electrons
N_n nuclei

Schrödinger equation for interacting particles

$$\hat{H}\Psi(\{R\},\{r\}) = E\Psi(\{R\},\{r\})$$

$$\hat{H} = \hat{T}_n(\{R\}) + \hat{V}_{nn}(\{R\}) + \hat{T}_e(\{r\}) + \\ + \hat{V}_{ee}(\{r\}) + \hat{U}_{en}(\{R\},\{r\})$$

Many body hamiltonian in more detail

$$\widehat{T}_n = \sum_{I=1}^{N_n} -\frac{\nabla_I^2}{2M_I}$$

Kinetic energy of nuclei

$$\widehat{T}_e = \sum_{i=1}^{N_e} -\frac{\nabla_i^2}{2m_e}$$

Kinetic energy of electrons

$$\widehat{V}_{nn} = \frac{1}{2} \sum_{I,J,I\neq J}^{N_n} \frac{Z_I Z_J}{|R_I - R_J|}$$

Ion-ion interactions

$$\widehat{V}_{ee} = \frac{1}{2} \sum_{i,j,i\neq j}^{N_e} \frac{1}{|r_i - r_j|}$$

Electron-electron interactions

$$\widehat{U}_{en} = -\sum_{j,J}^{N_e,N_n} \frac{Z_J}{|R_J - r_j|}$$

Electron-ion interactions

Exactly solvable for two particles (analytically) and very few particles (numerically)

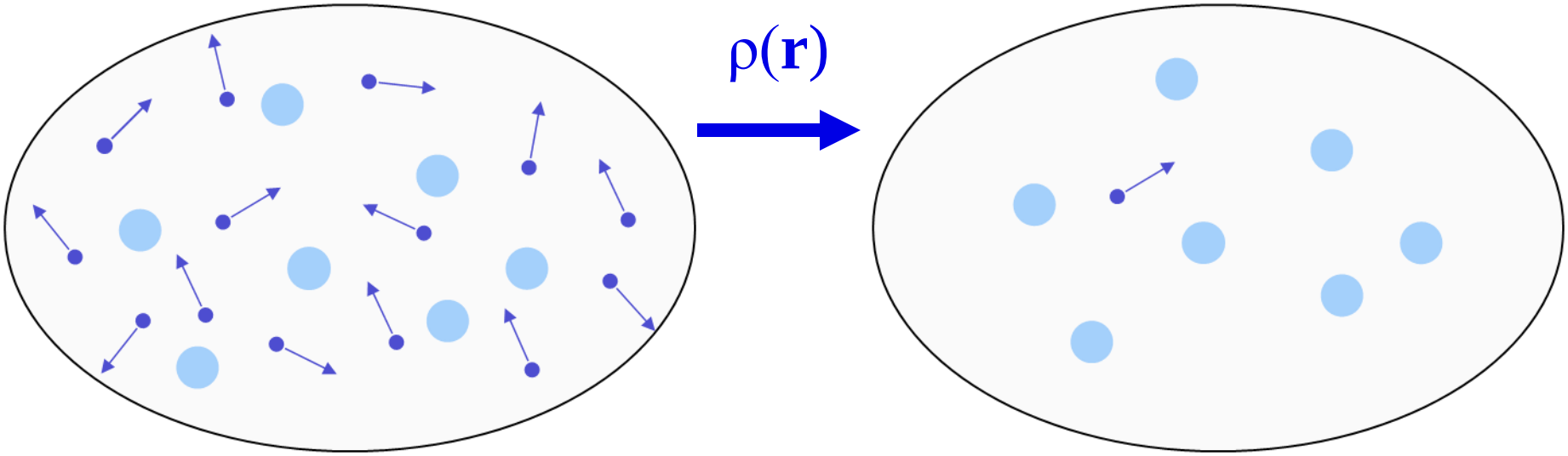
How to deal with N ~ 10^{23} particles?

Density Functional Theory (DFT)

W. Kohn
Nobel Prize in Chemistry in 1998

It can map, exactly, the **interacting** problem to a **non-interacting** one

Hohenberg and Kohn, Phys. Rev. B 136, 864 (1964)



interacting particles in a real external potential

a set of non-interacting electrons (with the same density as the interacting system) in some effective potential

Some comments

• In principle it is exact and pure predictive, but in practice it needs some approximations (exchange-correlation functional)

• Good scaling of computational cost with system size

• Calculations on large and complex systems (surfaces, interfaces, nanostructures, defects)

• Accuracy of properties prediction is well known (i.e. 3% for bond length, 10% for bulk modulus and phonon frequencies)

• Good compromise between accuracy and computational time

Computational details

Density Functional Theory - DFT

- Kohn and Sham Equations: Self Consistent Solutions
- Exchange-Correlation Functional: LDA
- Total Energy Minimization: Ions and Electrons

PWSCF S. Baroni *et al*. http://www.pwscf.org

- Periodic Supercell
- Vacuum space ~ 10 Å
- Number of k-points: 16x1x1 Monkhorst-Pack mesh
- Bulk lattice parameter: a_{Si}=5.40 Å; a_{Ge}=5.59 Å; a_{SiGe}=5.49 Å (Vegard's law)
- Pseudo-potentials: norm-conserving
- Ecut-off: 30 Ry

SIESTA J. M. Soler *et al*. http://www.icmab.es/siesta/

- Linear Combination of Atomic Orbitals (LCAO)
- Periodic Supercell
- Vacuum space ~ 10 Å
- Number of k-points: 16x1x1 Monkhorst-Pack mesh
- Pseudo-potentials: norm-conserving
- Basis set: double-ς plus polarization functions
- Supercells made of 6 primitive cells to avoid interactions between the periodic image of the impurity

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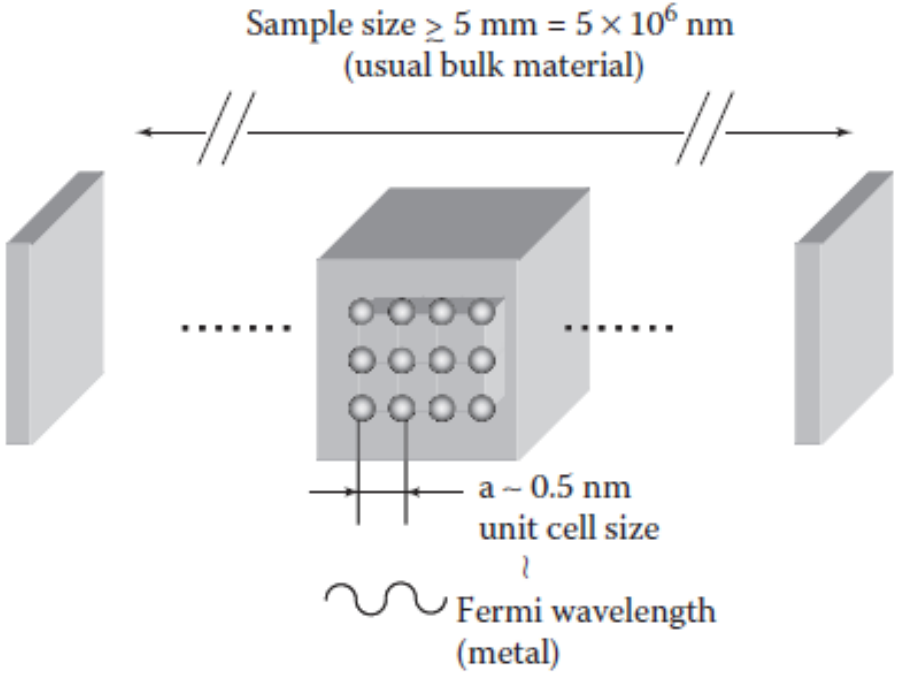
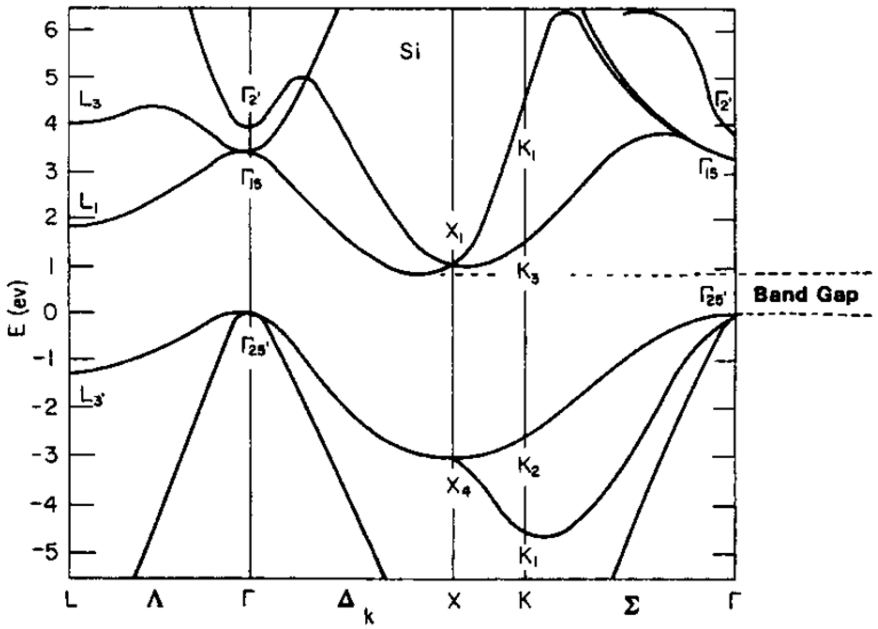
III. *Quantum confinement in Si nanowires*

Space for electrons in materials



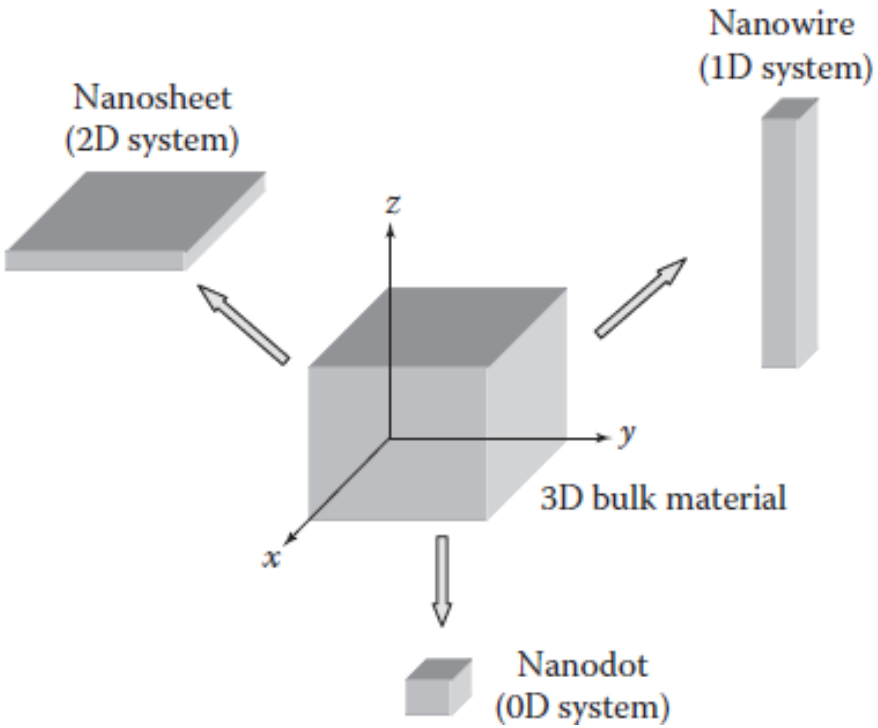


Si band structure

T. Tsurumi et al. *Nanoscale physics for materials science*, Taylor and Francis (2010)

- In macroscopic materials the Fermi wave length is of the same order as the unit cells
- Thus the inner space is too large for electrons to feel boundaries
- The possible energy levels for electrons $\varepsilon(k)=(\hbar^2/2m^*)k^2$ are dense with very small energy spacing

Quantum confinement effect (QCE)



T. Tsurumi et al. *Nanoscale physics for materials science*, Taylor and Francis (2010)

Quantum confinement effect (QCE) is defined as: a reduction in the degrees of freedom of the carrier particles, implying a reduction in the allowed phase space

E.G. Barbagiovanni et al. Appl. Phys. Rev. 1, 011302 (2014)

Consequences of QCE

- Electrons traveling along the direction that has been reduced in size reach the boundaries and are confined

- This confinement causes the quantization of the electron wavelength and of the energy spectrum

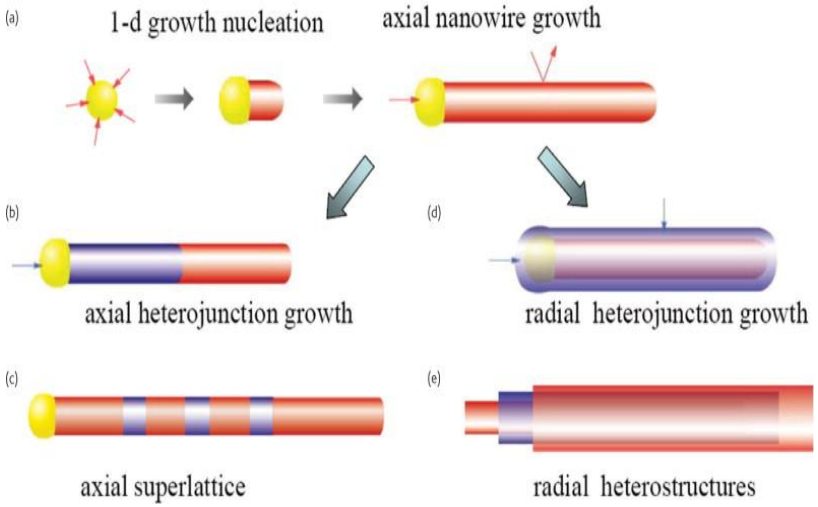
- The contribution of edge-localized surface states can become relevant

- Size effects dominate the physics of nanostructures

The case of silicon nanowires (Si NWs)

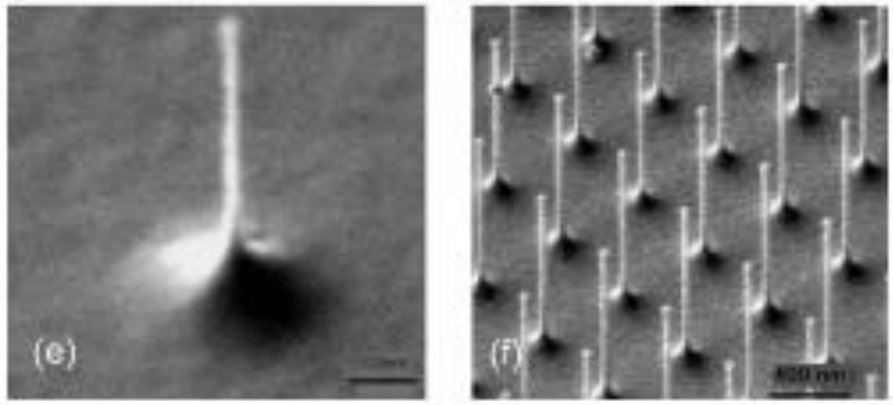
One-dimensional nanostructures with precise composition, morphology, interfaces and electrical properties (d=2-3 nm)

Vapor-Liquid-Solid (VLS) growth



O. Hayden et al., Nanotoday 3 5-6 (2008)

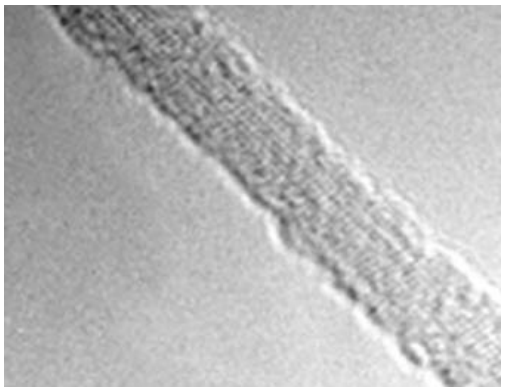
Lithography and etching processes



N. Singh et al., IEEE Trans. Electron Devices 55, 11 (2008)

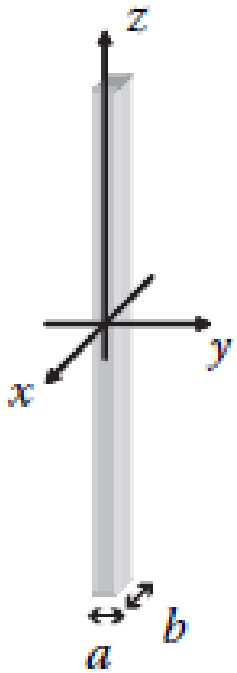
QCE in Si NWs: Electronic Structure

Real system



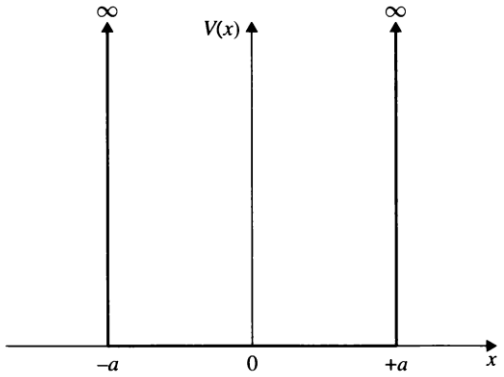
Wu et al., Nano Lett. 4, 433 (2004)

Geometrical model



T. Tsurumi et al., Taylor and Francis (2010)

Infinite potential well (particle-in-a-box model)



B.H. Brandsen and Joachin, *Quantum Mechanics* (2000)

QCE in Si NWs: Electronic Structure

The motion of electrons is restricted to be in the direction of confinement

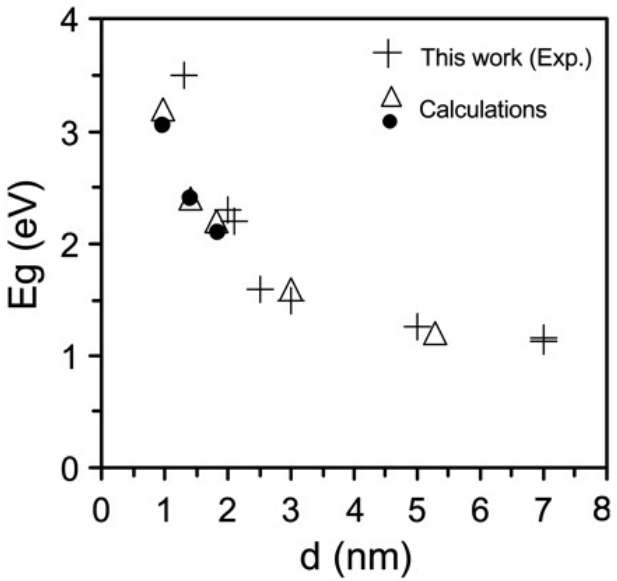
Their kinetic energy increases and the eigenstates energies are given by:

$$E_n = \frac{\hbar^2 n^2 \pi^2}{2m^* d^2}$$

m*=effective mass
d=width of the well

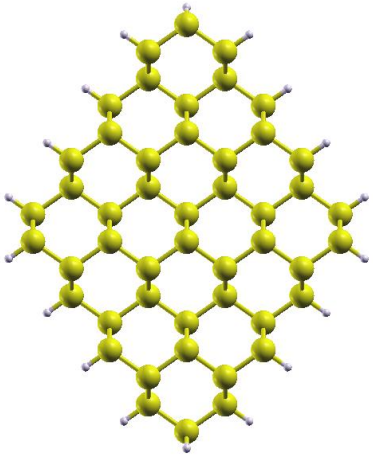
Not only the energy levels but even the spacing between them increase when the diameter is reduced (QCE increases)

QCE has a dramatic effect on semiconductor NWs (like Si NWs) because it affects the **energy band gap**

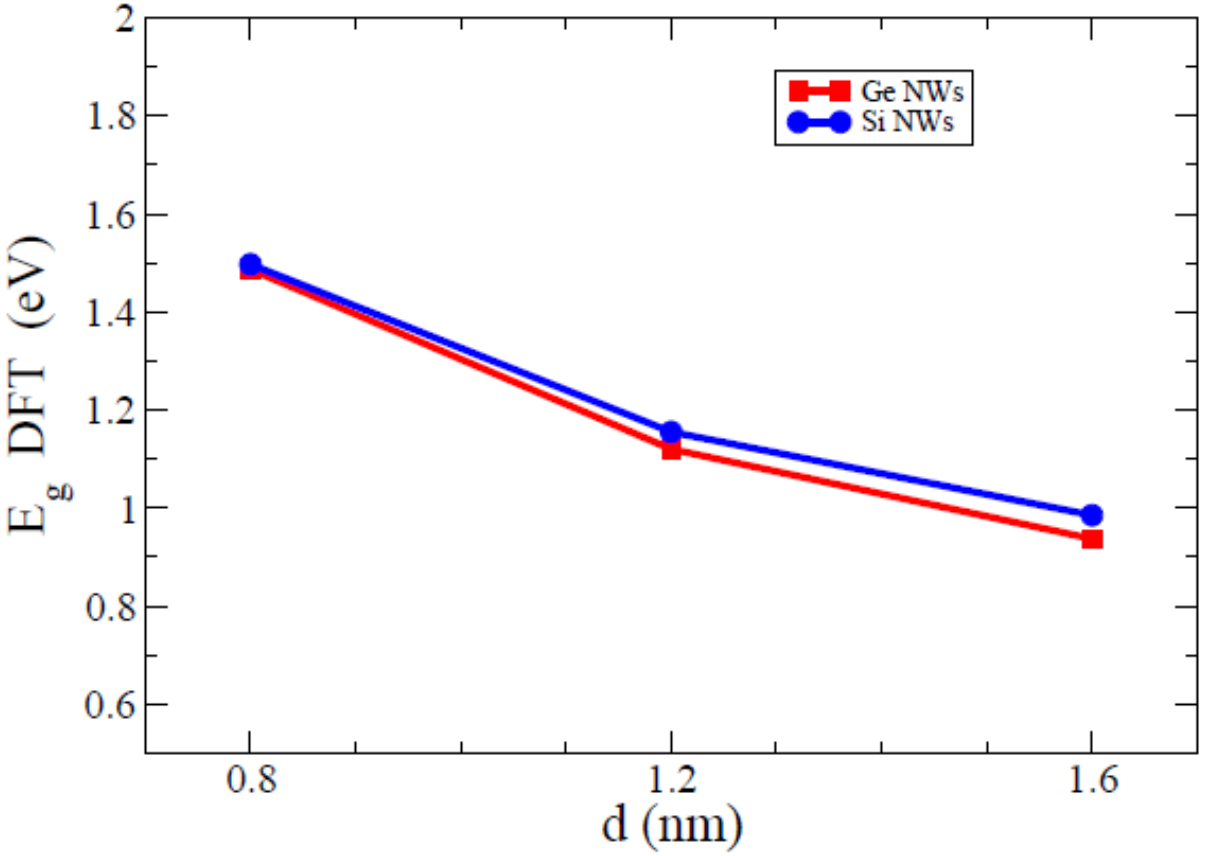


D.D.D. Ma et al., Science 299, 1874 (2003)

QCE in Si NWs: DFT scaling of the gap



Si NWs cross-section



M. Amato et al., Phys. Rev. B 79, 201302(R) (2009)

$$E_{gap} = E_{gap}^{bulk} + C(1/d)^{\alpha}$$

M. Bruno et al., Phys. Rev. B 72 (2005)
S. Beckman et al., Phys. Rev. B 74 (2006)

with α=0.9 - 1.1

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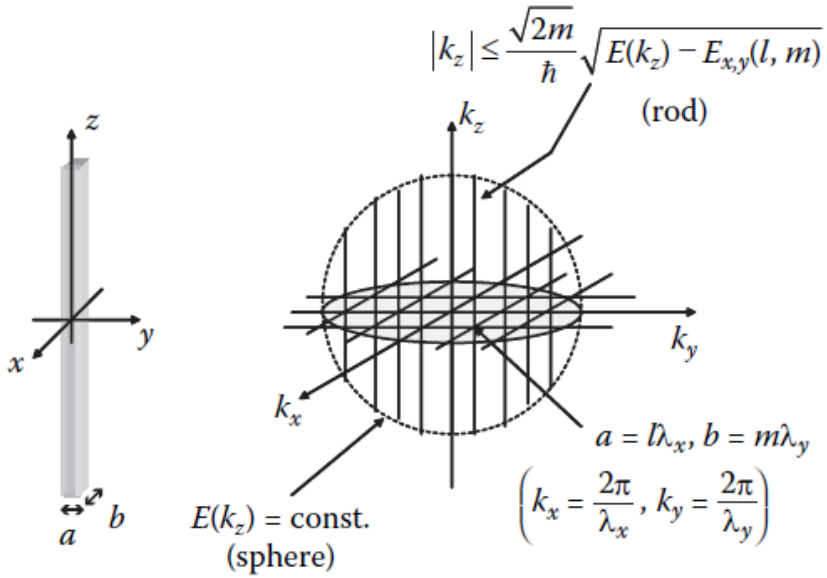
QCE in NWs: energy quantization

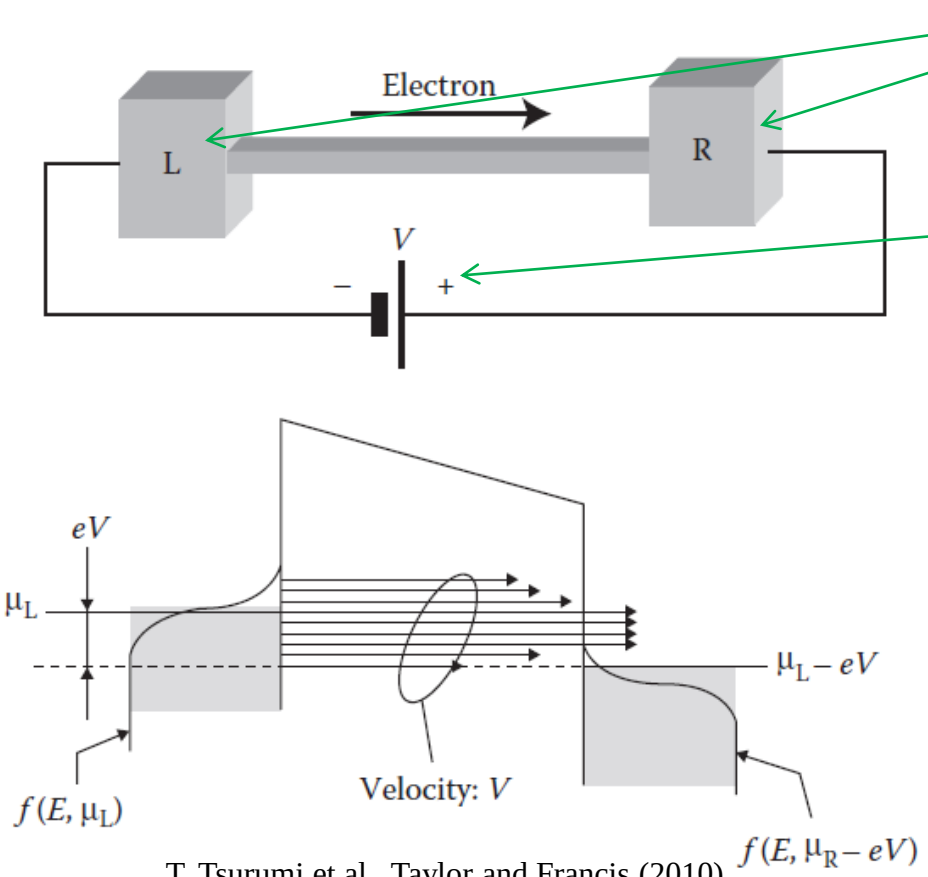


T. Tsurumi et al., Taylor and Francis (2010)

The total energy of electrons is given by the formula:

$$E\left(k_z\right) = \underbrace{\frac{\hbar^2}{2m^*}k_z^2}_{\text{Kinetic energy}} + \underbrace{E_{x,y}(l,m)}_{\text{Quantized energy in the plane}}$$

QCE in NWs: Landauer approach

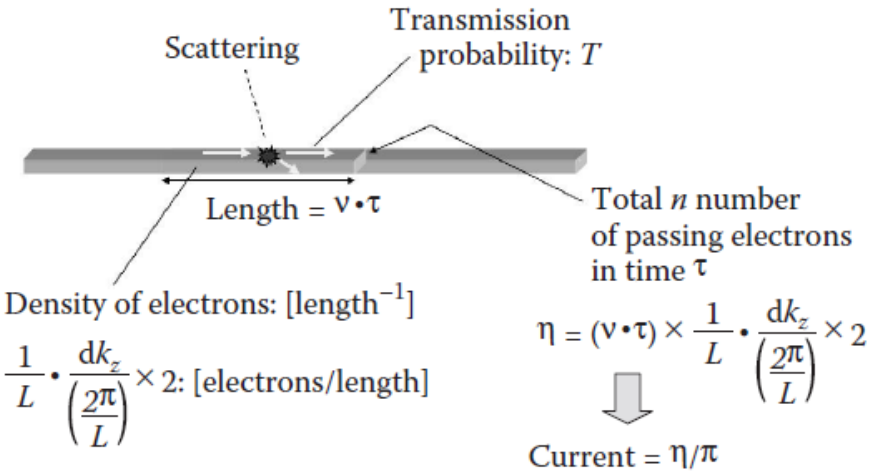


T. Tsurumi et al., Taylor and Francis (2010)

Electrons move with a group velocity v(k) and transmission probability T(k)

Can we calculate the current between electrodes?

QCE in NWs: quantized conductance



T. Tsurumi et al., Taylor and Francis (2010)

Current

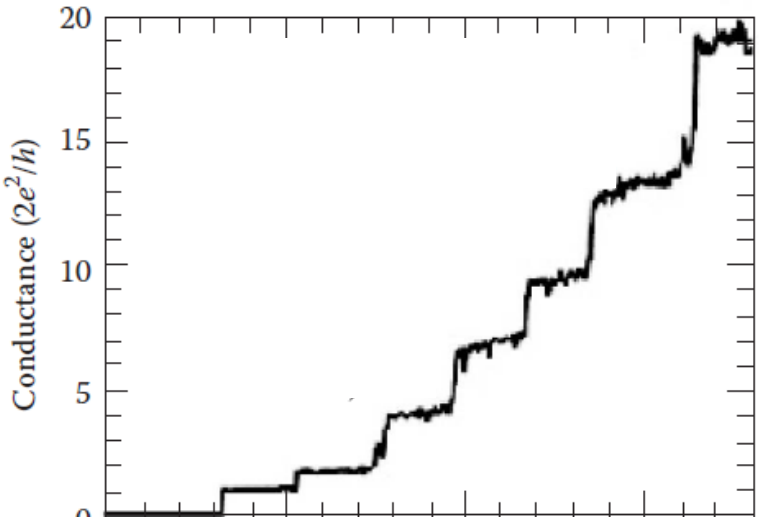
$$I = \frac{2e}{h} \int_0^\infty \{f(E,\mu) - f(E,\mu - eV)\} T(E) dE$$

Conductance (if the bias is small)

$$G = \frac{2e^2}{h} \int_0^\infty \left\{ -\frac{\partial f(E,\mu)}{\partial E} \right\} T(E) dE \equiv \frac{2e^2}{h} T_\mu$$

QCE in NWs: quantized conductance

- In 1D systems the conductance of electrons is quantized in units of $2e^2/h$
- Electrons states along the wire are associated with quantized states in the plane
- Each of the quantum states in the plane has equal unit of conductance $(2e^2/h)T_\mu$ along the wire axis
- The conductance of NWs is hence the product of the number of quantum states and their quantized conductance $(2e^2/h)T_\mu$



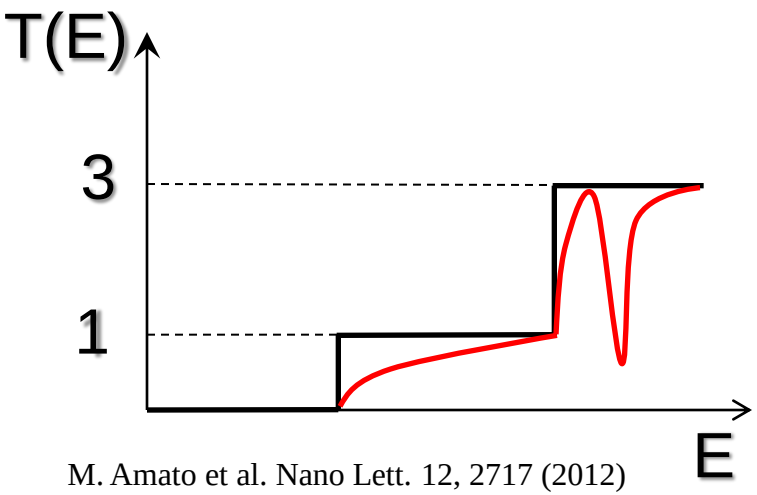
G. Rubio et al. Phys. Rev. Lett. 76, 2302 (1996)

STM experimental demonstration on gold NWs

QCE in Si NWs: DFT + Landauer approach

Conductance is calculated in terms of transmission probability T(E) through the available transmitting channels

How many?
For an infinitely long NW: as many as electron states at that energy



M. Amato et al. Nano Lett. 12, 2717 (2012)

For a pristine Si NW: T(E) = 1
For a defected NW: T(E) < 1

Outline

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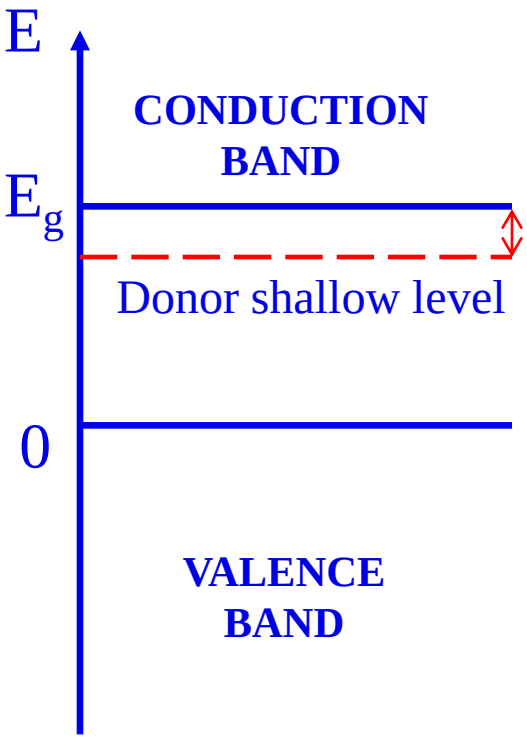
QCE in Si NWs: impurity deactivation

Si bulk P-doped



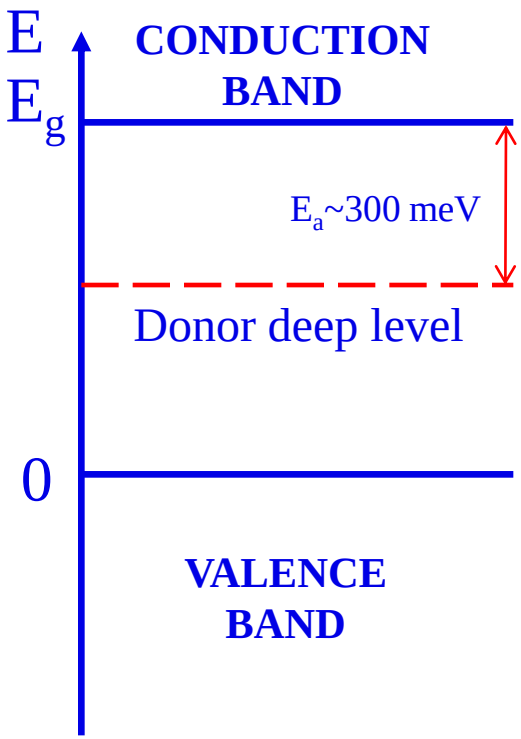
Quantum confinement

G. W. Bryant, Phys. Rev. B 29, 6632 (1984)

Dielectric mismatch

M. T. Bjork et al., Nat. Nanotechnol. 4 (2009)
M. Diarra et al., Phys. Rev. B 75, 045301 (2007)

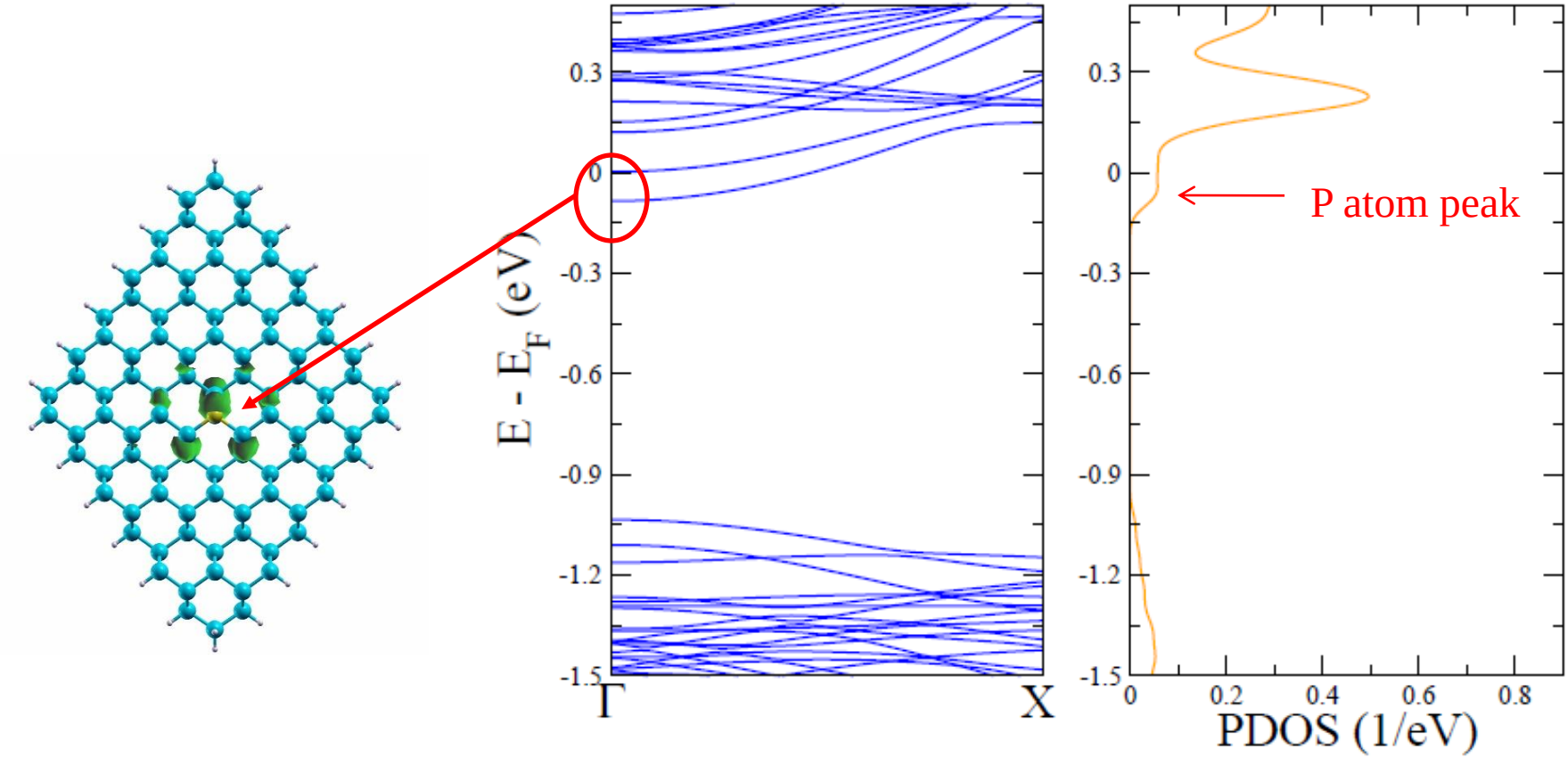
Si NW P-doped (d<10nm)



- Ionization energy ~ few hundredths of eV
- Ionized impurity at room temperature
- High doping efficiency

- Ionization energy increase
- Donor level deep into the band gap
- Doping deactivation with respect to bulk

QCE in Si NWs: P deactivation with DFT



M. Amato et al., Nano Lett. 11, 594–598 (2011)

P-impurity state deep into the band gap
Activation energy is too high (~ 100 meV)

Some comments on QCE in Si NWs

The diameter is a powerful tool to modulate physical properties

• Electronic Structure. Reducing the size can induce an opening of the bulk band gap that can cause a modulation of optical properties

• Transport. The quantization due to the confiment leads to a quantization of the electrical conductance. Si NWs are hence quantum confined ballistic conductors

• Doping. Intentional addition of impurities in Si NWs is not efficient as for bulk systems due to the impurity deactivation

Is it possible to further modify the physical properties of Si NWs?

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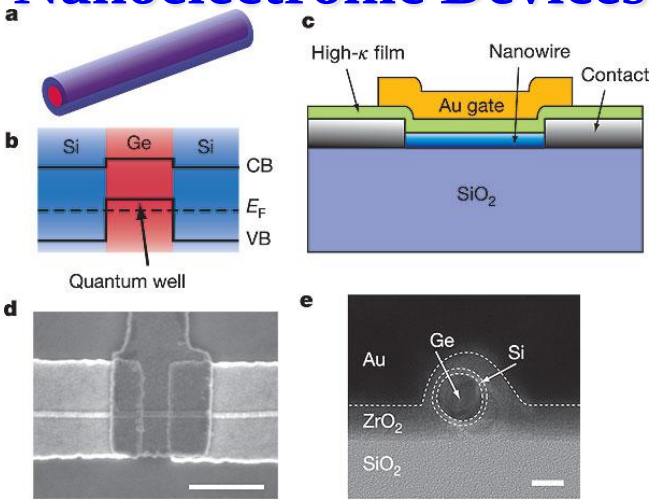
IV. *Physical properties of SiGe nanowires*

Why SiGe NWs ?

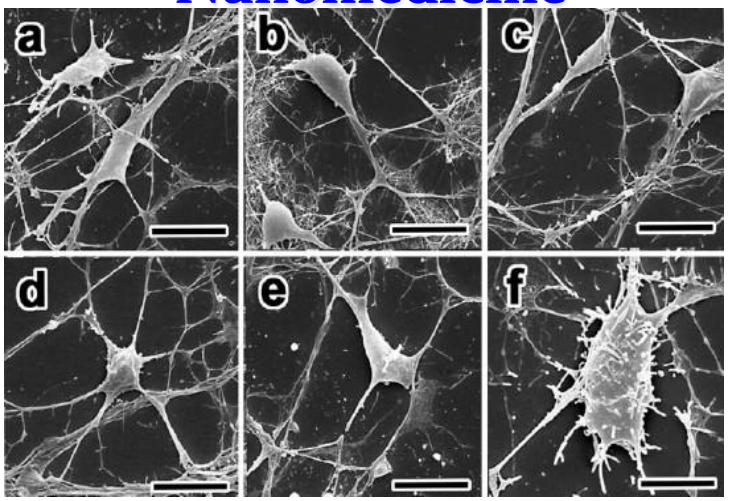
M. Amato et al. Chem. Rev. 114 (2), 1371 (2014)

Nanoelectronic Devices



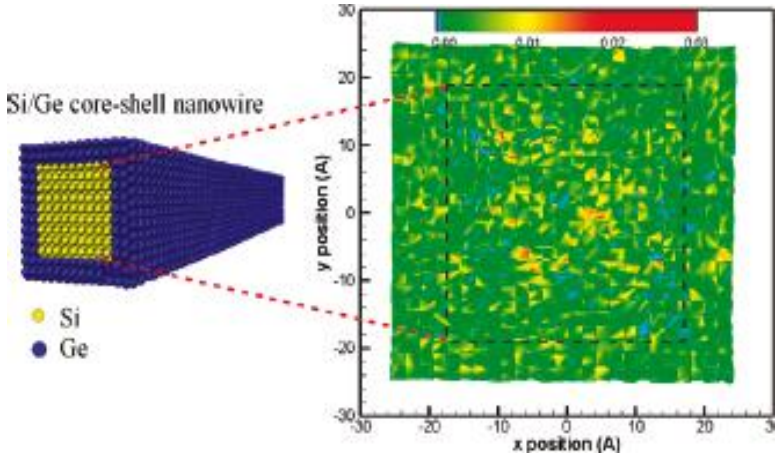
J. Xiang et al., Nature (London) 441, 489 (2006)

Nanomedicine



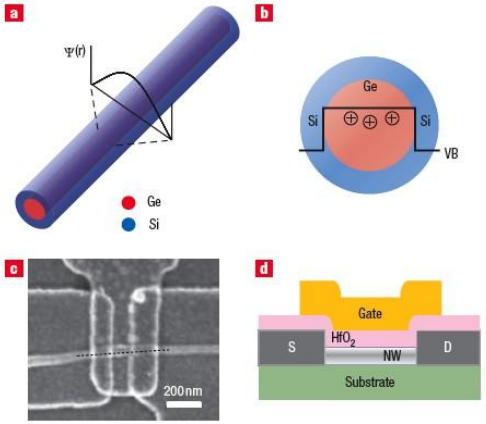
K.-Y. Lee et al., Nanoscale Res. Lett. 5, 410 (2010)

Thermoelectrics



M. Hu et al., Nano Lett. 11, 618-623 (2011)

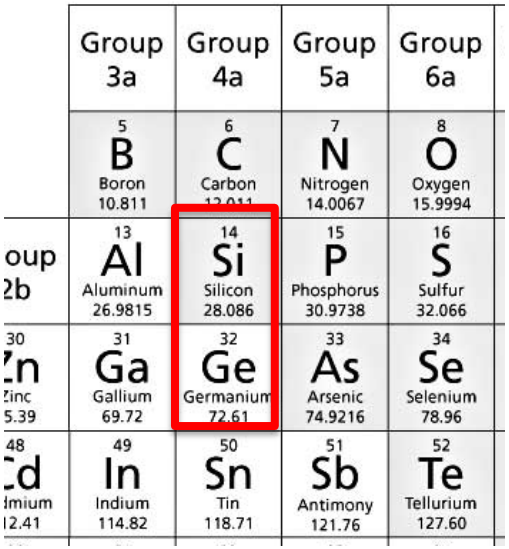
Superconductivity



J. Xiang et al., Nat. Nanotechnol. 1, 208 (2006)

Why SiGe NWs ?

By bringing together **Silicon** and **Germanium** within a nanowire geometry a surprisingly rich physics and a wealth of new properties emerge



	Group 3a	Group 4a	Group 5a	Group 6a
	5 B Boron 10.811	6 C Carbon	7 N Nitrogen 14.0067	8 O Oxygen 15.9994
oup 2b	13 Al Aluminum 26.9815	14 Si Silicon 28.086	15 P Phosphorus 30.9738	16 S Sulfur 32.066
30 Zn Zinc 5.39	31 Ga Gallium 69.72	32 Ge Germanium 72.61	33 As Arsenic 74.9216	34 Se Selenium 78.96
48 Cd dmium 12.41	49 In Indium 114.82	50 Sn Tin 118.71	51 Sb Antimony 121.76	52 Te Tellurium 127.60

Why SiGe NWs ?

- These materials can improve the electronic and optoelectronic performance of nanowire devices - A.Goldthorpe *et al*., Nano Lett. **20** (2008)

- They represent a realistic way to modulate the electronic and optical properties of NWs by changing composition and geometry - D.B. Migas *et al*., PRB **76** (2007)

- The interaction between Si and Ge atoms leads to a QCE different from that of pure nanostructures - R. Musin *et al*., PRB **74** (2006)

- The type II band offset between the two different materials creates a spatial localization of electrons and holes, which changes remarkably transport properties and creates a very suitable material for doping and photovoltaic application - A. Nduwimana *et al*., Nano Lett. **6** (2008)

- The band alignement between Si and Ge represents a useful key to modulate absorption and emission spectra - J. Yang *et al*., Nano Lett. **6** (2006); A. Goldthorpe *et al*., Nano Lett. **9** (2009)

Why SiGe NWs ?

SiGe NWs
electronic, transport and optical properties

Extrinsic parameters

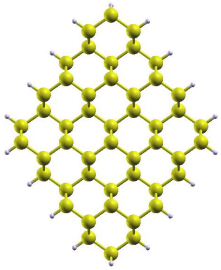
- **Diameter of the wire**
- **Doping with B and P impurities**

Intrinsic parameters

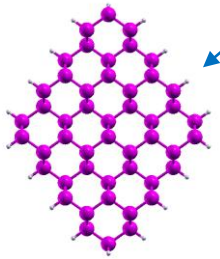
- **Relative composition of Si and Ge atoms**
- **Geometry of Si/Ge interface**

Ab initio simulations on [110] SiGe NWs

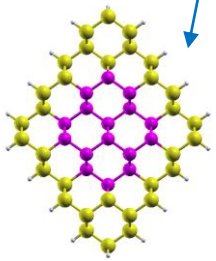
The model:
hydrogenated freestanding nanowires
Si NWs, Ge NWs, SiGe NWs



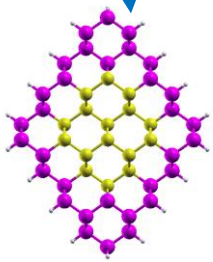
Si NWs



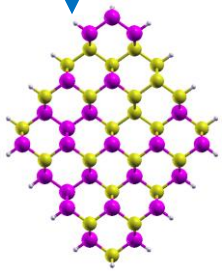
Ge NWs



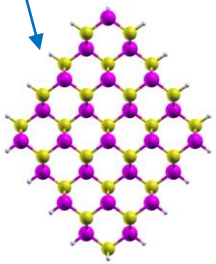
Ge_{core} / Si_{shell} **NWs**



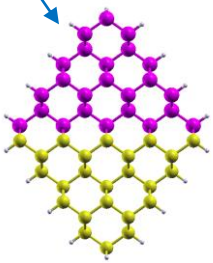
Si_{core} / Ge_{shell} **NWs**



Random **SiGe NWs**



Mixed **SiGe NWs**



Abrupt **SiGe NWs**

Diameter range
0.8 to 2.4 nm

Calculated quantities:

- Optimized geometry
- Band structure and band gap
- Electronic wave function localization
- Band offset

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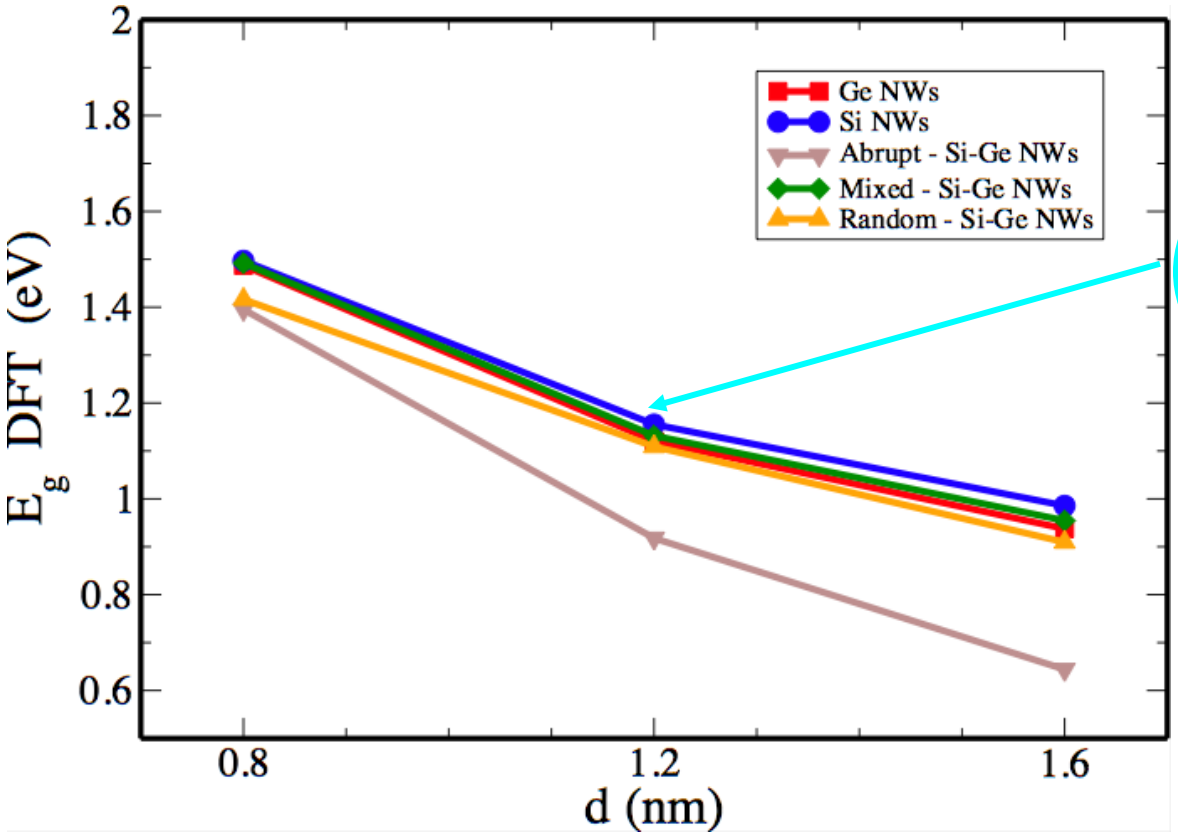
Reduced QCE (x_{Ge}=0.5)



Trend for pure NWs:
good agreement
with other theoretical works

M. Bruno et al., Phys. Rev. B 72 (2005)
S. Beckman et al., Phys. Rev. B 74 (2006)

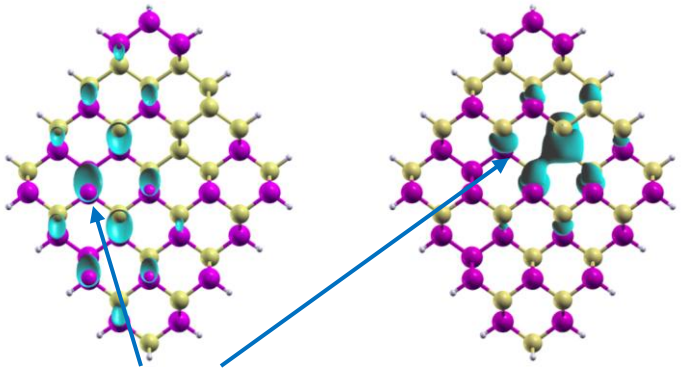
M. Amato et al., Phys. Rev. B 79, 201302(R) (2009)

Abrupt NWs show a reduced QCE (RQCE) which is more pronounced increasing the diameter and is principally related to the geometry; the origin of this effect is due to the type II band offset between Si and Ge

Type II offset and localization of the wave function

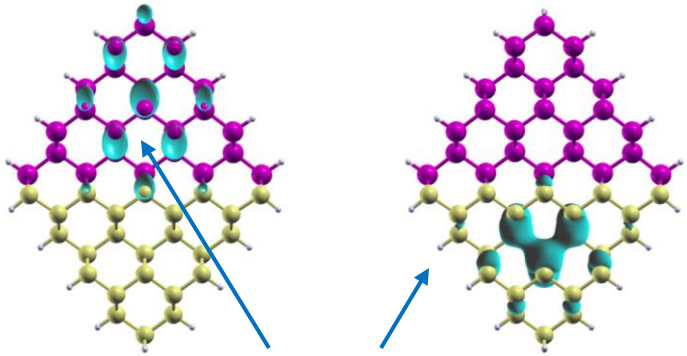
This type of offset implies that the minimum of the conduction band (CBM) and the maximum of the valence band (VBM) are on different materials

VBM CBM



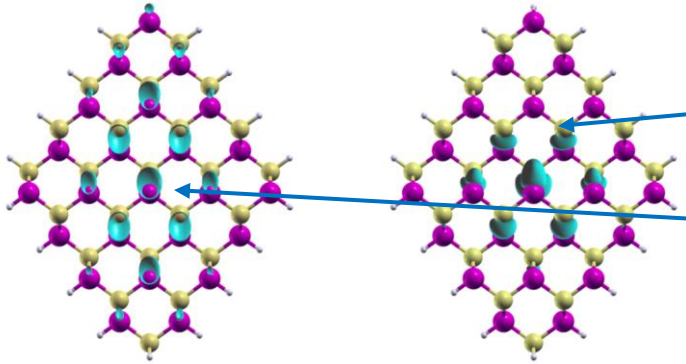
Random SiGe NWs
Partial localization

VBM CBM



Abrupt SiGe NWs
Complete localization

VBM CBM



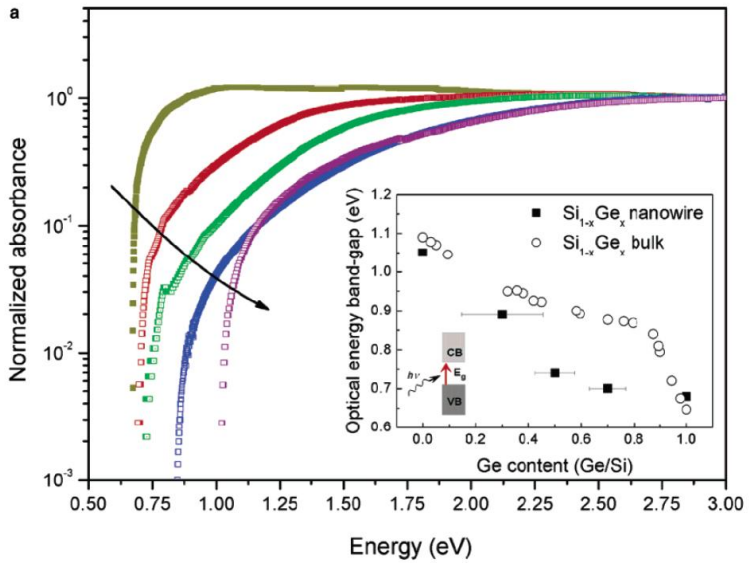
Mixed SiGe NWs
No localization

M. Amato et al., Phys. Rev. B 79, 201302(R) (2009)

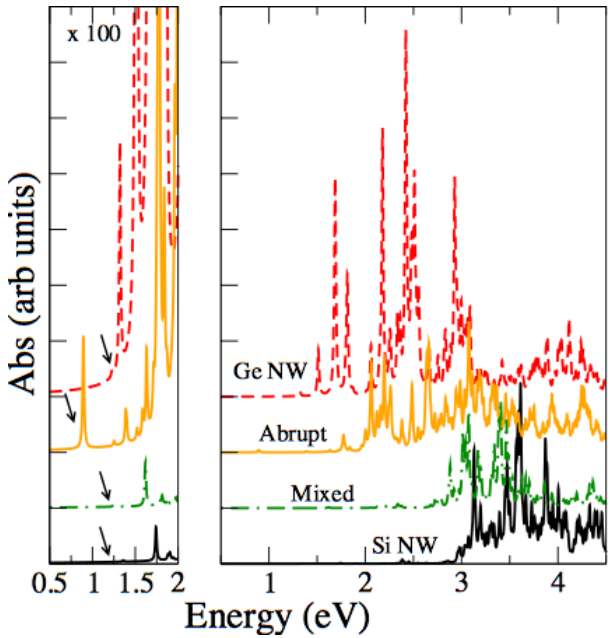
Effect on the optical properties

In $Si_{1-x}Ge_x$ NWs the electronic and optical properties can be continuously modulated by controlling the Ge content *x*

The optical gap decreases increasing the Ge concentration



Yang et al., Nano Lett. 6, 2679 (2006)



M. Palummo et al. Phys. Rev. B 82, 073305 (2010)

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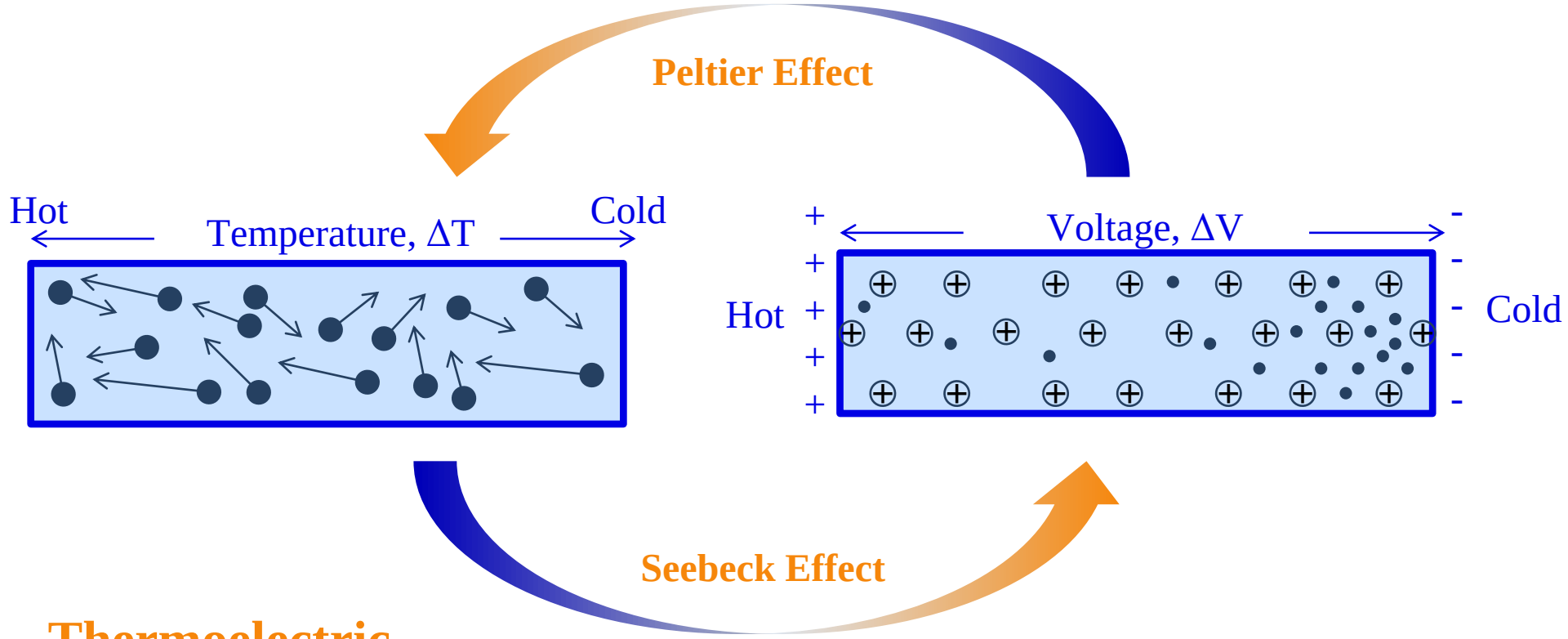
Thermoelectric Energy Conversion



Thermoelectric Efficiency

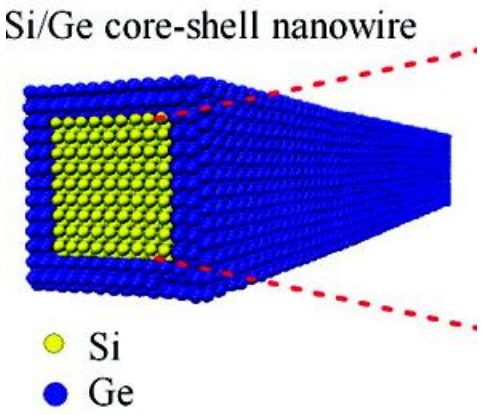
$$ZT = S^2 T \frac{\sigma_e}{\sigma_T}$$

- Electrical Conductivity
- Thermal Conductivity
- Seebeck Coefficient

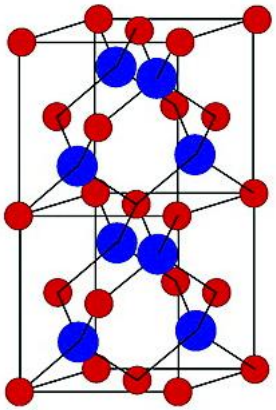
How do we increase ZT?

- Increasing $S^2\sigma_e$
- Decreasing σ_T

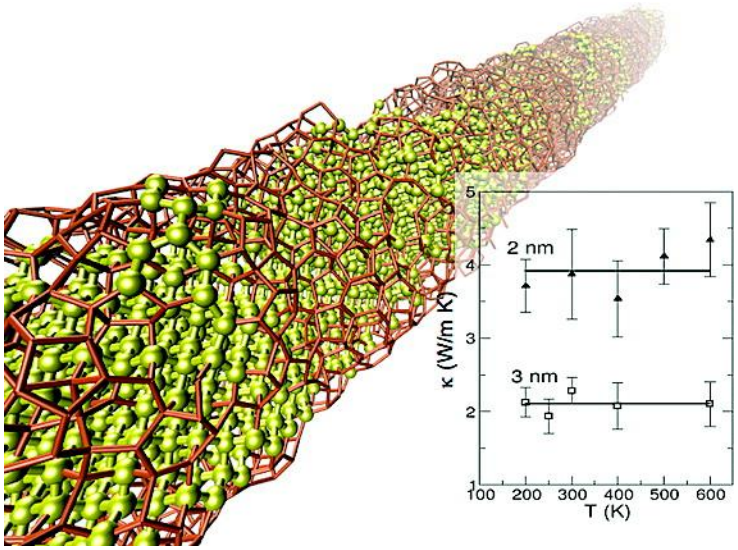
Nanostructures for Thermoelectrics



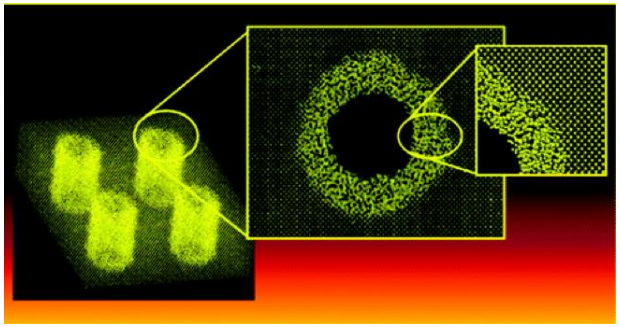
Hu et al., Nano Lett. 11, 618 (2011)



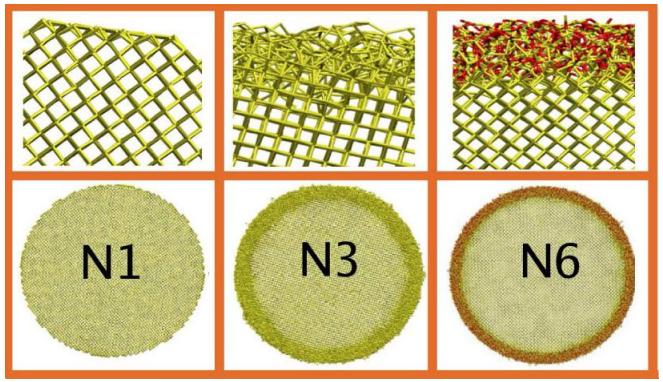
Garg et al., Nano Lett. 11, 5135 (2011)



Donadio et al., Nano Lett. 10, 847 (2010)



He et al., ACS Nano 5, 1839 (2011)



He et al., ACS Nano 5, 1839 (2011)

The main aim

M. Amato, et al. Nano Lett. 12, 2717 (2012)

Study of the electrical conductivity of SiNWs in the ballistic regime upon Ge-alloying

It is known that thermal conductivity goes down

M. Amato et al. Chem. Rev. 114 (2), 1371 (2014)

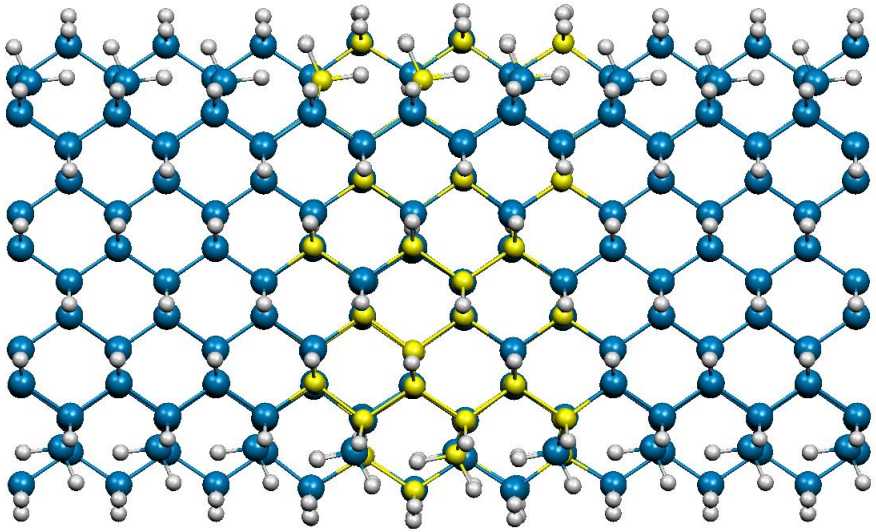
Is electrical conductivity reasonably preserved?

Theoretical Model

Si NW / $Si_{1-x}Ge_x$ NW / Si NW

Diameter 2.4 nm

x = 0.1 -0.9



First-principles DFT calculations

SIESTA code

www.icmab.es/siesta

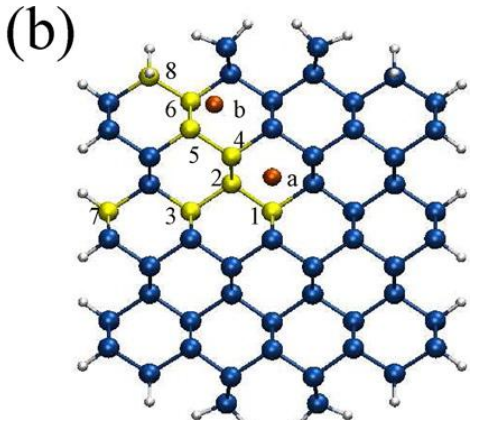
Calculated quantities:

- Optimized geometry
- Band structure
- Wave function localization

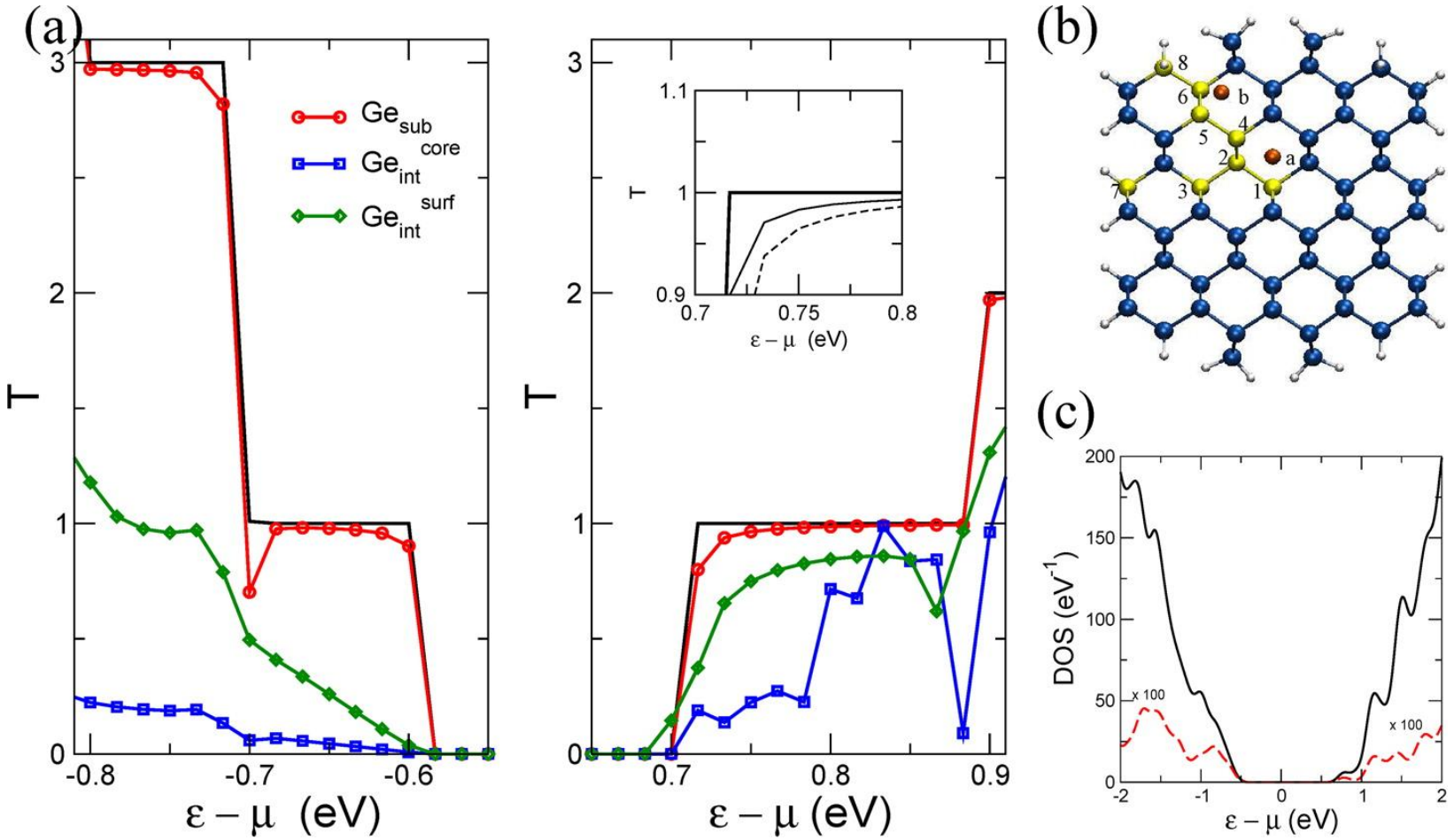
Single impurity scattering

At first we have studied the scattering of ***individual Ge impurities*** in a pristine Si NW

We considered both
substitutionals
and **interstitials**



Single impurity scattering

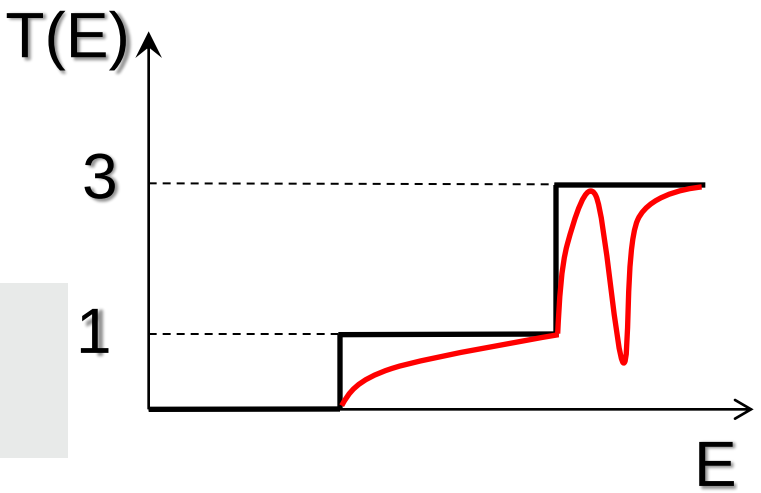


- $E_f^s << E_f^i$
- Minimal scattering associated to substitutionals
- Larger scattering in the valence band

Landauer Theory

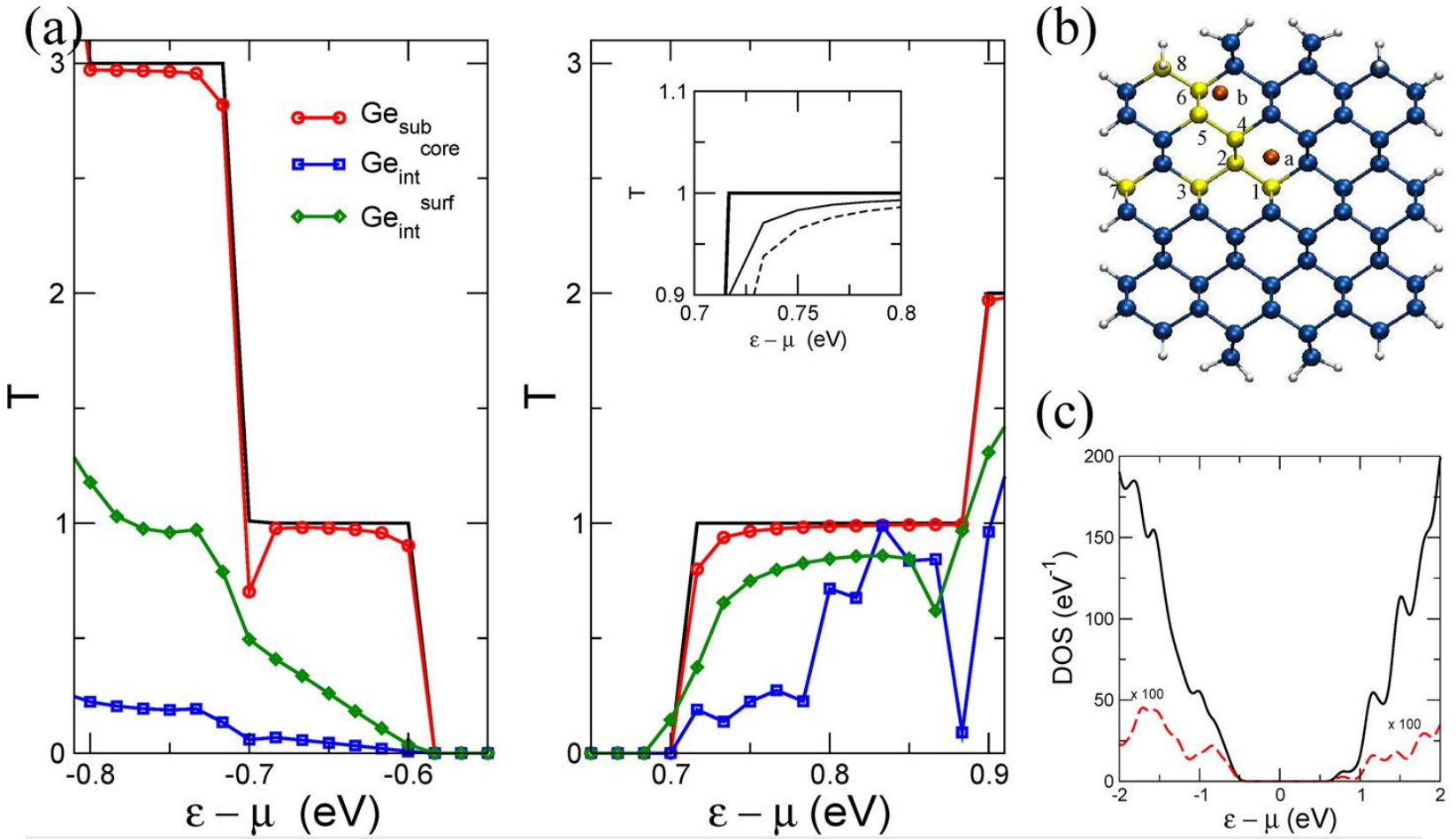
Conductance is calculated in terms of transmission probability T(E) through the available transmitting channels

How many?
For an infinitely long NW: as many as electron states at that energy



For a pristine Si NW: T(E) = 1
For a defected NW: T(E) < 1

Single impurity scattering



- $E_f^s << E_f^i$
- Minimal scattering associated to substitutionals
- Larger scattering in the valence band

Single impurity scattering

The assumption that Ge impurities do not worsen the conductive properties of Si NW seems reasonable:

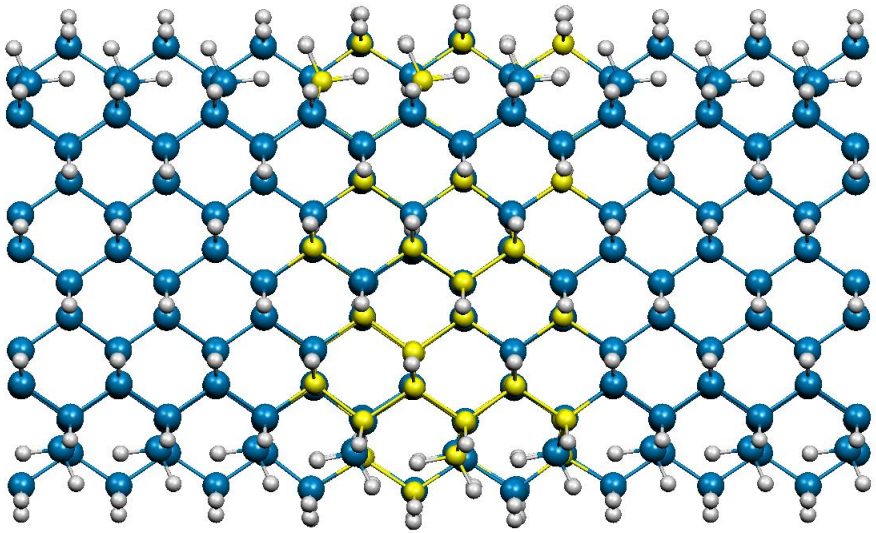
• only interstitial defects act as efficient scattering centers, but their concentration is expected to be negligible ($E_f^s << E_f^i$)

• substitutional defects are easily incorporated in the Si lattice ($E_f^s \sim 0$) and the transport channels of the pristine wire are only marginally affected

$Si_{1-x}Ge_x$ scattering

In realistic alloyed-NWs large amount of Ge impurities can be added (up to 70%!)

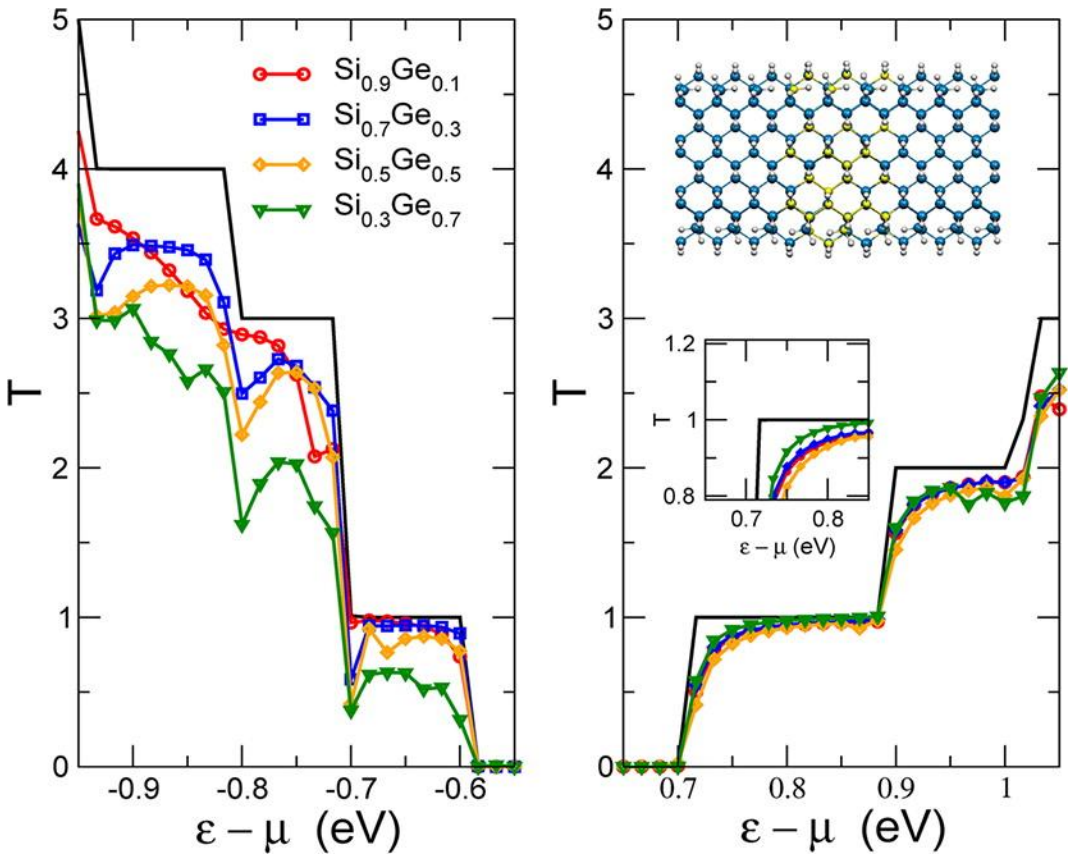
Therefore, although the scattering of individual Ge impurities is promisingly low, the study of $Si_{1-x}Ge_x$ regions has to be addressed directly



$Si_{1-x}Ge_x$ scattering

It is still true that the valence band scattering is stronger

Even more interesting: scattering in the conduction band is almost concentration independent!

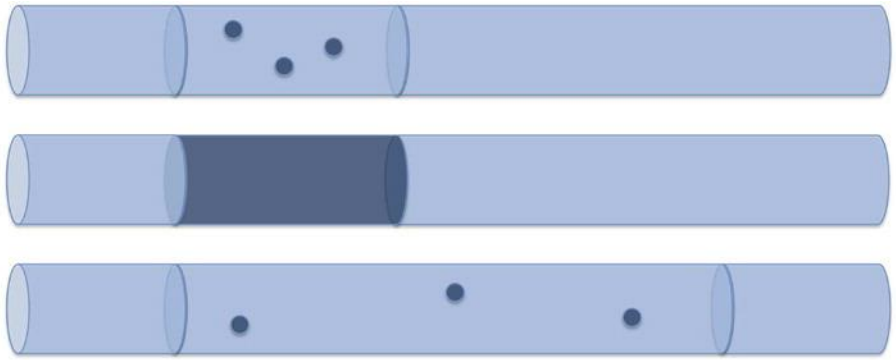


$Si_{1-x}Ge_x$ scattering

Many (many, really!) impurities give an unexpectedly low scattering

What happens if they are distributed over a longer wire segment?

$Si_{1-x}Ge_x$ scattering



Let us consider three cases:

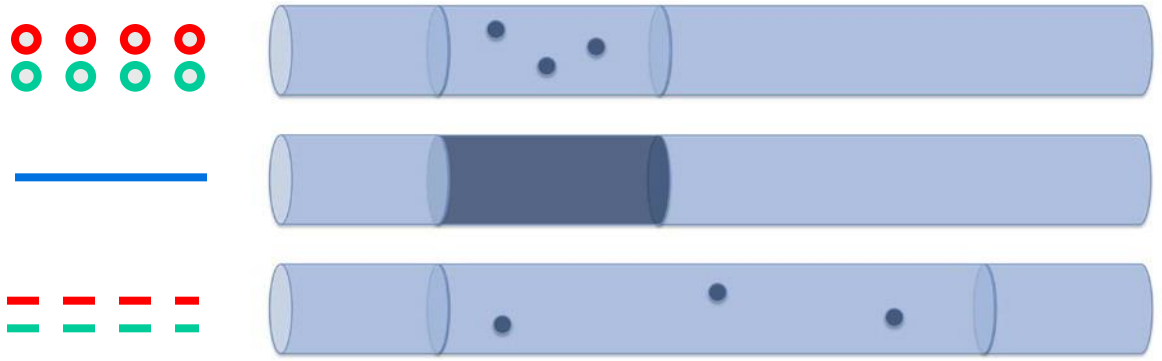
- abrupt Ge inclusion
- $Si_{1-x}Ge_x$ alloyed segment
- distributed, well-spaced *N* impurities

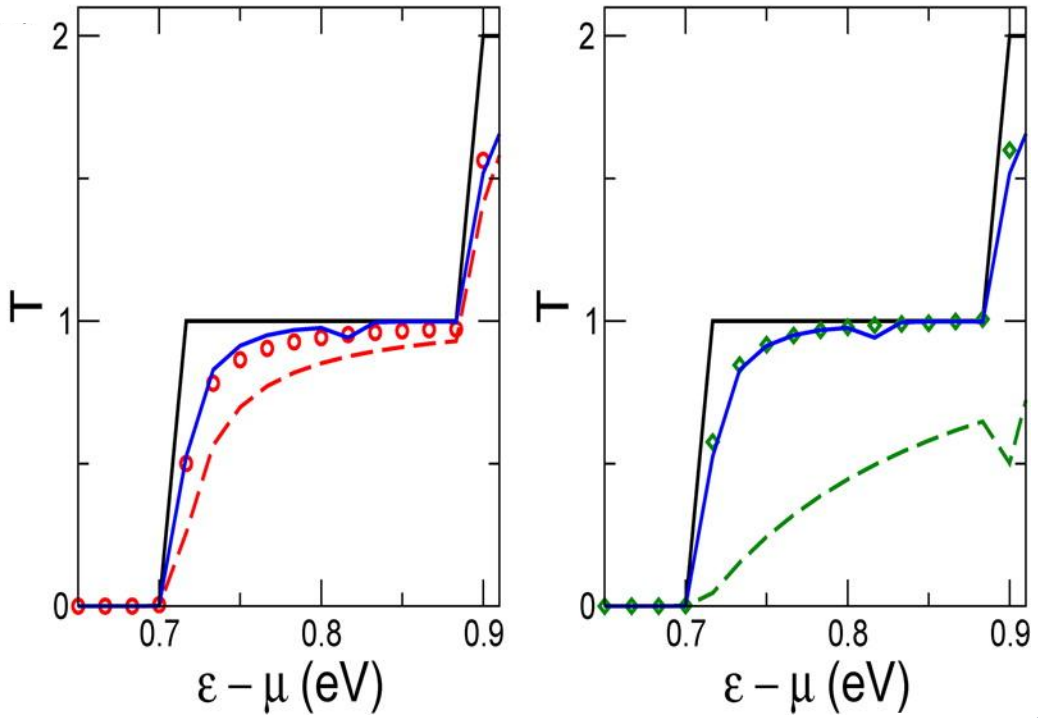
$Si_{1-x}Ge_x$ scattering

For both x=0.1 and x=0.7 the alloyed segment behave effectively like an all-Ge inclusion

Scattering is weakly dependent on x

Concentrating the impurities reduces the scattering





Some comments

• The assumption that Ge impurities do not worsen the conductive properties of Si NW seems reasonable. Single-impurity certainly do not.

• In alloyed NWs, at experimentally relevant Ge concentration, scattering is almost independent on it

• At practical effect, $Si_{1-x}Ge_x$ segments scatter carriers like all-Ge inclusion (interface scattering dominates)

• Given *N* Ge impurities, the resulting scattering is much lower in heavily alloyed segments than if distributing the impurities over a longer length of the NW

Outline

- Introduction on nanoscience
- Ab initio simulations: Density Functional Theory (DFT)
- Quantum confinement in Si nanowires (Si NWs)
  - Electronic structure
  - Transport properties
  - Doping effects
- Physical properties of SiGe nanowires (SiGe NWs)
  - Reduced quantum confinement effect
  - A good thermoelectric material
  - Efficient p- and n-type doping
- Conclusions

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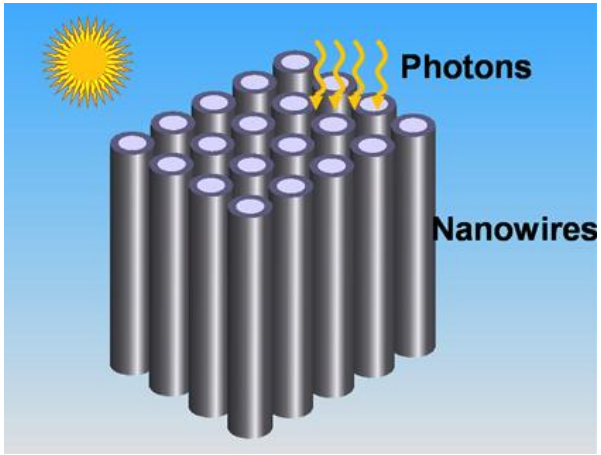
Si NWs for new concept solar cells



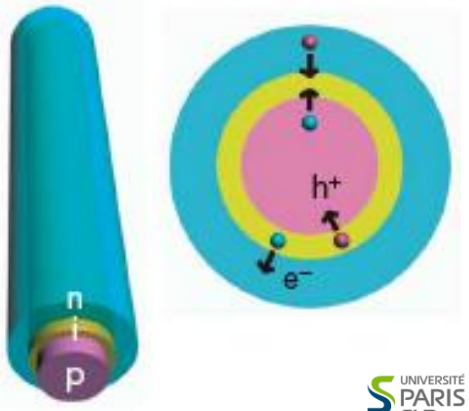
L. Hu and G. Chen, Nano Lett. 7, 3249 (2007)

Strong optical absorption in the solar spectrum and enhanced light trapping

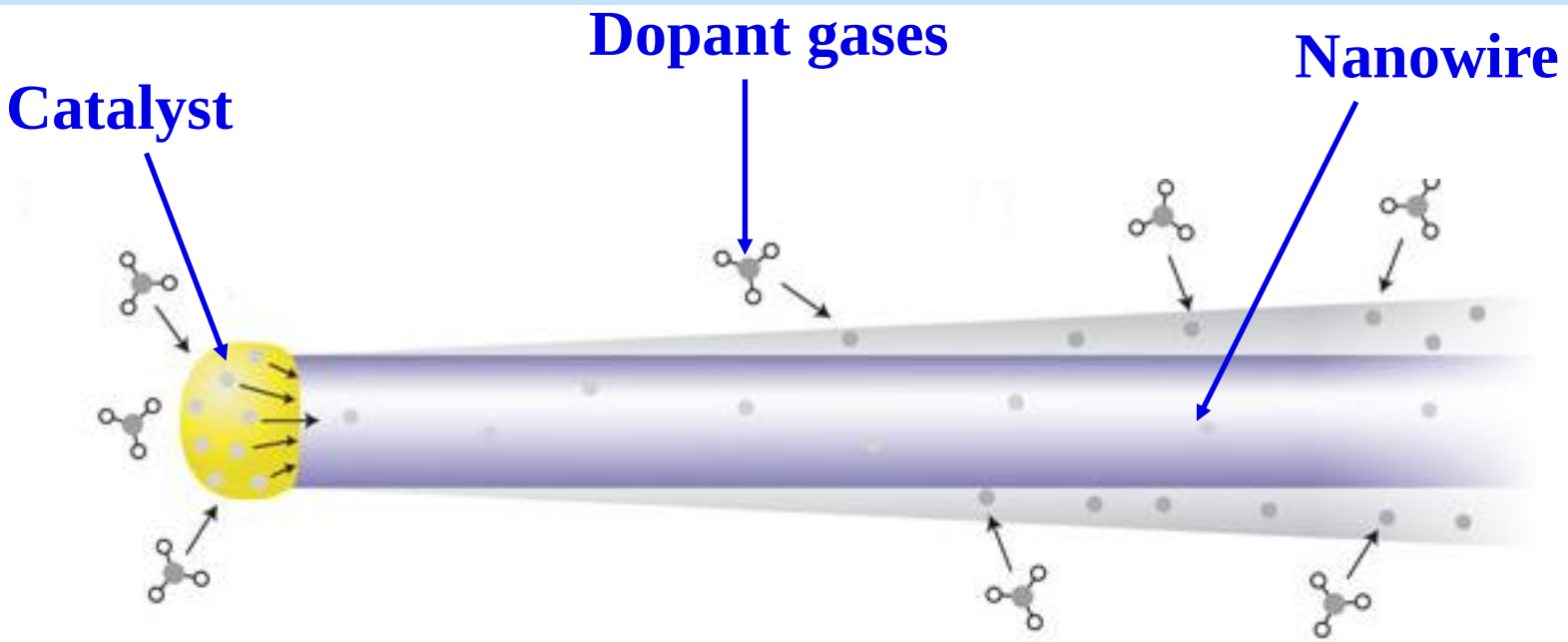
Excellent transport and electrical characteristics

B. Tian et al., Nature 449, 885 (2007)

Radial p-n junctions that offer a short collection length for charge carriers



Doping NWs with B and P impurities

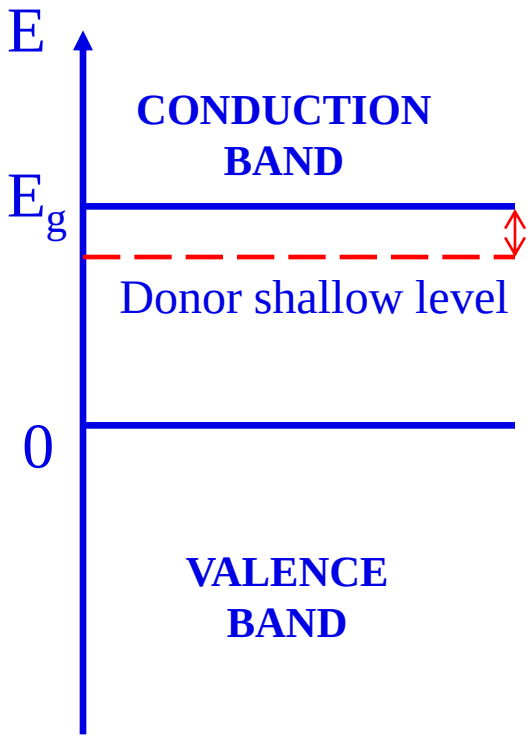


D. E. Perea et al., Nat. Nanotechnol. 4, (2009)

- Many device applications require a controlled doping
- n-type and p-type doping can be easily achieved for NWs with VLS
- It's not well understood how transport properties depend on the doping level

Impurity deactivation in ultrathin pure NWs

Si bulk P-doped



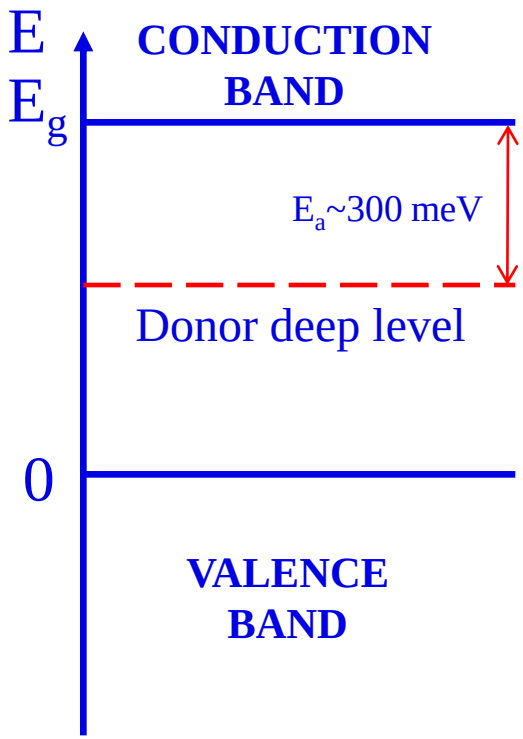
Quantum confinement

G. W. Bryant, Phys. Rev. B 29, 6632 (1984)

Dielectric mismatch

M. T. Bjork et al., Nat. Nanotechnol. 4 (2009)
M. Diarra et al., Phys. Rev. B 75, 045301 (2007)

Si NW P-doped (d<10nm)



- Ionization energy ~ few hundredths of eV
- Ionized impurity at room temperature
- High doping efficiency

- Ionization energy increase
- Donor level deep into the band gap
- Doping deactivation with respect to bulk

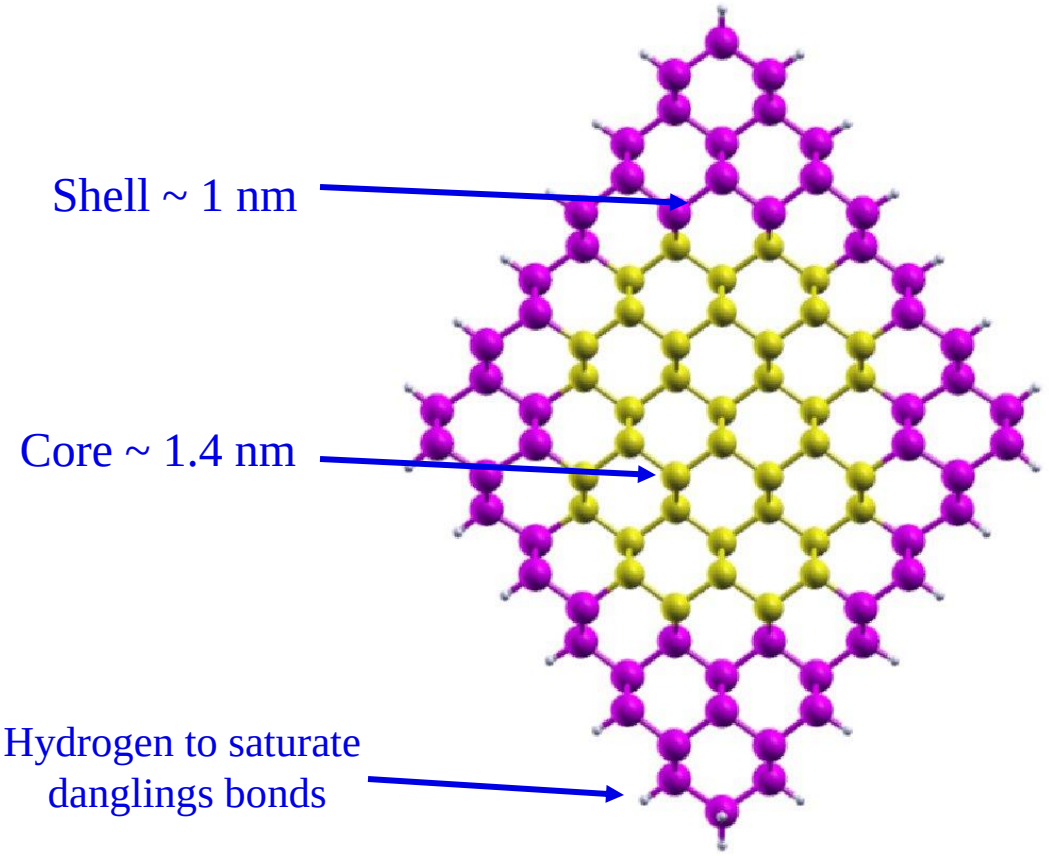
Theoretical model

Ge_{core}/Si_{shell} NW

Si_{core}/Ge_{shell} NW

Diameter 2.4 nm
B and P substitutional impurities

Core-Shell Theoretical Model

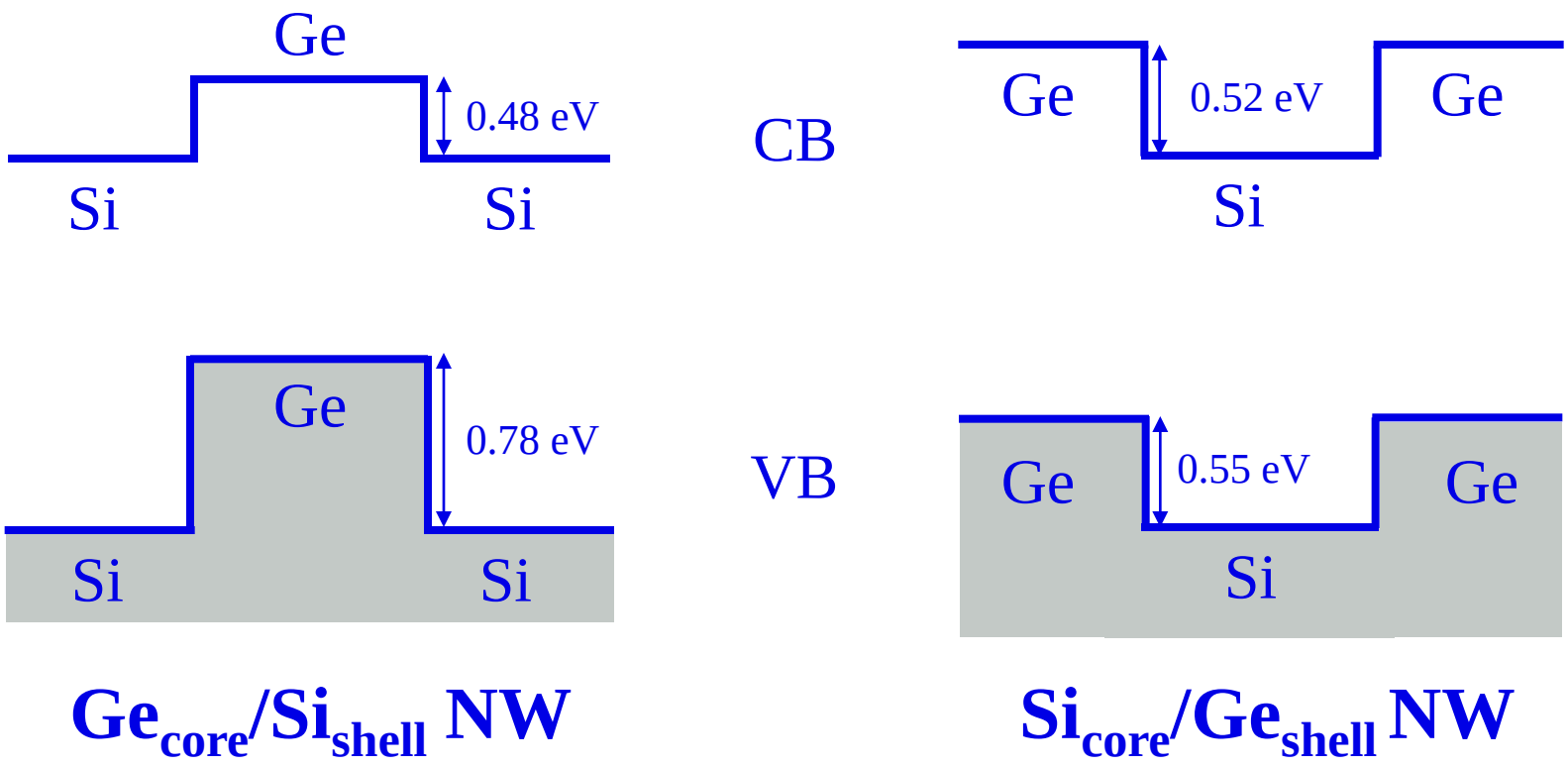


Calculated quantities:

- Optimized geometry
- Band structure
- Wave function localization

Electronic structure of undoped SiGe NWs

Type II band-offset

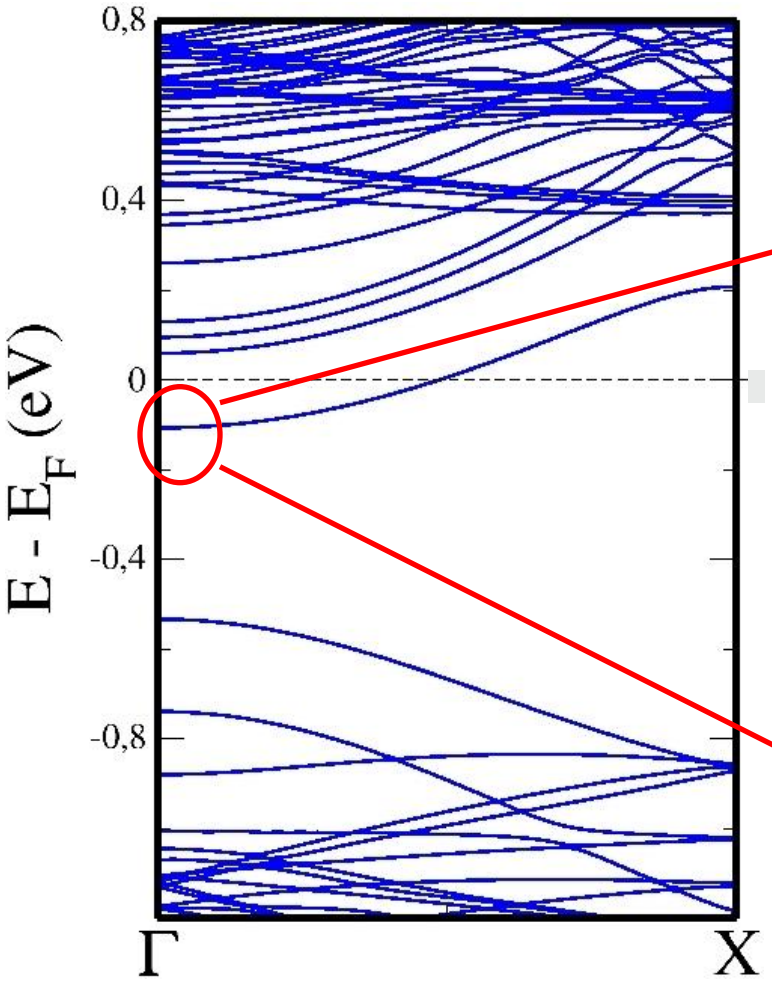


Ge_{core}/Si_{shell} NW **Si_{core}/Ge_{shell} NW**

M. Amato et al., Phys. Rev. B 80, 2355333 (2009)

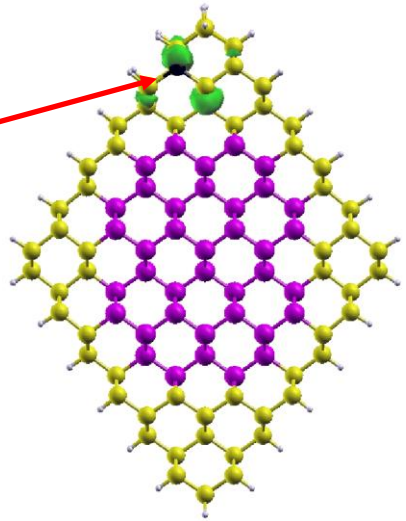
Valence states located on Germanium
Conduction states located on Silicon

Ge_{core}/Si_{shell}: P impurity into the Si shell

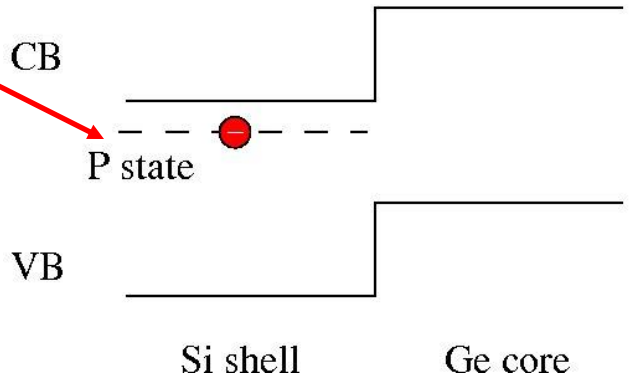


M. Amato et al., Nano Lett. 11, 594–598 (2011)

Impurity state localization



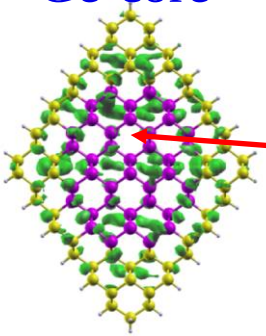
P-impurity state deep into the band gap
No difference with the P-doping of a pure NW



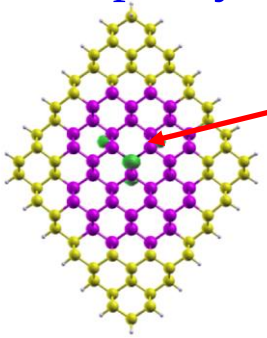
Ge_{core}/Si_{shell}: P impurity into the Ge core

Efficient doping

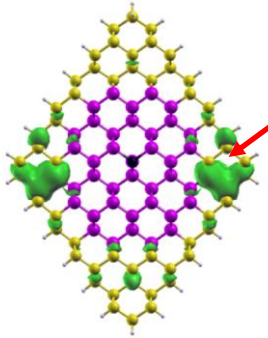
Ge-core

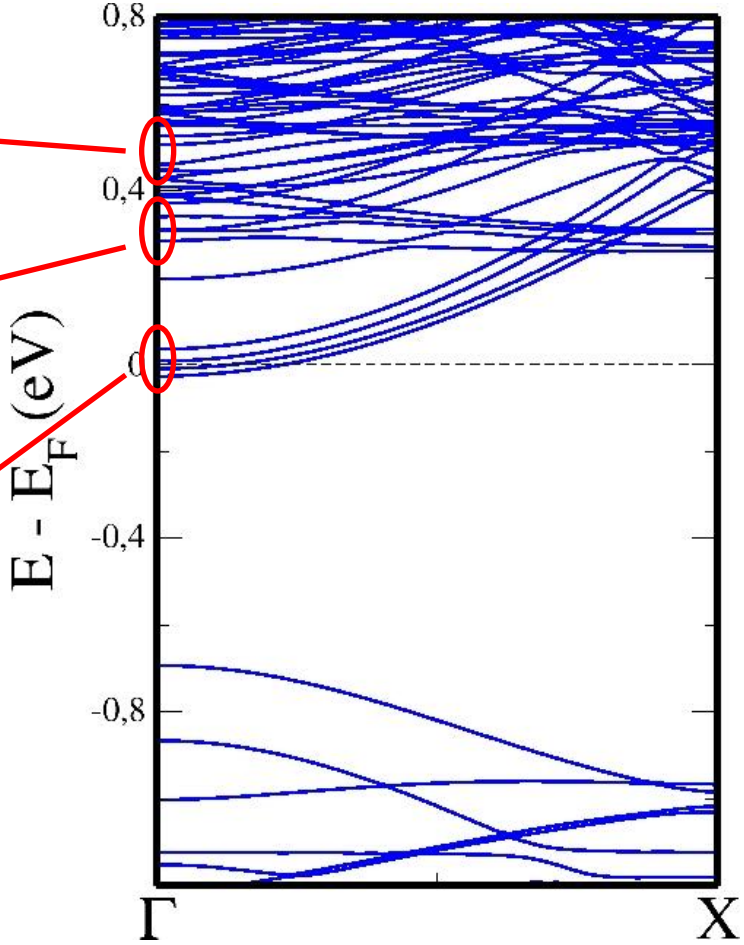


P-impurity

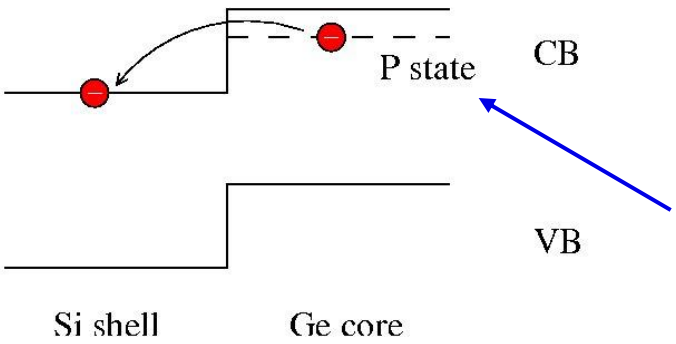


Si-shell





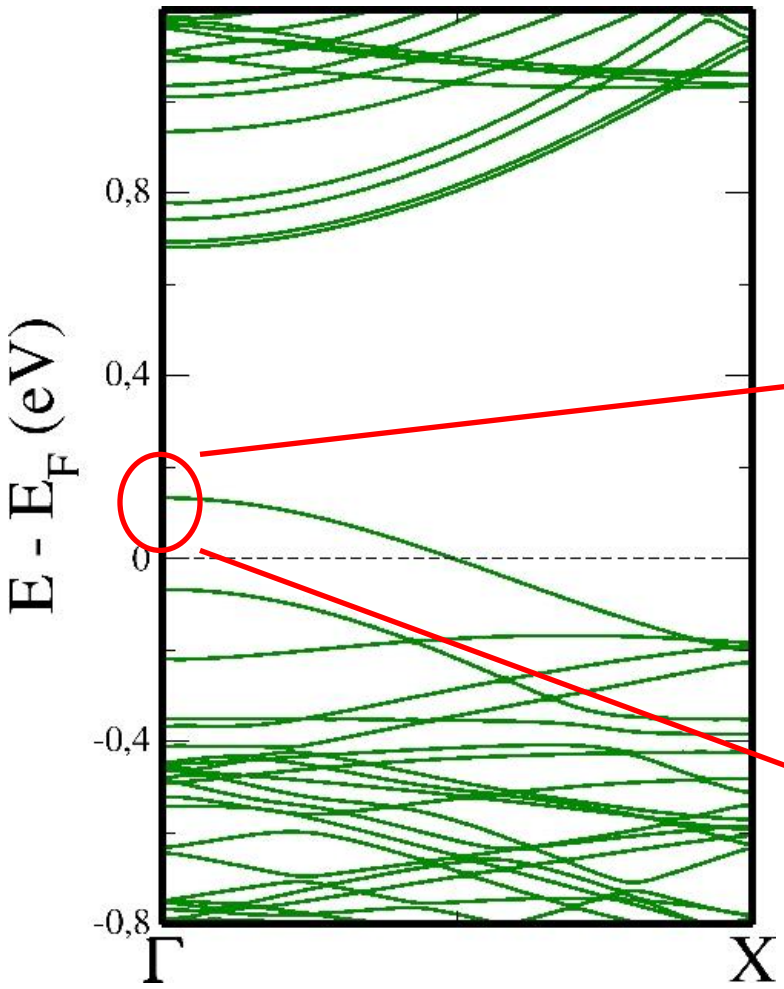
M. Amato et al., Nano Lett. 11, 594–598 (2011)



P-impurity state located deep into the CB

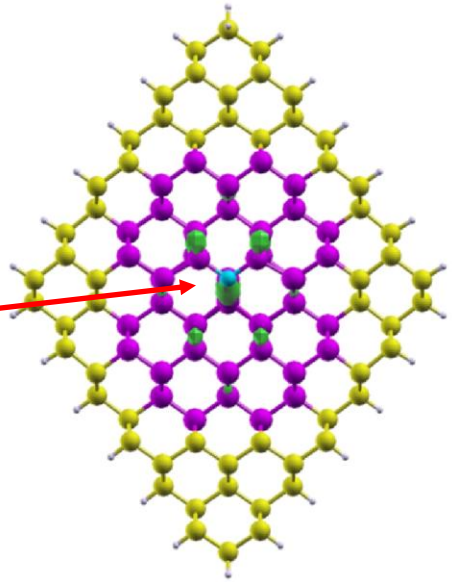
Creation of an electron 1D-gas

Ge_{core}/Si_{shell}: B impurity into the Ge core

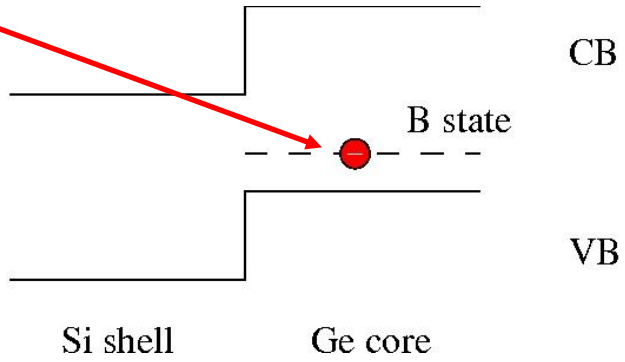


M. Amato et al., Nano Lett. 11, 594–598 (2011)

Impurity state localization



B-impurity state deep into the band gap
No difference with the B-doping of a pure NW

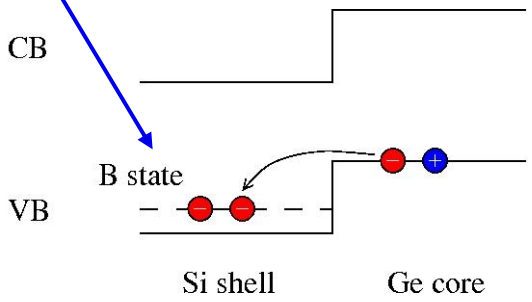


Ge_{core}/Si_{shell}: B impurity into the Si shell

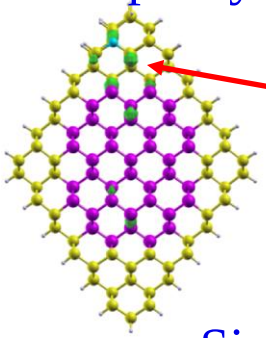
Efficient doping

B-impurity state located deep into the VB

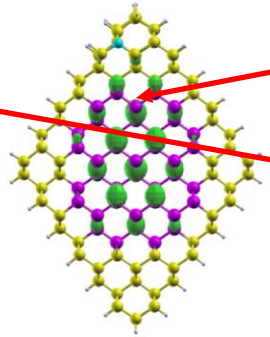
Creation of a hole 1D-gas



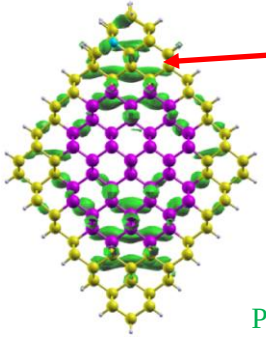
B-impurity

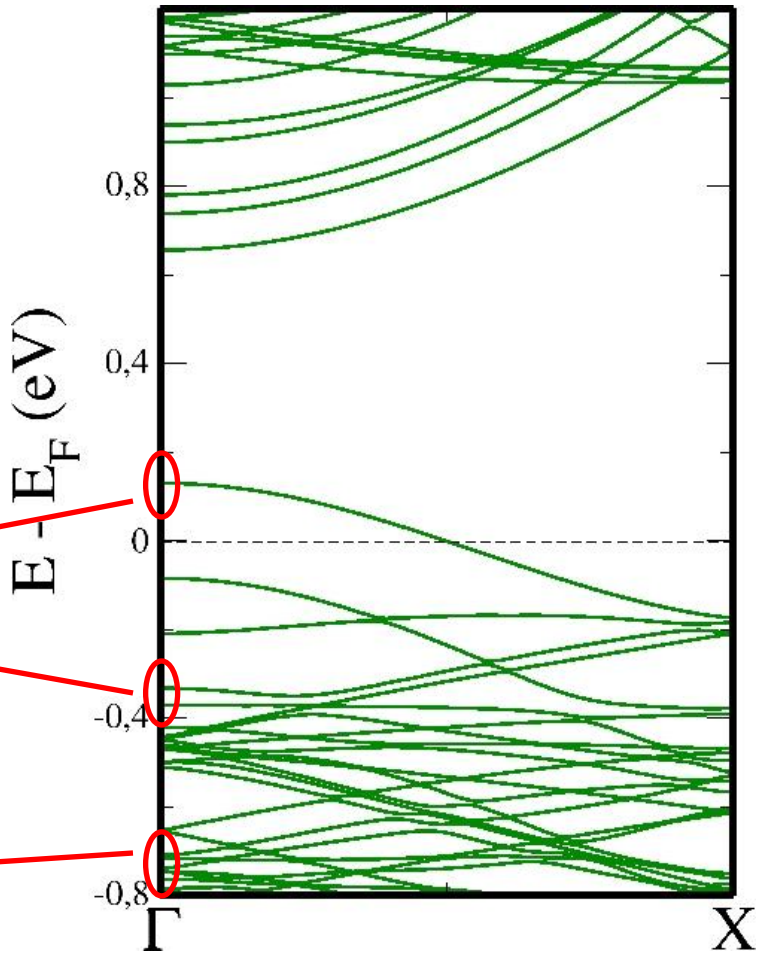


Ge-core



Si-shell





M. Amato et al., Nano Lett. 11, 594–598 (2011)

Experimental evidences. I

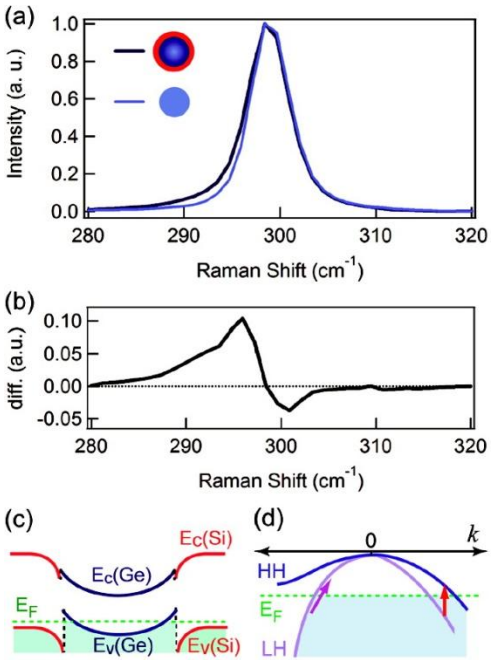
NANO LETTERS

pubs.acs.org/NanoLett

Direct Detection of Hole Gas in Ge–Si Core–Shell Nanowires by Enhanced Raman Scattering

Shixiong Zhang, Francisco J. Lopez, Jerome K. Hyun, and Lincoln J. Lauhon*

Department of Materials Science and Engineering, Northwestern University, Evanston, Illinois 60208, United States



Direct detection of hole accumulation in the core of Ge_{core}/Si_{shell} nanowires with B impurities into the silicon shell through analysis of a Fano resonance spectra

Experimental evidences. II

NANO LETTERS

LETTER

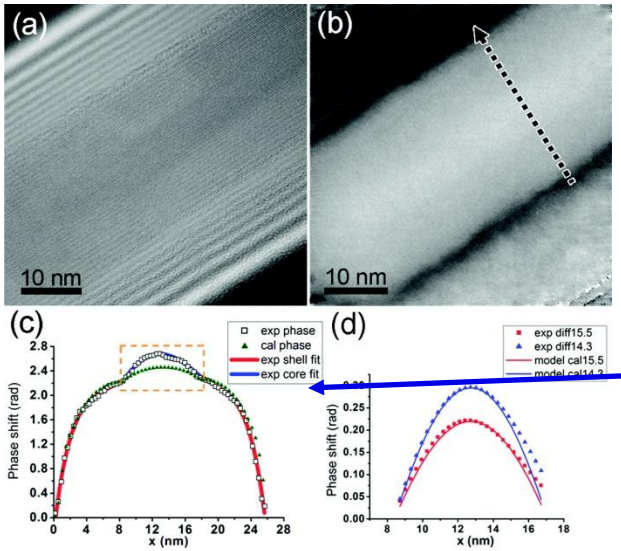
pubs.acs.org/NanoLett

Observation of Hole Accumulation in Ge/Si Core/Shell Nanowires Using off-Axis Electron Holography

Luying Li,*,† David J. Smith,† Eric Dailey,‡ Prashanth Madras,‡ Jeff Drucker,† and Martha R. McCartney†

†Department of Physics, Arizona State University, Tempe, Arizona 85287-1504, United States

‡School of Mechanical, Aerospace, Chemical and Materials Engineering, Arizona State University, Tempe, Arizona 85287-6106, United States



Hole accumulation in Ge_{core}/Si_{Shell} nanowires observed and quantified using off-axis electron holography and other electron microscopy techniques

Some comments on doping efficiency

- We have demonstrated how it is possible to obtain an efficient n- and p- type doping for Ge_{core}/Si_{shell} NWs and to overcome the limit of impurity deactivation in NWs

- The two cases of interest are P impurity into the Ge core and B impurity into the Si shell

- This physical phenomen can be also observed, with the appropriate differences, in Si_{core}/Ge_{shell} NWs [M. Amato et al. J. Comput. Elec. 11, 3, 272-279 (2012)]

- SiGe core-shell NWs provide a system ideally suited for photovoltaic applications, since it fulfils two of their fundamental applications, i.e. to separate electrons and holes and to render both carriers active [M. Amato et al. Chem. Rev. 114 (2), 1371 (2014)]

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Conclusions

Physical properties of SiGe NWs can be strongly modified by changing diameter and composition

• Electronic Structure. Adding Ge atoms into a Si NW reduce the effect of QCE offering the possibility to choose the desired gap

• Transport. SiGe alloyed NWs preserve the electrical ballistic conductance of Si NWs while they strongly reduce the thermal conductivity

• Doping. An efficient n- and p- type single-doping for Ge_{core}/Si_{shell} NWs can be obtained overcoming the limit of impurity deactivation in pure systems

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Rome, Italy

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Modena, Italy