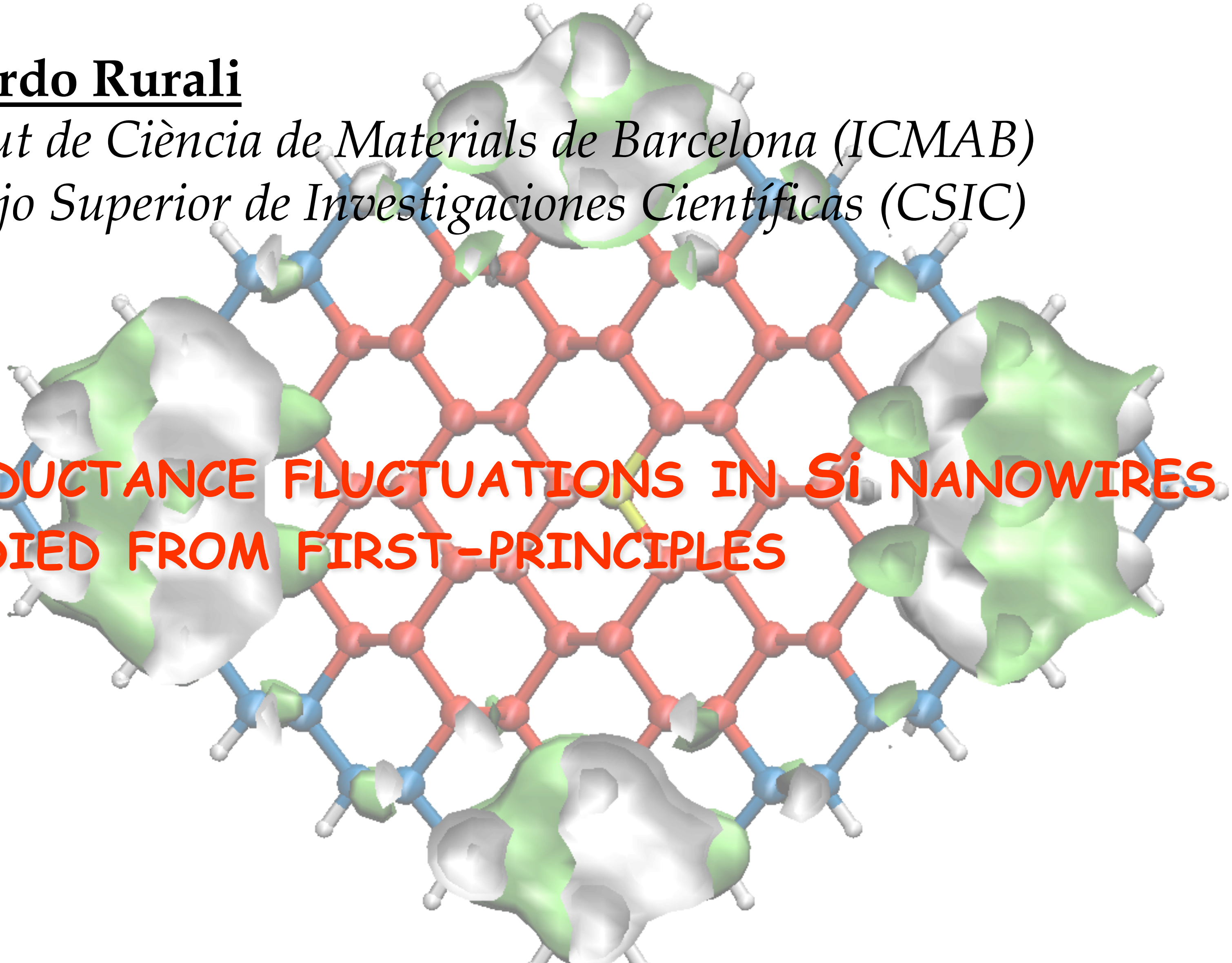
Riccardo Rurali
Institut de Ciència de Materials de Barcelona (ICMAB)
Consejo Superior de Investigaciones Científicas (CSIC)

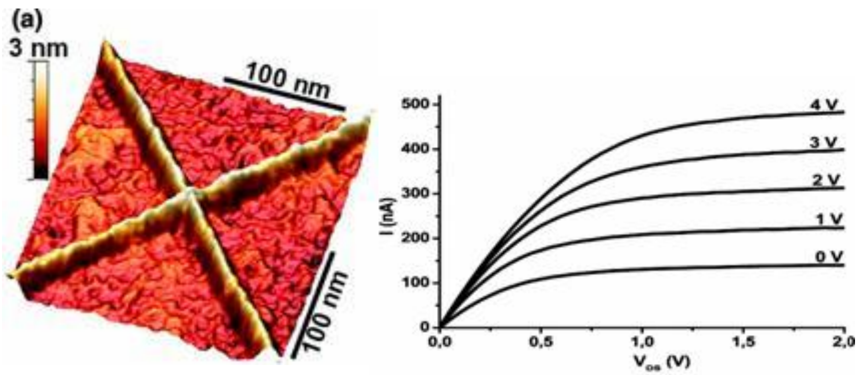


CONDUCTANCE FLUCTUATIONS IN Si NANOWIRES STUDIED FROM FIRST-PRINCIPLES

7th International Conference on Unsolved Problems on Noise (UPoN)
Casa Convalescència, Barcelona (Spain), July 13-17, 2015

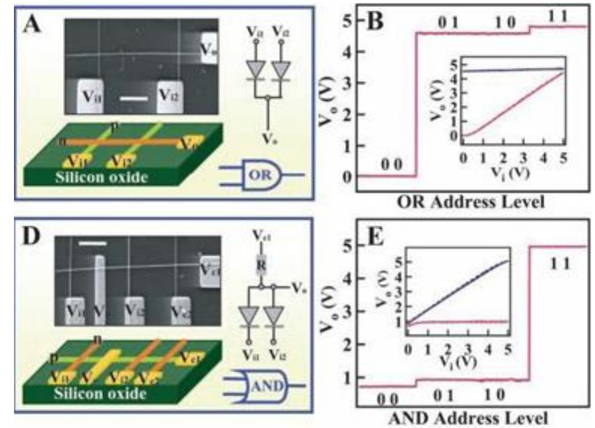
Why Nanowires?

Devices



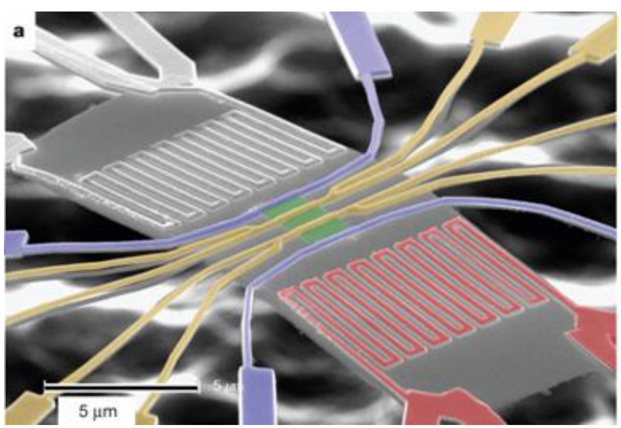
Martínez *et al.*, Nano Lett. **8**, 3636 (2008)

Logic gates



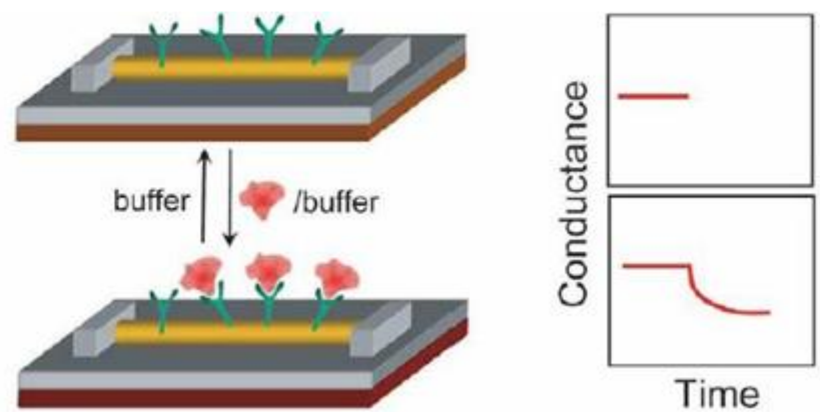
Huang *et al.*, Science **294**, 1317 (2001)

Thermoelectrics



Boukai *et al.*, Nature **451**, 168 (2008)

Chemical sensors



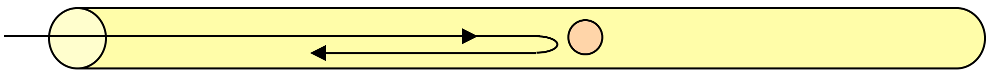
Cui *et al.*, Appl. Phys. Lett. **78**, 2214 (2001)

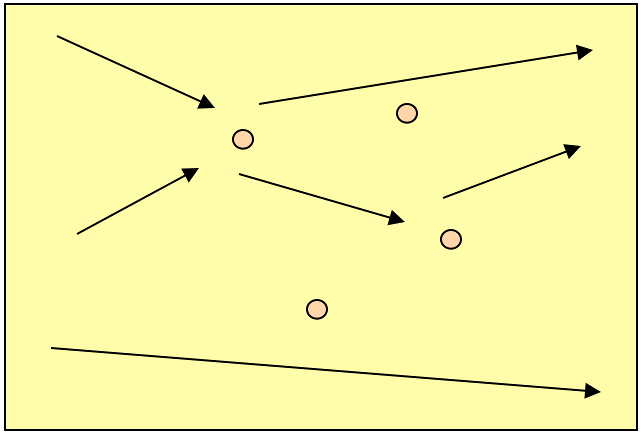
The scattering problem: why bother?

The impurity scattering cross-section can be of the same order of the wire diameter → serious limitation of the conductive performances

We cannot neglect backscattering (actually we expect it to take place!)

Simplified pictorial view: nano 1D vs bulk 3D





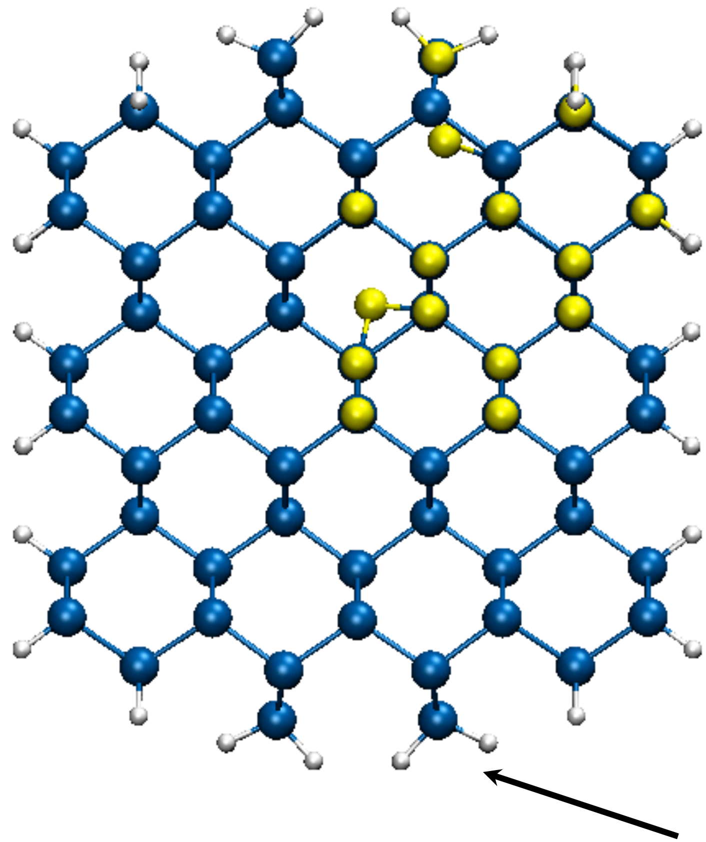
Theoretical framework

First-principles DFT calculations
SIESTA code www.icmab.es/siesta

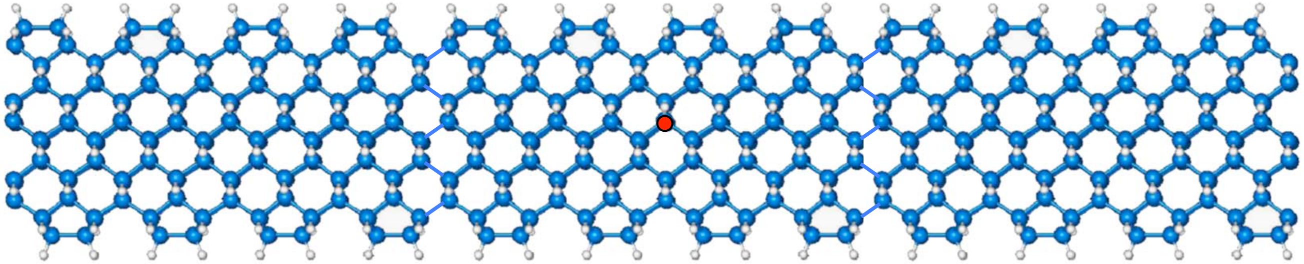
Calculated quantities:
- Optimized geometry
- Band structure
- Wave function localization

Conductance
Ballistic transmission within Landauer theory

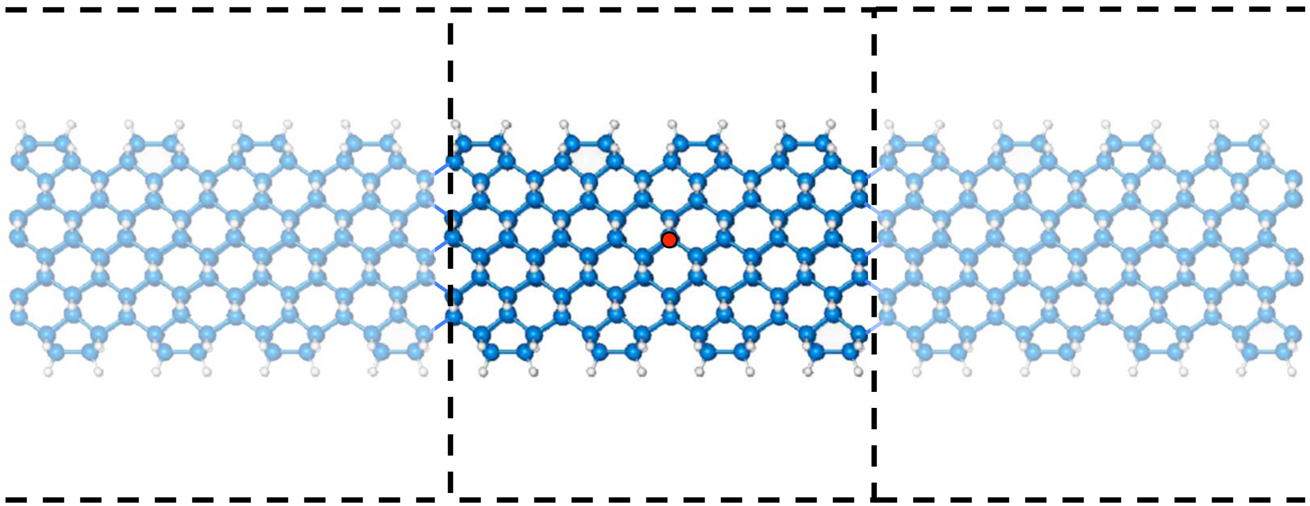
Atomistic description of the NW and its impurities



Theoretical framework



Theoretical framework

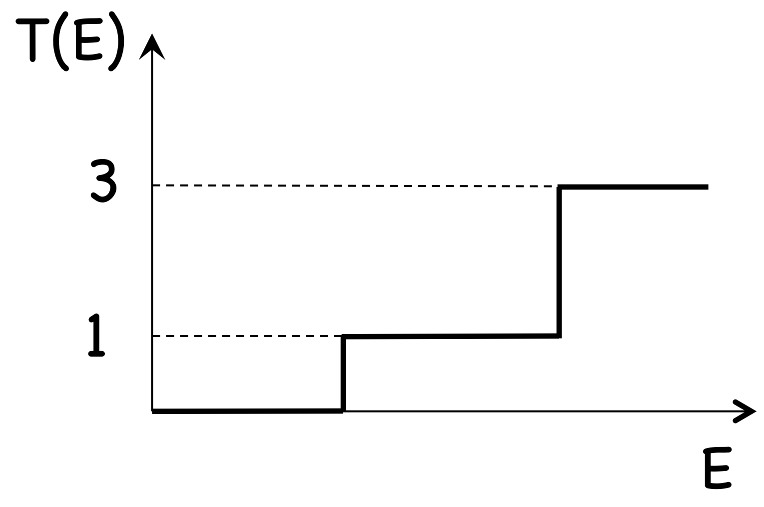


Theoretical framework

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

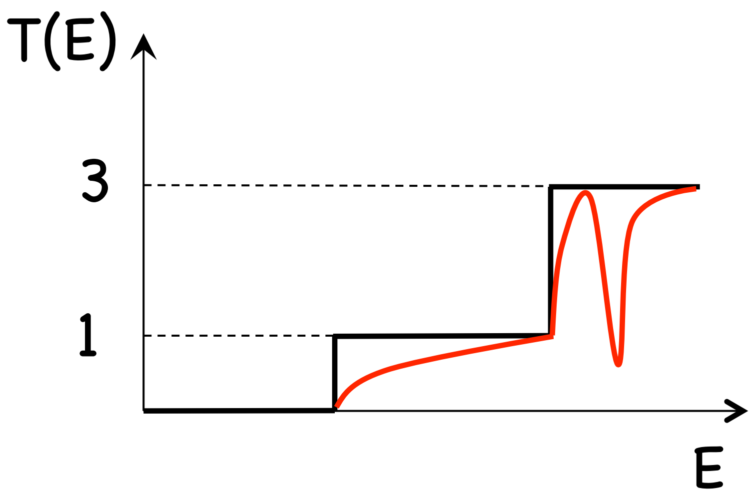


Theoretical framework

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

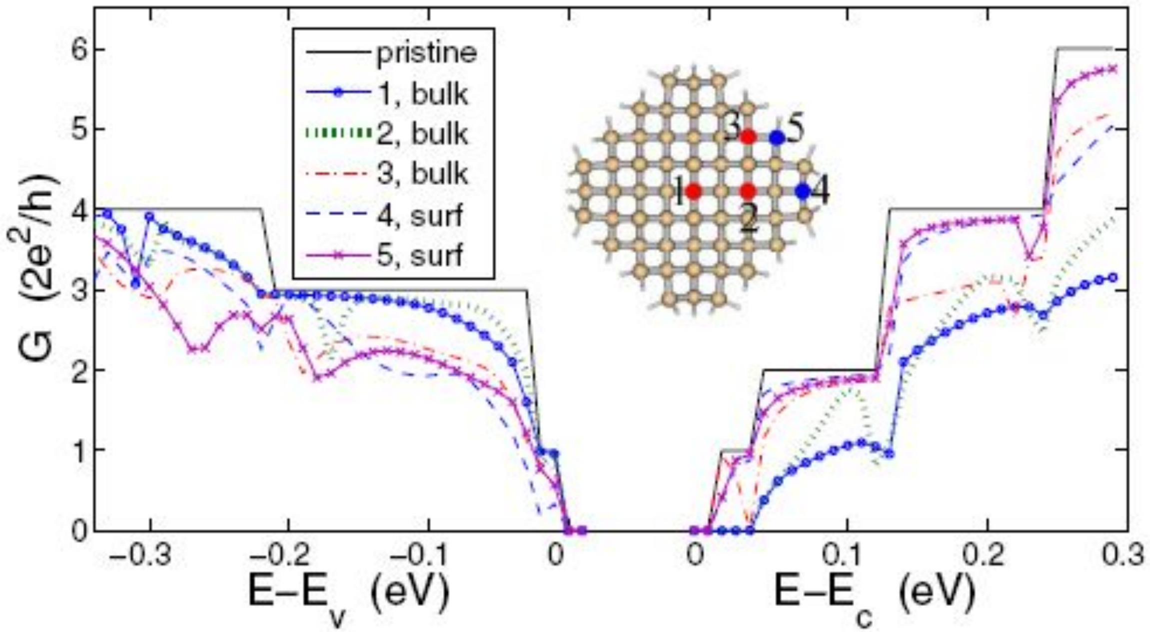
How many?
For an infinitely long NW: as many as electron states at that energy

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



Single-impurity scattering

The physical origin of dopant scattering related variability: lattice sites are no longer radially equivalent (as they were in bulk)



Impurities at different lattice (or interstitial) sites, **scatter differently**

M. V. Fernández-Serra, Ch. Adessi, and X. Blase, *Phys. Rev. Lett.* **96**, 166805 (2006)

M. V. Fernández-Serra, Ch. Adessi, and X. Blase, *Nano Lett.* **6**, 2674 (2006)

T. Markussen, R. Rurali, A.-P. Jauho, and M. Brandbyge, *Phys. Rev. Lett.* **99**, 076803 (2007)

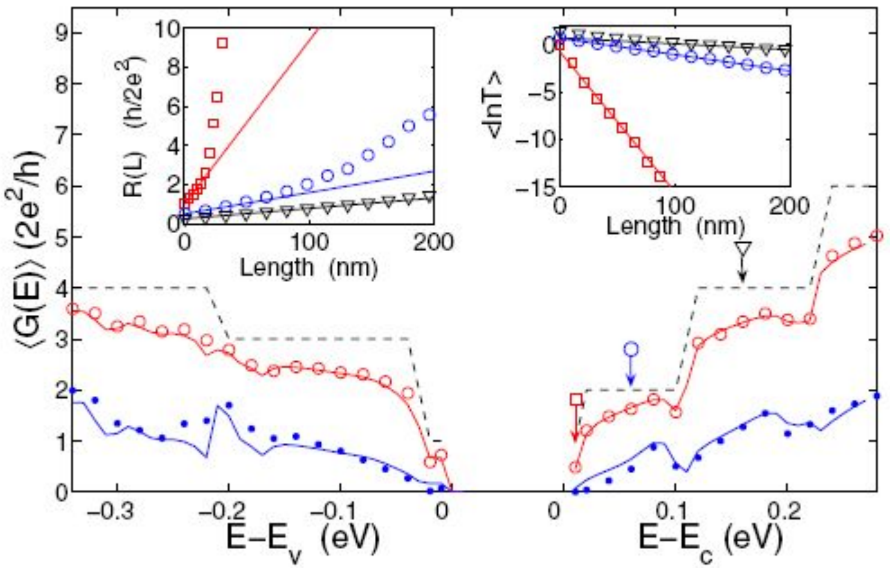
Single-impurity scattering

Real nanowires contain several dopants and, because of interference effects between successive scattering events, it is not obvious if the single-dopant results carry over to the long wire case (with many impurities present)

How much can we know from separate single-impurity calculation? **Is some kind of averaging meaningful at all?**

Multi-impurity scattering

The T(E) of a long wire with a **distributions** of defects can be entirely predicted on the basis of single-impurity calculations



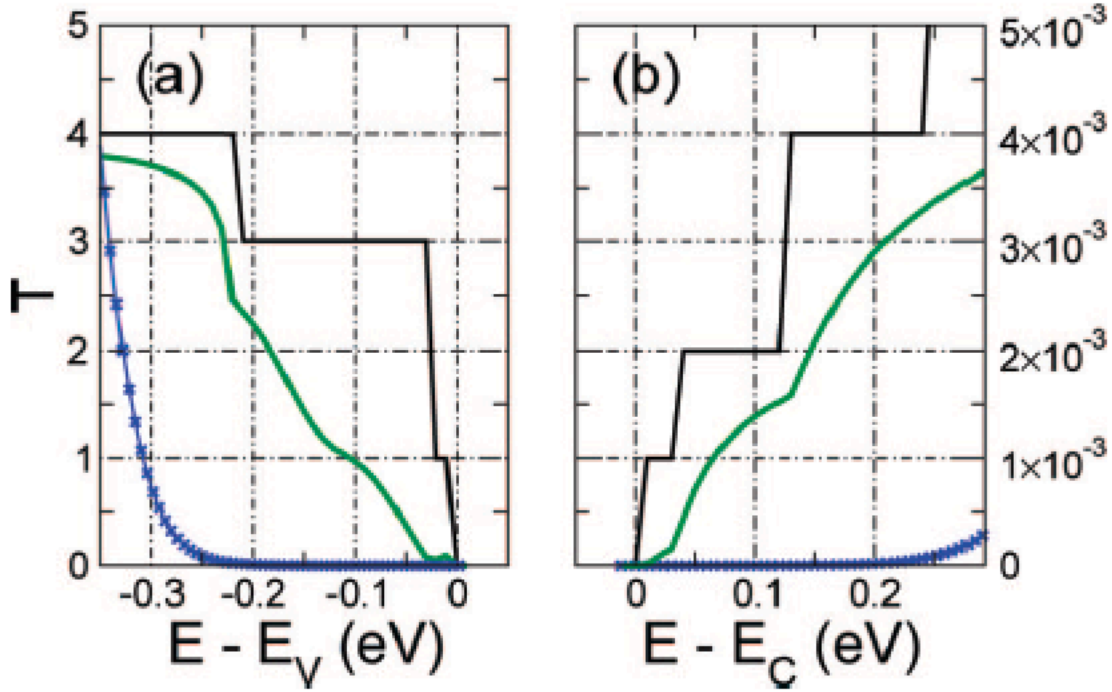
- Solid lines( ): averaging following: $\langle R(L,E)\rangle = R_C(E) + \langle R_S(E)\rangle\ L/d$
- Symbols ( ): long-wire calculation

Tackling long wires allows extracting experimentally relevant quantities such as the mean free paths of or resistance vs length curves

T. Markussen, R. Rurali, A.-P. Jauho, and M. Brandbyge, *Phys. Rev. Lett.* **99**, 076803 (2007)

(Charged impurity scattering)

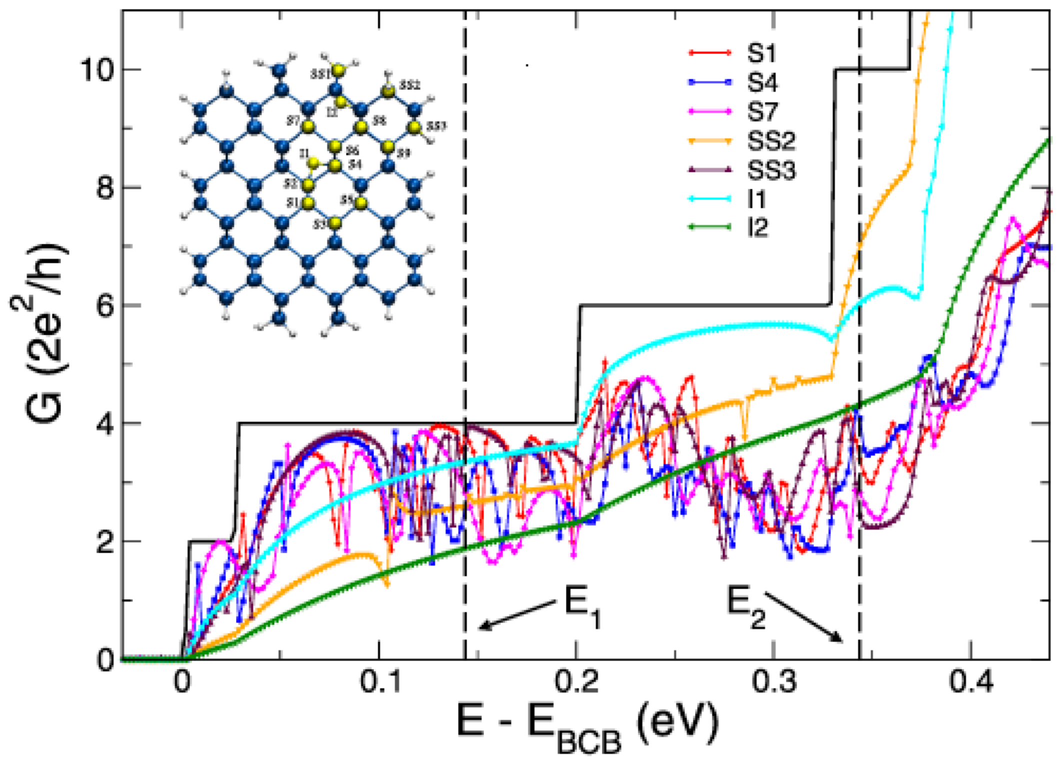
A parenthesis on **impurity charge state**: it must be taken into account for quantitative estimates, especially for minority carriers



R. Rurali, T. Markussen, J. Suñé, M. Brandbyge, and A.-P. Jauho, *Nano. Lett.* **8**, 2825(2008)

Impurity scattering induced variability

We carried out a systematic study of single-dopant (P) scattering in a [111] Si nanowire, sampling substitutionals and interstitials



The expected strong variability of the resistance associated to each kind of impurity is evident in this figure

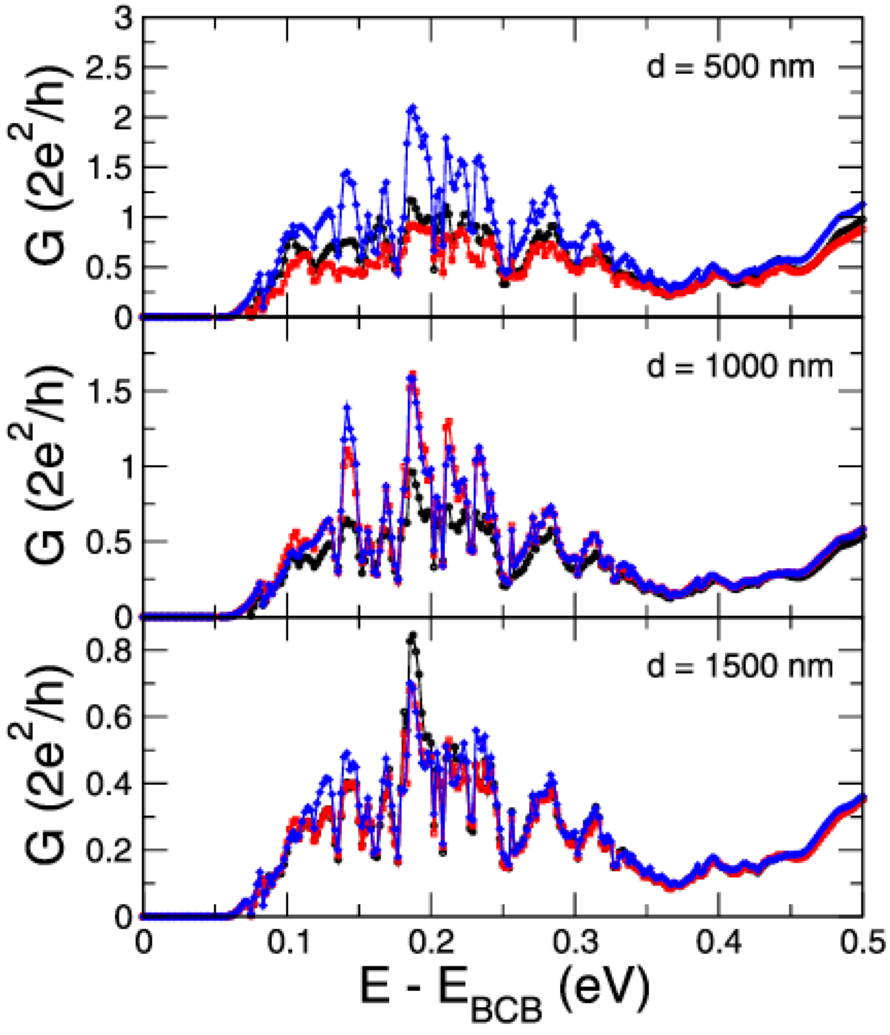
The stronger scattering center is an interstitial defect

F. Iori, S. Ossicini, and R. Rurali, *J. Appl. Phys.* **116**, 074303 (2014)

Impurity scattering induced variability

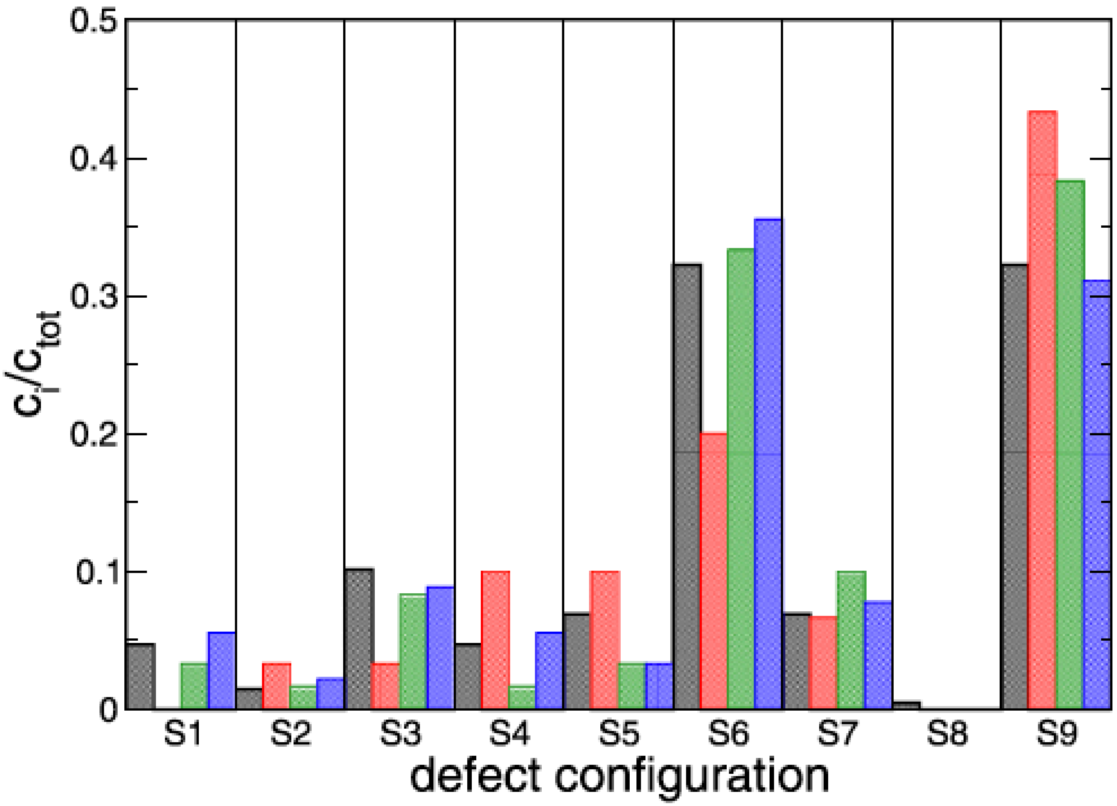
- We created random distribution of defects, the probability of occurrence of each defect is weighted with its formation energy
  - ✓ This guarantees that the equilibrium concentration is correct
- We calculated the Landauer conductance by classically adding up the resistance associated to each individual scattering event

$$R(L,E) = R_c(E) + \sum_{i=0}^{L/d} R_s^i(E)$$



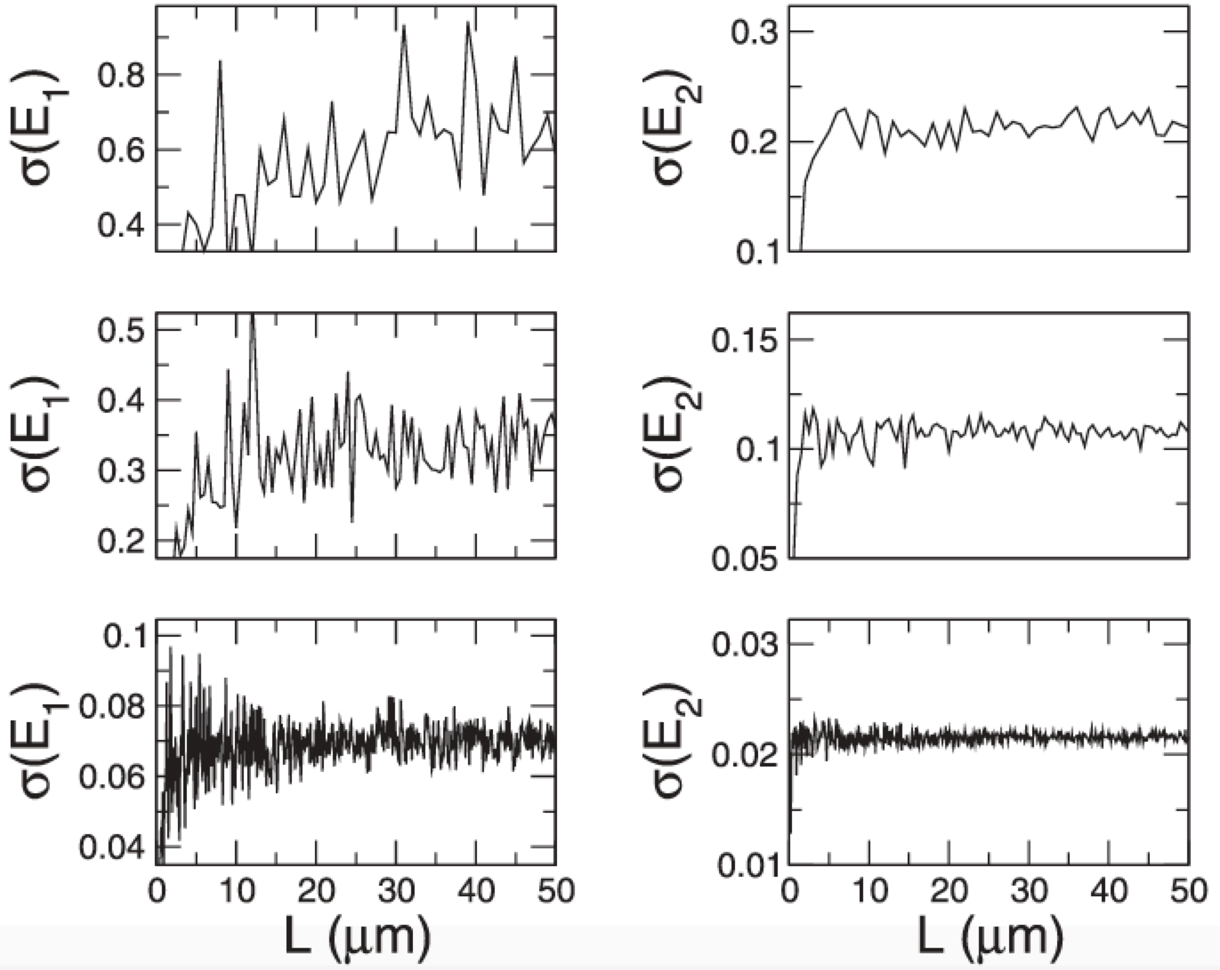
Impurity scattering induced variability

Expected equilibrium concentration of the nine substitutionals (black column), with the **mean concentration** (averaging over three realizations) of the 0.5, 1.0, and 1.5 lm nanowires (red, green, and blue column).



As a general rule, <u>the shorter the wire, the larger the deviation</u> from the expected concentration

Impurity scattering induced variability



Conductivity at selected energies as a function of wire length for increasing dopant concentration ($5 \cdot 10^{20}$, 10^{20}, $5 \cdot 10^{21}$ cm^{-3})

Conclusions

- You need to add impurity to dope the NW, i.e. give it a controlled conductivity

- Dopants induce scattering

- To have some average properties, the NW has to be longer than some minimal length L_{min}

- NW longer than L_{min} will not be in the ballistic regime

IF YOU WANT A DOPED NW IN THE BALLISTIC REGIME (OR SIMPLY *SHORT*) YOU HAVE TO LIVE WITH THE INTRNISC VARIABILTY RELATED TO DOPANT SCATTERING

Conclusions

Want to know more??? rrurali@icmab.es

This work

F. Iori, S. Ossicini, and R. Rurali, J. Appl. Phys. **116**, 074303 (2014)

related

Markussen *et al.*, Phys. Rev. Lett. **99**, 076803 (2007)

Rurali *et al.*, Nano. Lett. **8**, 2825(2008)

Review papers on NWs

R. Rurali, Rev. Mod. Phys. **82**, 427 (2010)

M. Amato, M. Palummo, R. Rurali, and S. Ossicini, Chem. Rev. **114**, 1371 (2014)