CNR-IMM
Laboratorio MDM

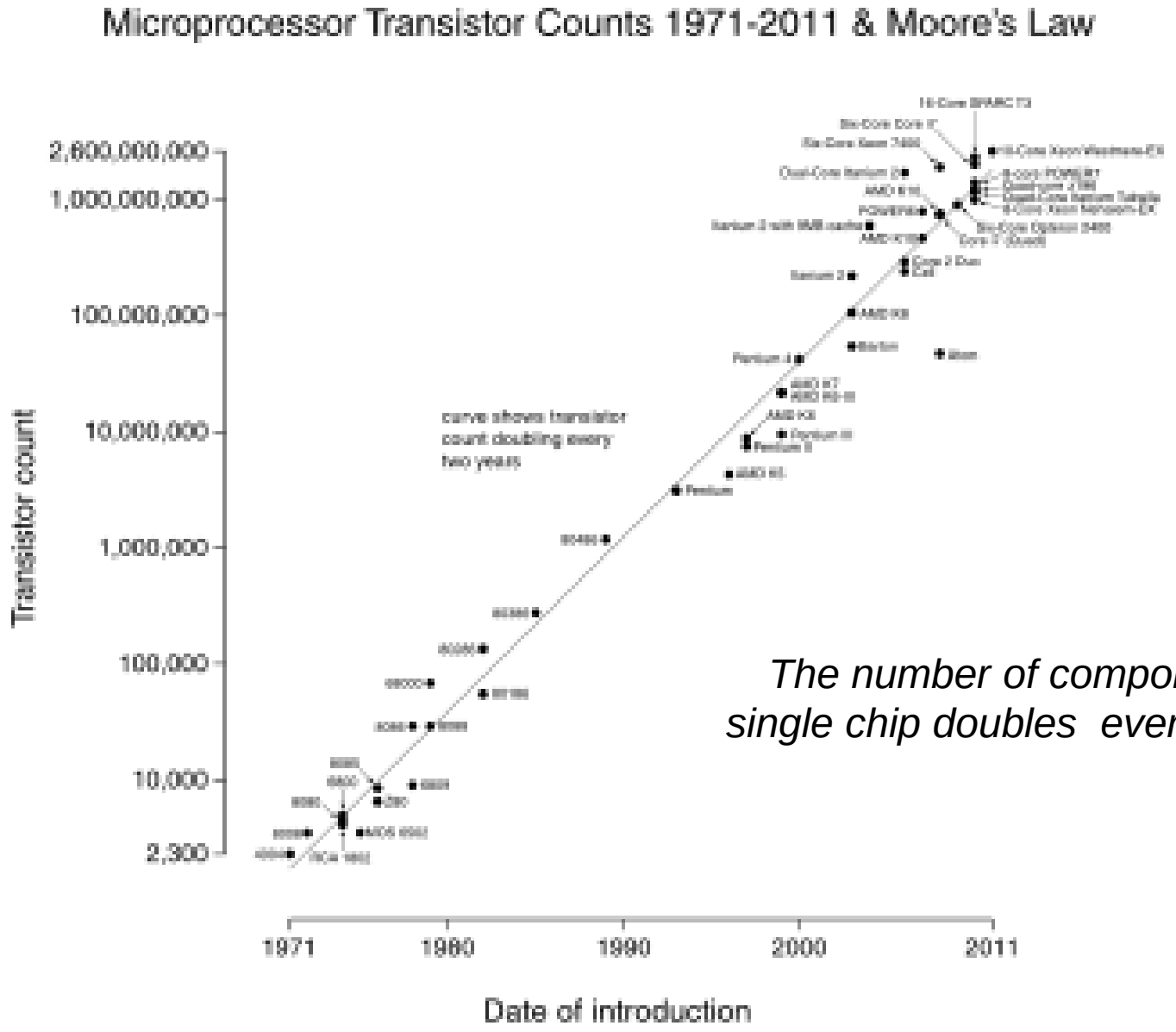
Nanostrutture a base di Si e Ge per nuovi dispositivi nano-elettronici

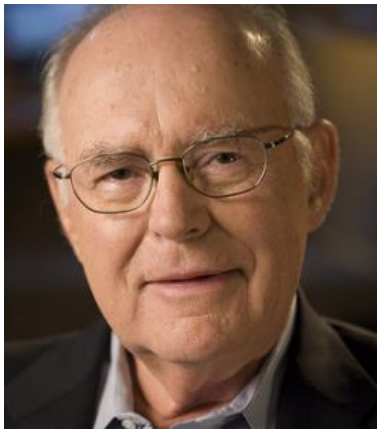
Alberto Debernardi
Laboratorio MDM, IMM-CNR
Agrate Brianza (Italy) – www.mdm.imm.cnr.it

Plan of the talk

- Scaling down electronic devices (Moore's law)
- P or Se doped Si-nanowires for quantum computing
- Delocalization of P(Se) wave-function Si NW [001], [011], [111] oriented
- Ab initio spectroscopy (Hyperfine parameters, MOKE)
- Conclusion and Discussion

Scaling down of CMOS logic devices

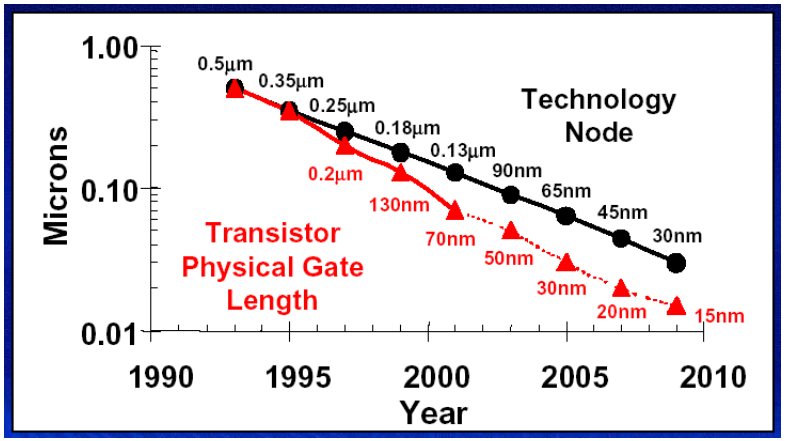




Moore's law

The number of components in a single chip doubles every 18 months

Scaling down of CMOS logic devices



INTEL Presentation SPIE 03/2003

La dimensione dei chip si riduce constantemente …

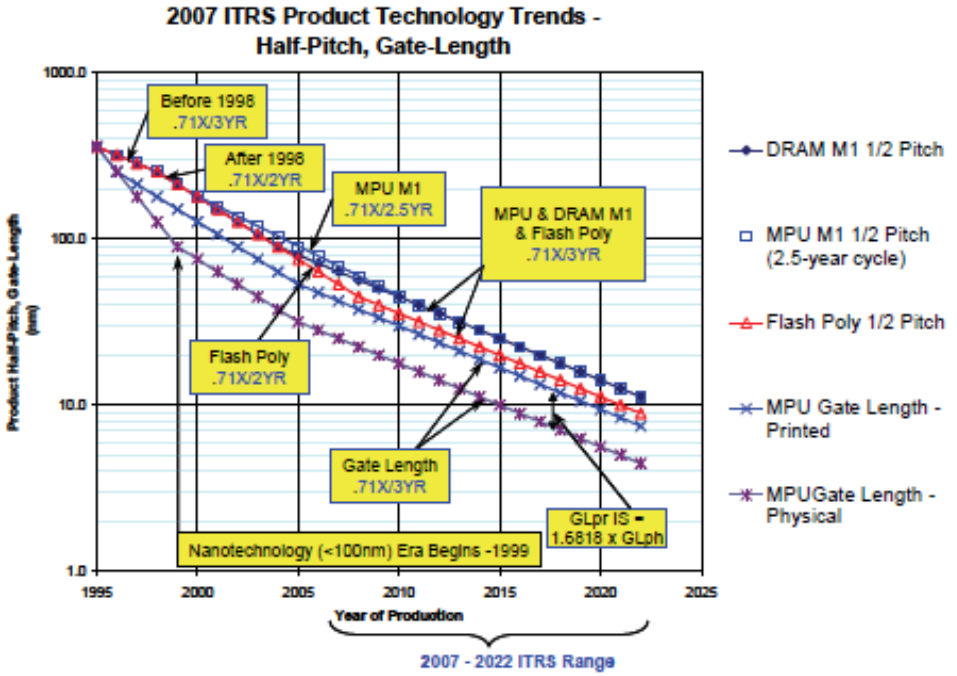
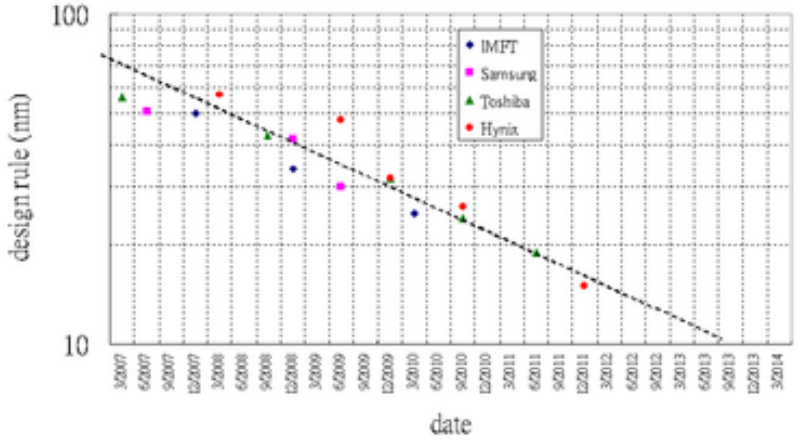


Figure 7 2007 ITRS—Half Pitch and Gate Length Trends

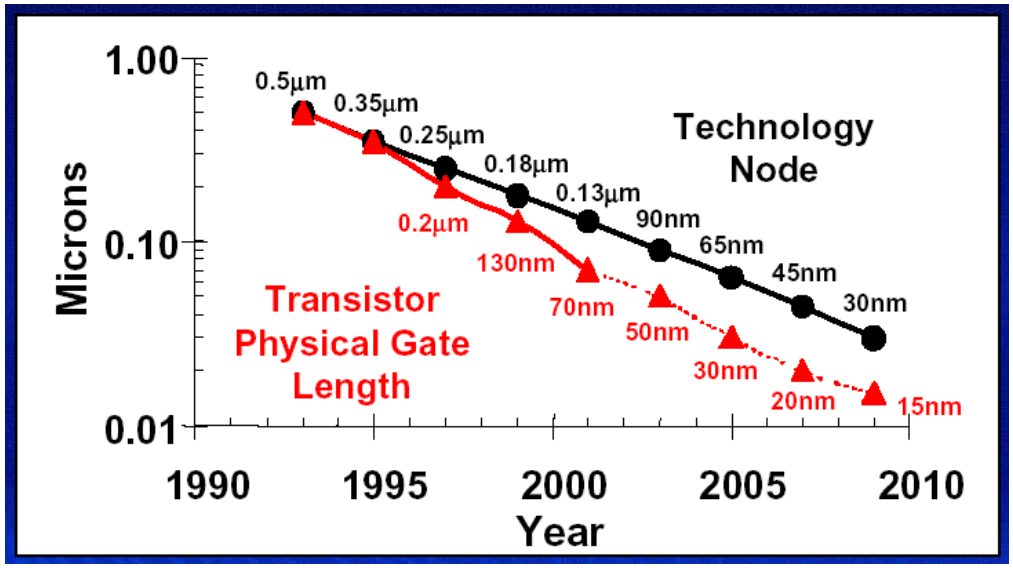


International Technology Roadmap for Semiconductors (ITRS)

http://www.itrs.net/

… fino a raggiungere le dimensioni atomiche ?!

Scaling down of electronic devices



Moore's law

Nanodevices whose size is a few nanometers

Quantum effect are relevant➔ first principles simulations techniques

Three strategies

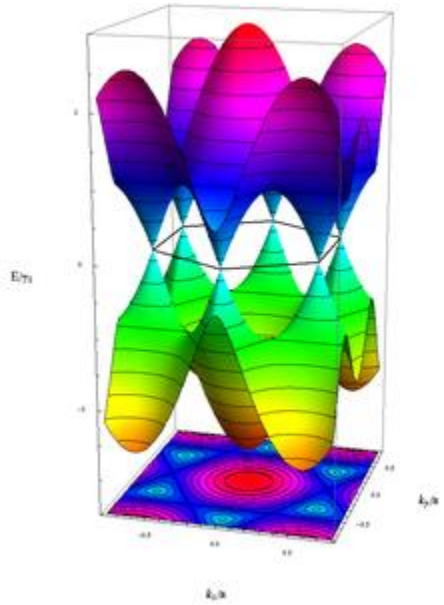
Ultra-scaled CMOS devices

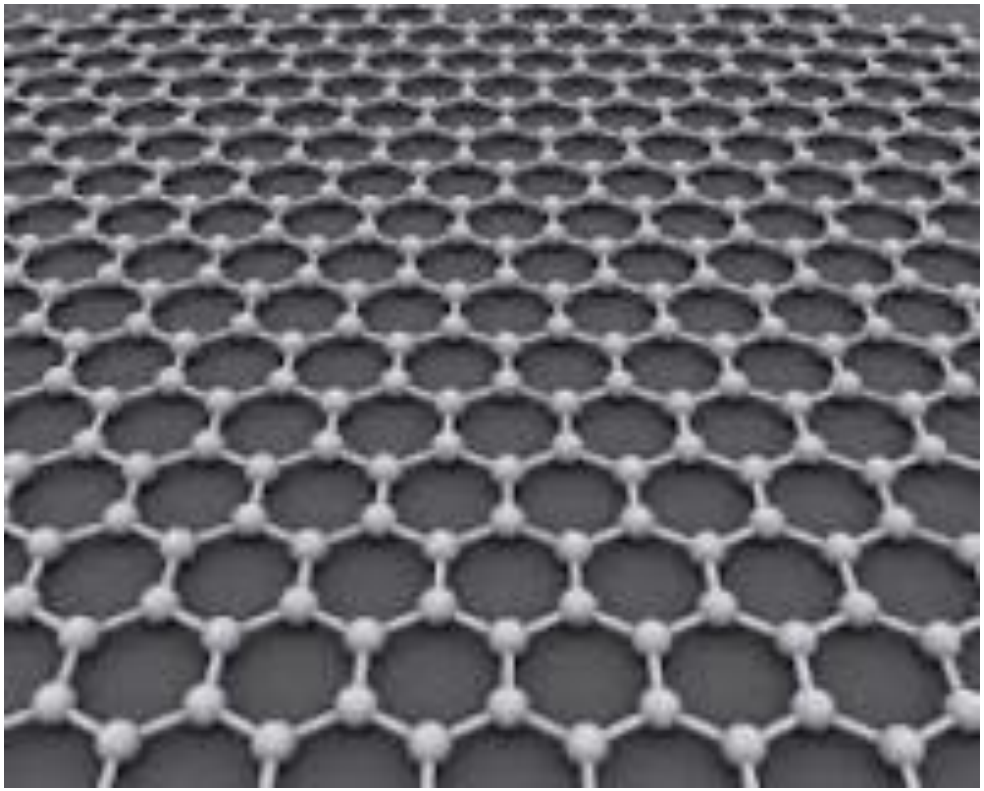
Nano structures as building block of novel device

More than Moore, new concept for ultra-scaled devices

Il nuovo mondo bidimensionale

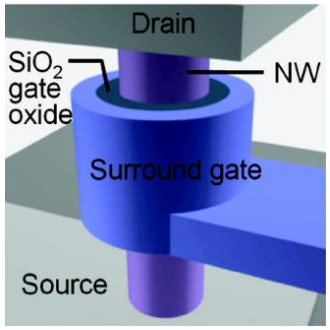
- Grafene (C)
- Silicene (Si)
- Germanene (Ge)
- Stanene (Sn)



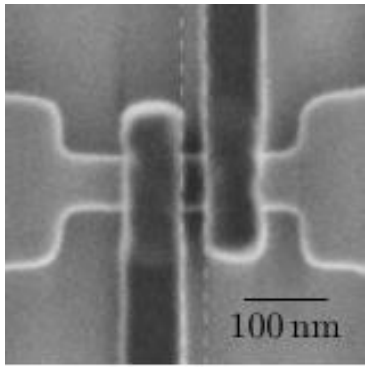


Dispositivi ultra-veloci
Nuovi Sensori
Nuova elettronica

Si-Nanostructures Applications



Ultra-scaled electronic devices



Gate controlled quantum dot

Quantum computation

Photovoltaics

Nanosensors (DNA, ...)

- What are the limits of Conventional computing ?

Density Functional Theory

For a give external potential

$$v\left(\vec{r}\right) \rightarrow E[n]$$

Target:
to compute the total energy

Total energy is a unique functional of the density

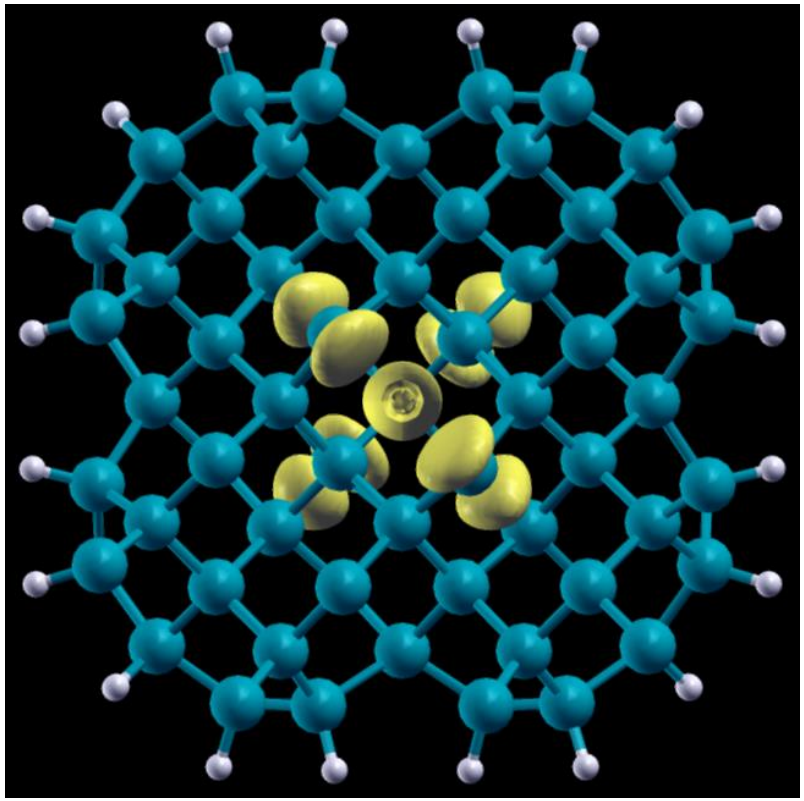
Plane-waves pseudo-potential techniques

$$E[n] = \sum \varepsilon_{\mathrm{v}} - \frac{1}{2}\int \frac{n\left(\vec{r}\right)n\left(\vec{r'}\right)}{\left|\vec{r} - \vec{r'}\right|} d\vec{r}\,d\vec{r'} + E_{\mathrm{xc}}[n] - \int v\left(\vec{r}\right)n\left(\vec{r}\right)d\vec{r}$$

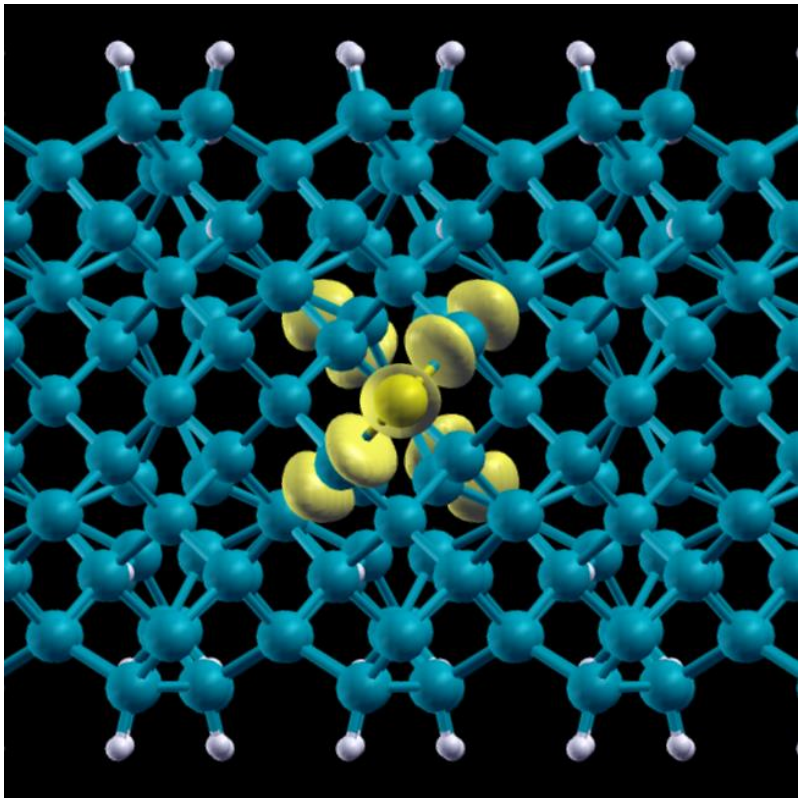
Ab initio: Simulazioni senza alcun parametro sperimentale !!!

Single atom electronics: Se impurity

Se doped H passivated Si nanowires
(nanoelectronics, quantum computer)

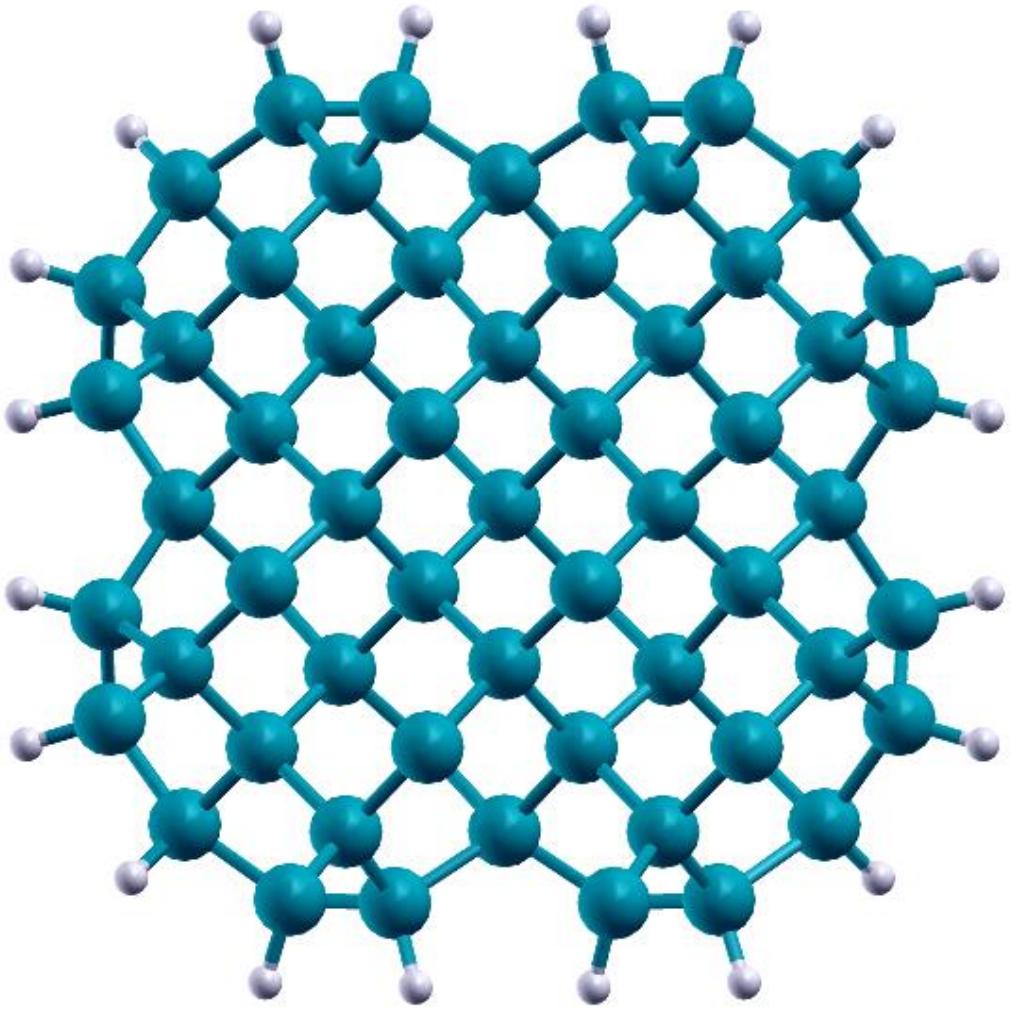


front view



side view

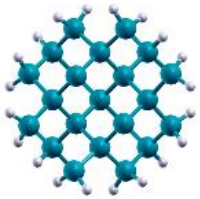
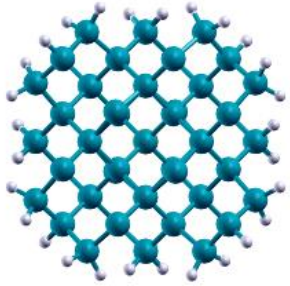
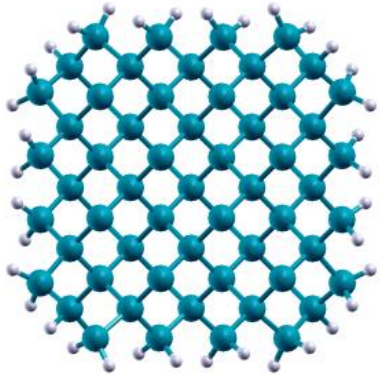
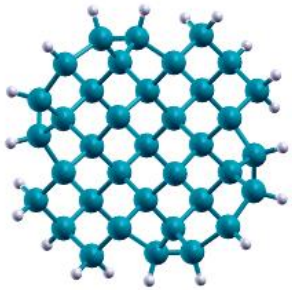
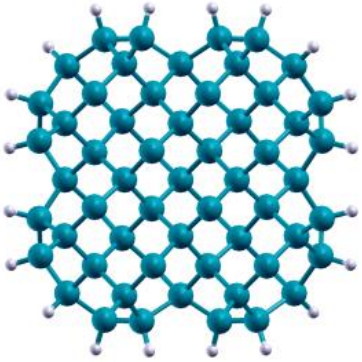
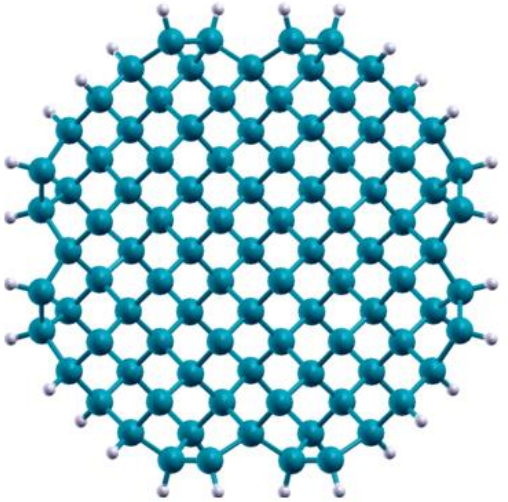
Nanowire passivation



H passivated Si nanowires

d≃0.8 nm d≃1.2 nm d≃1.5 nm d≃2 nm

Relaxed – Passivated and Relaxed again Distortion of NW for smal size is significant.

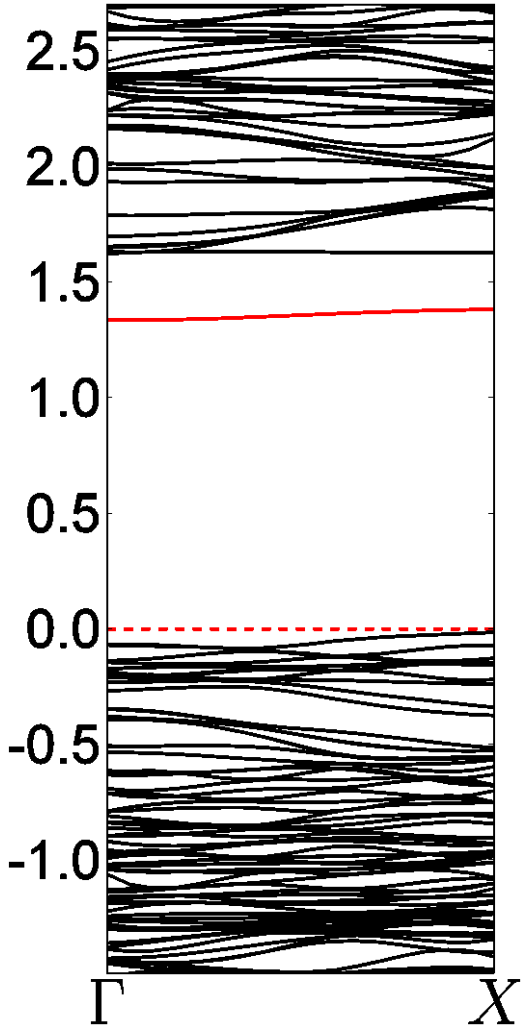







Passivated and relaxed

Se doped Si nanowires

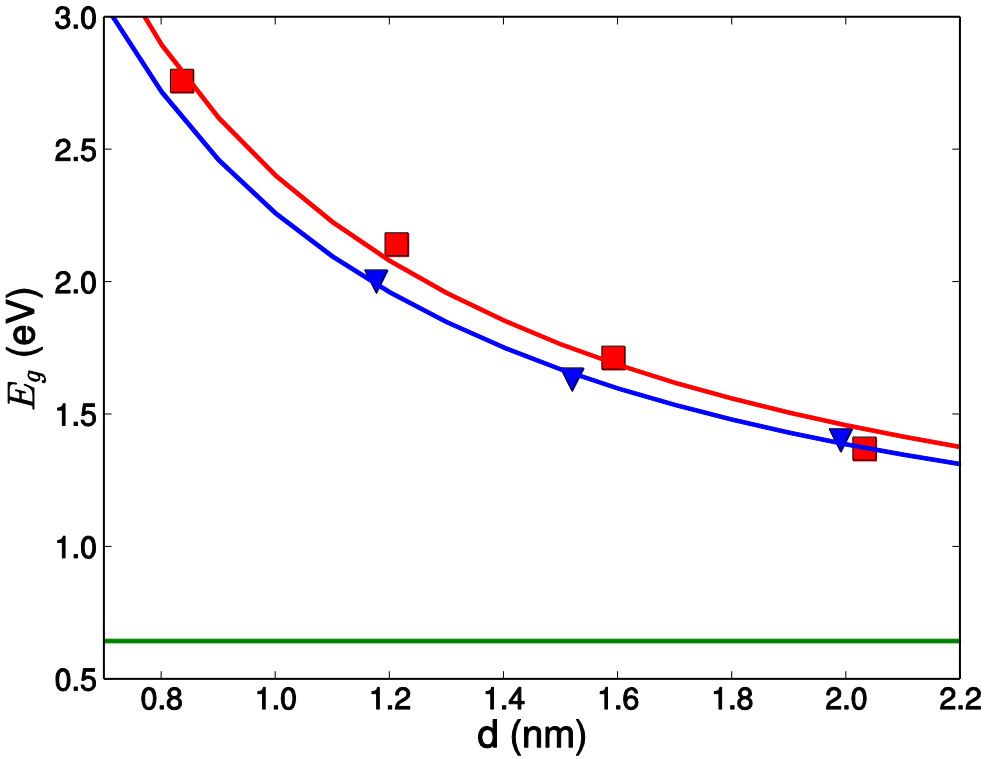
- One dimensional bandstructure
- Impurity level in the bandgap

- Correction to periodically repeated charged imeges (Rurali et al, Makov-Payne)



Band-gap of Si nano-wire

Band-gap as a function of NW diameter



- Trangles: NW with surface reconstruction
- Squares: NW without surface reconstruction

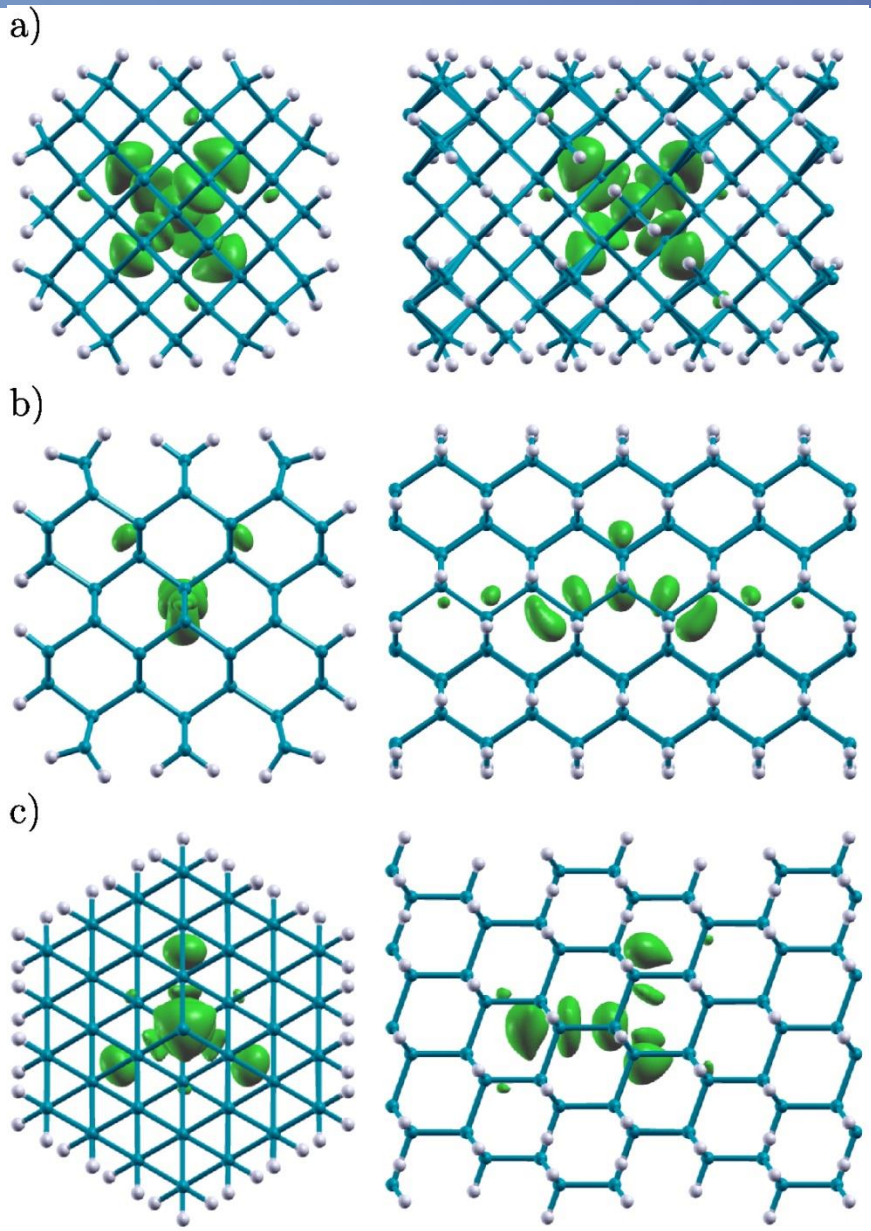
As an effect of confinemente the Bandgap increases as the diameter is reduced

Delocalization of donor wave-funnction

[001]

[011]

[111]



- Three orientations considered
- Diameter: 1.2-1.3 nm
- passivated→relaxed

Delocalization of donor wave-funnction

$$a_z \equiv \langle \Psi | \sqrt{z^2} | \Psi \rangle$$

[001]

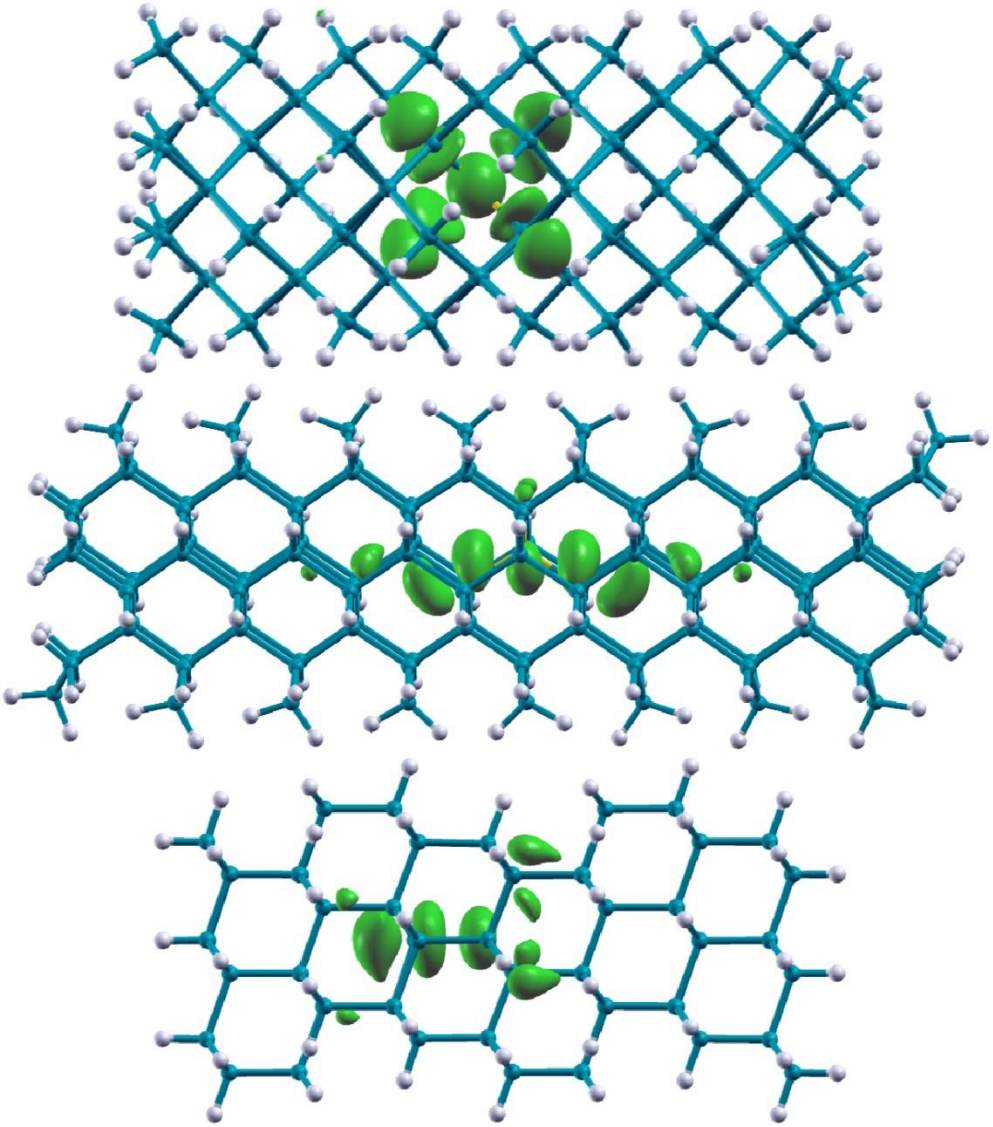
$$a_z = \int \|\Psi(x,y,z)\|^2 \sqrt{z^2} dxdydx$$

[011]

LUMO of ionized system (Niquet et al, 2010).

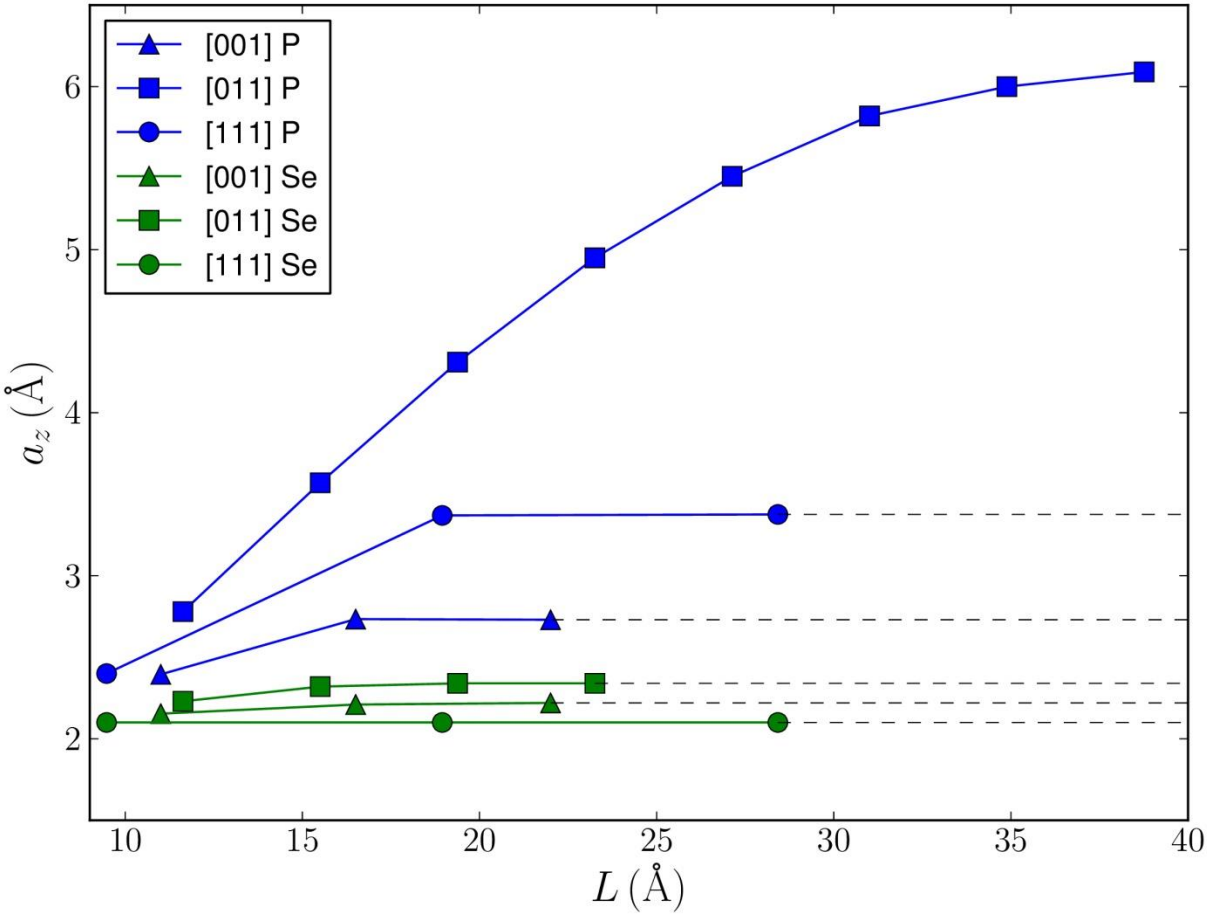
But HOMO of neutral system gives the same qualitative results

[111]



Delocalization of donor wave-function

- The a_z of Se wave-function is computed
- The a_z of Se wave-function for [011] should be extrapolated

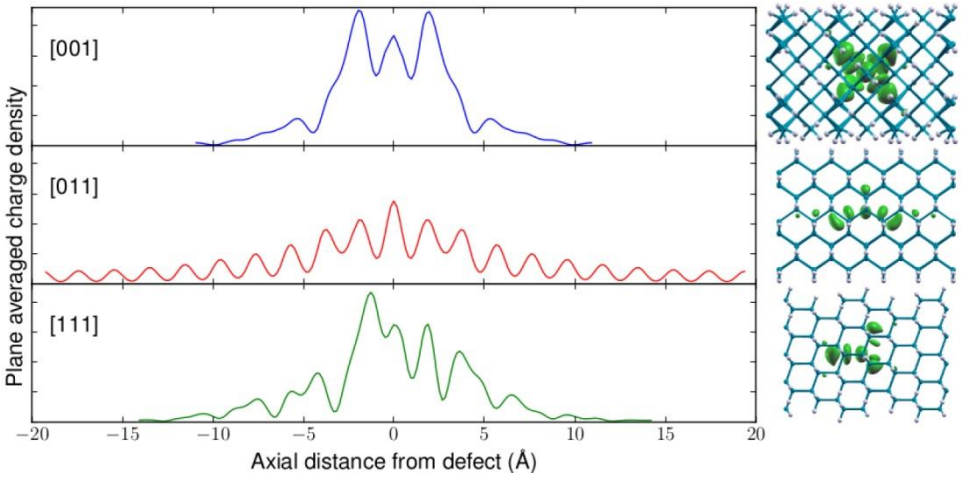


$$f(z, L) = e^{-z^2/a} + c$$

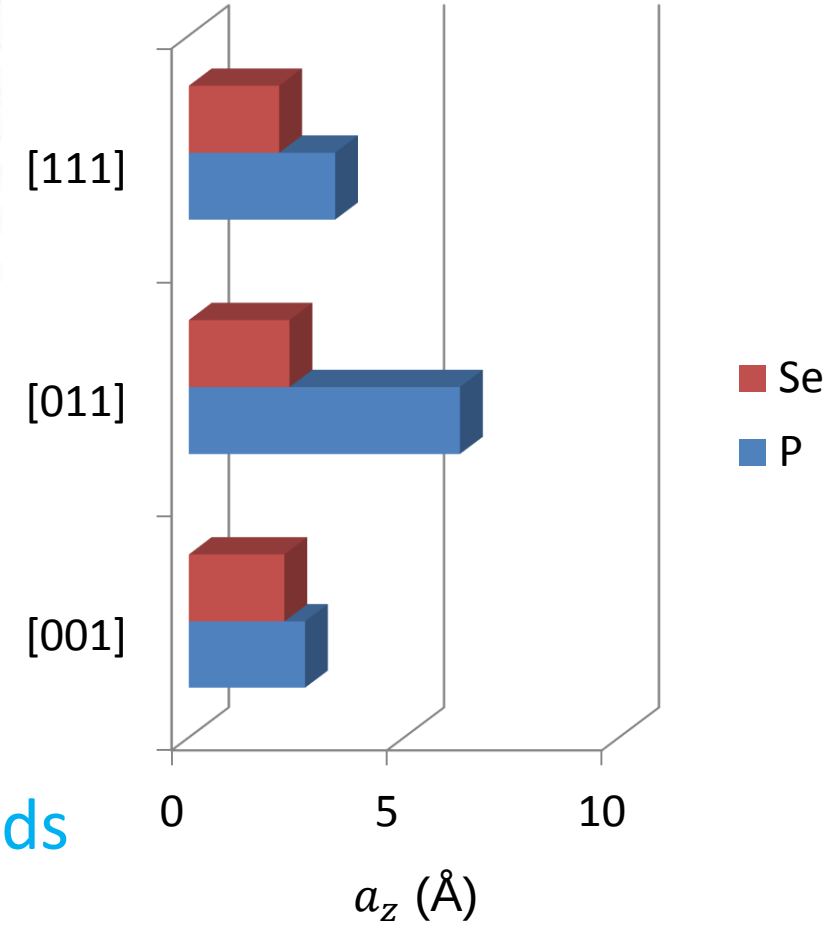
Delocalization of donor wave-function

The large delocalization of P wave-function along [011] direction …

$Si{:}\,P\ bulk \quad a_z \sim 25$ Å



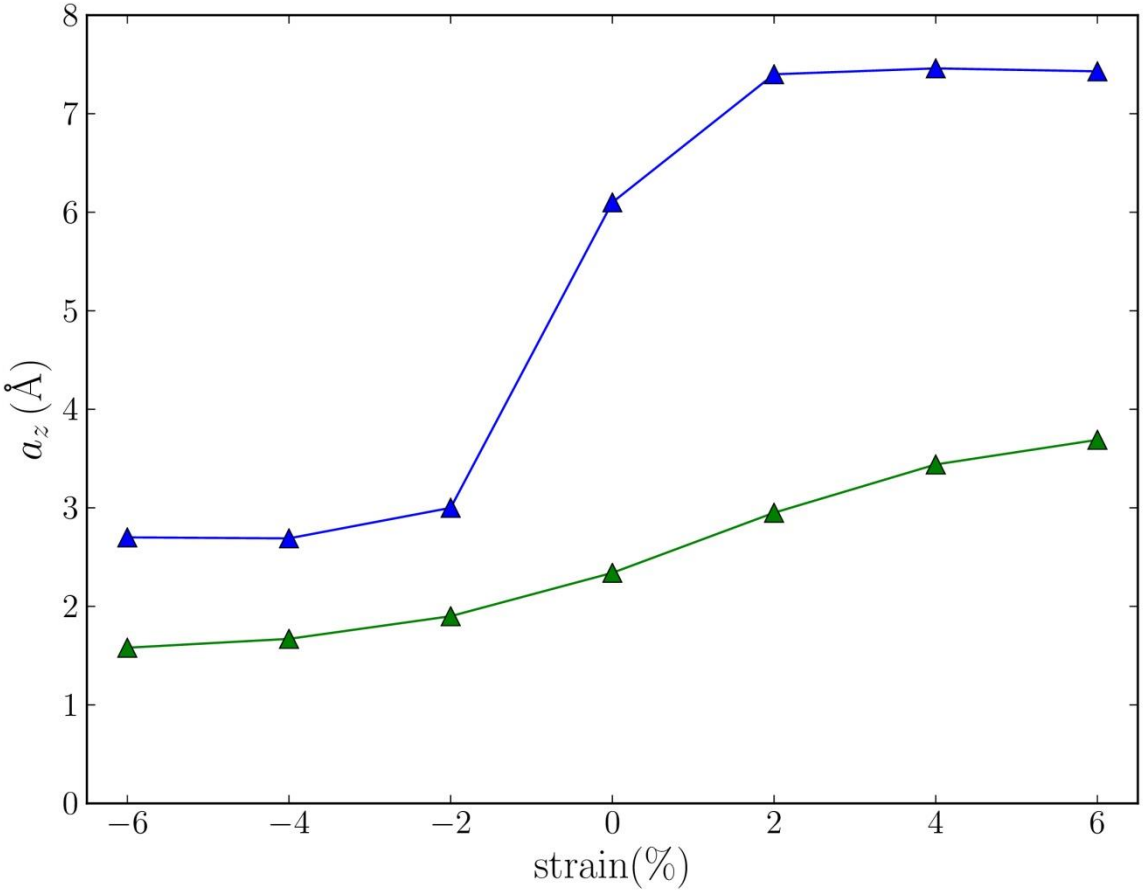
$$a_z^{[001]} < a_z^{[111]} < a_z^{[011]}$$



….we suggest it is a general tends

Strain along the NW axis

- The a_z of Se: non linear dependence of the strain
- The a_z of P: strong dependence

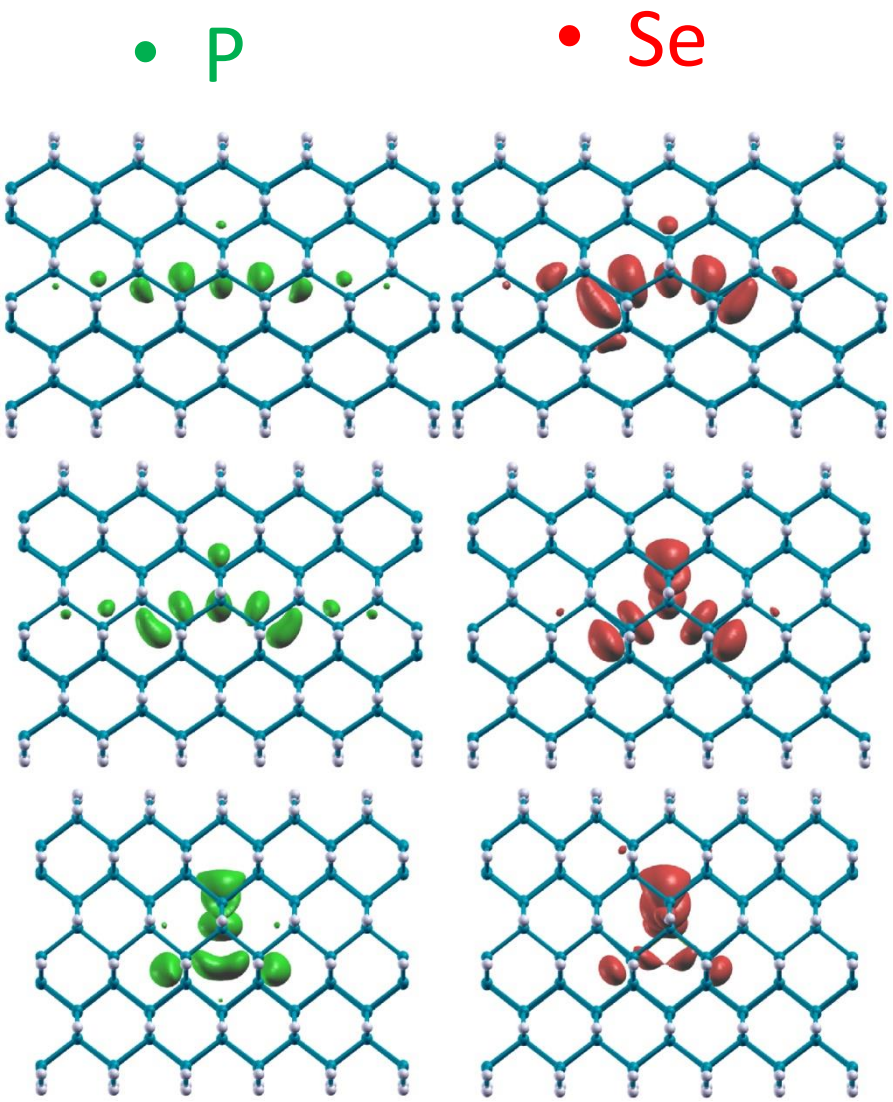


Modification of shallow wave-function by strain

Strain along the NW axis

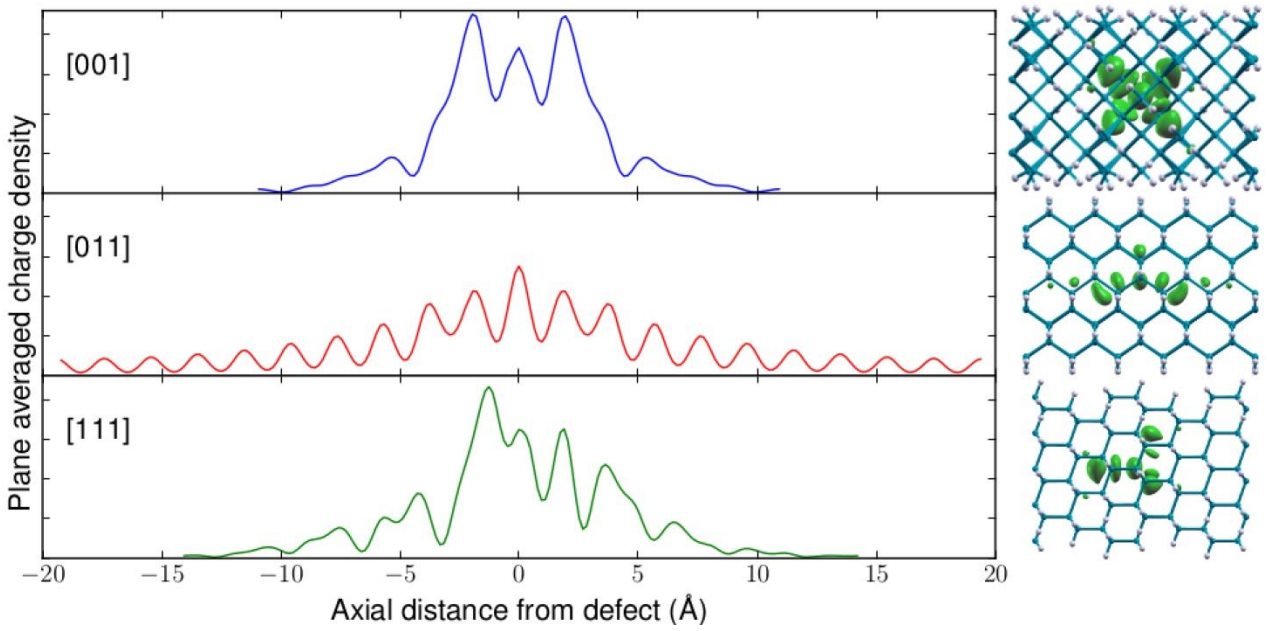
Quantum computing

The interaction between neighbour P can be tuned by piezoelectrical actuators



Conclusions

- **The [011] is the best direction for nano-electronic and quantum computing applications**
- **Stress allow to tune delocalization**

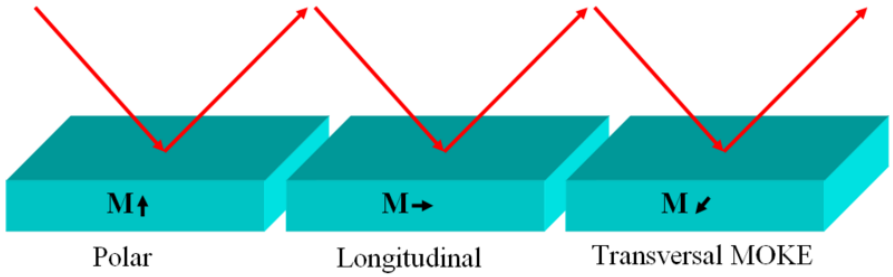


Ab initio spectroscopy

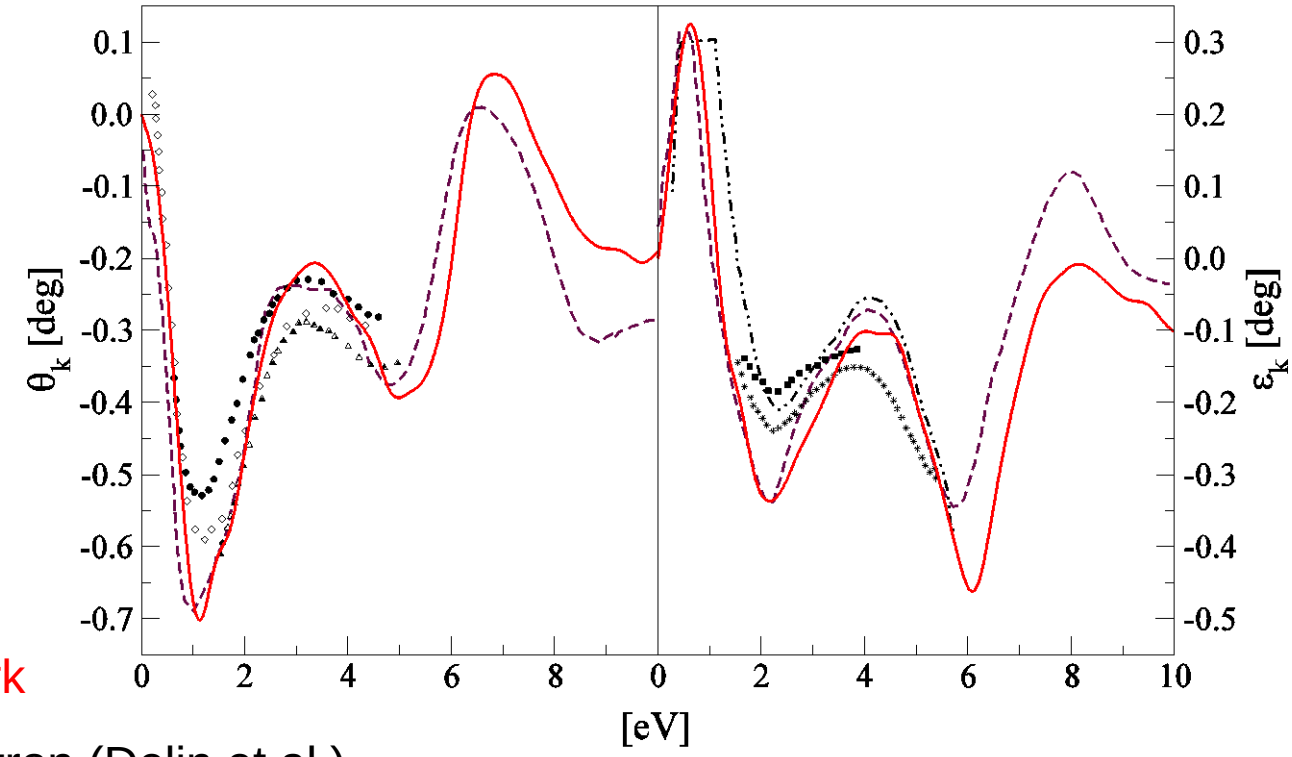
Interazione luce-materia
predizioni senza parametri aggiustabili

- Permette l'analisi dei dati sperimantali
- Individua i meccanismi microscopici responsabili di una data proprietà
- Predice quali sono le condizioni ottimali per ottenere un dato fenomeno
- E' più economica di un «vero» esperimento

Ab initio spectroscopy: MOKE



- MOKE spectra by plane-wave pseudopotential techniques
- Simulation of relatively large systems



----- our work

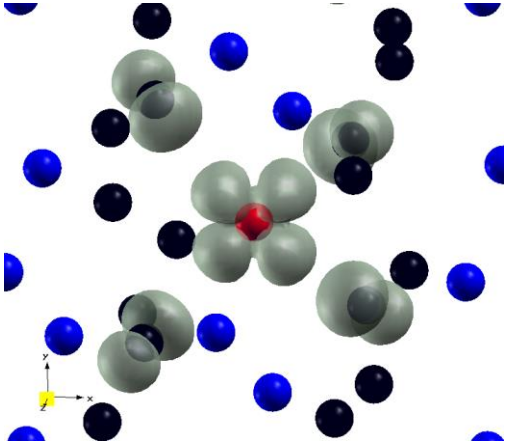
----- all electron (Delin et al.)

**** experiment

Bulk Fe

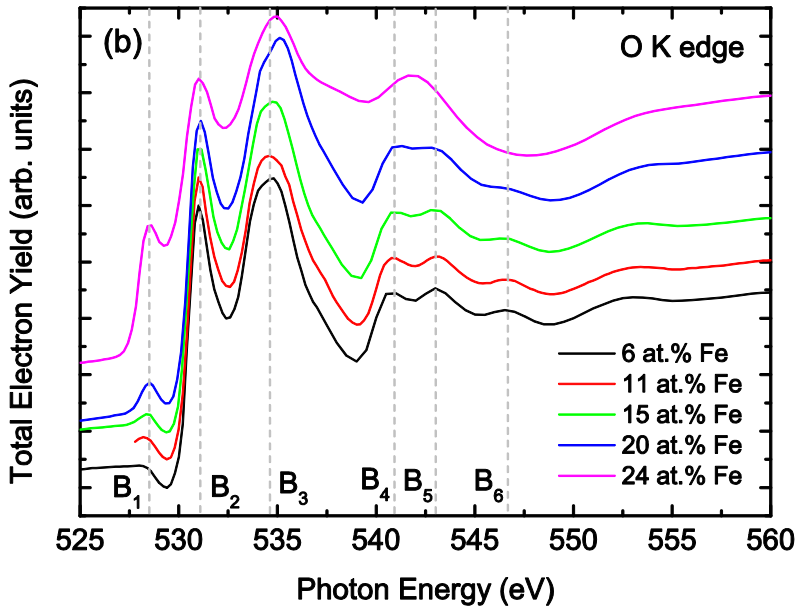
Ab initio spectroscopy: XAS

Interazione luce-materia, predizioni senza parametri aggiustabili

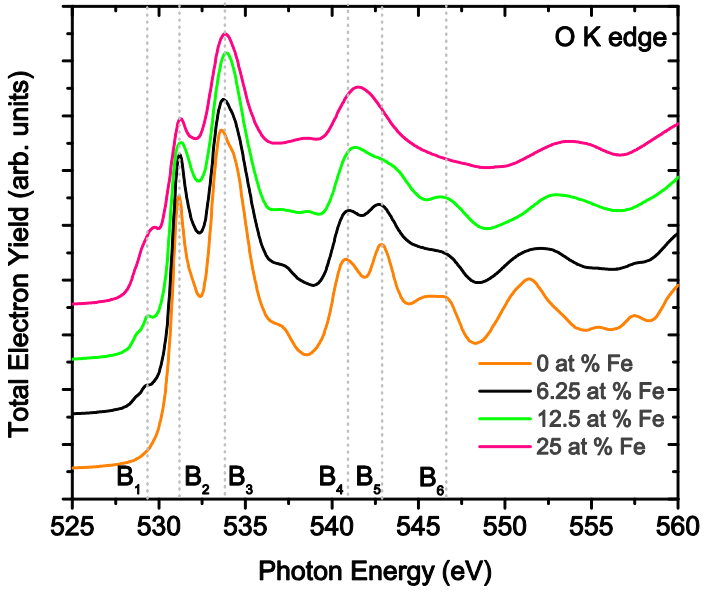


ZrO2:Fe Diluted Magnetic Oxide for spintronic applications (film di 29 nm)

Esperimento



Teoria

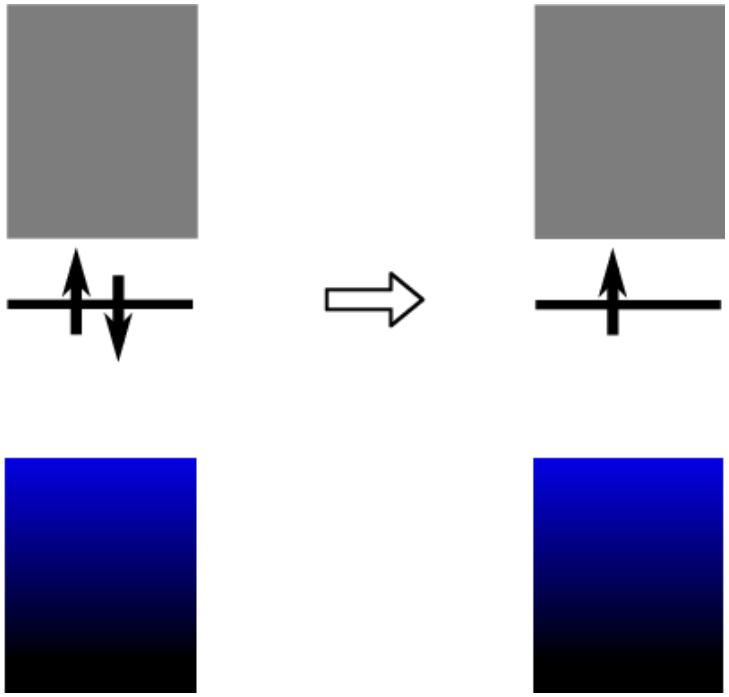


Hyperfine coupling constant: Charged defects

Hyperfine interaction requires a spin density≠0

Ionization of the impurity

$$\overleftrightarrow{A} = A_{iso}\,\overset{\leftrightarrow}{1} + \overleftrightarrow{A}_{dip}$$

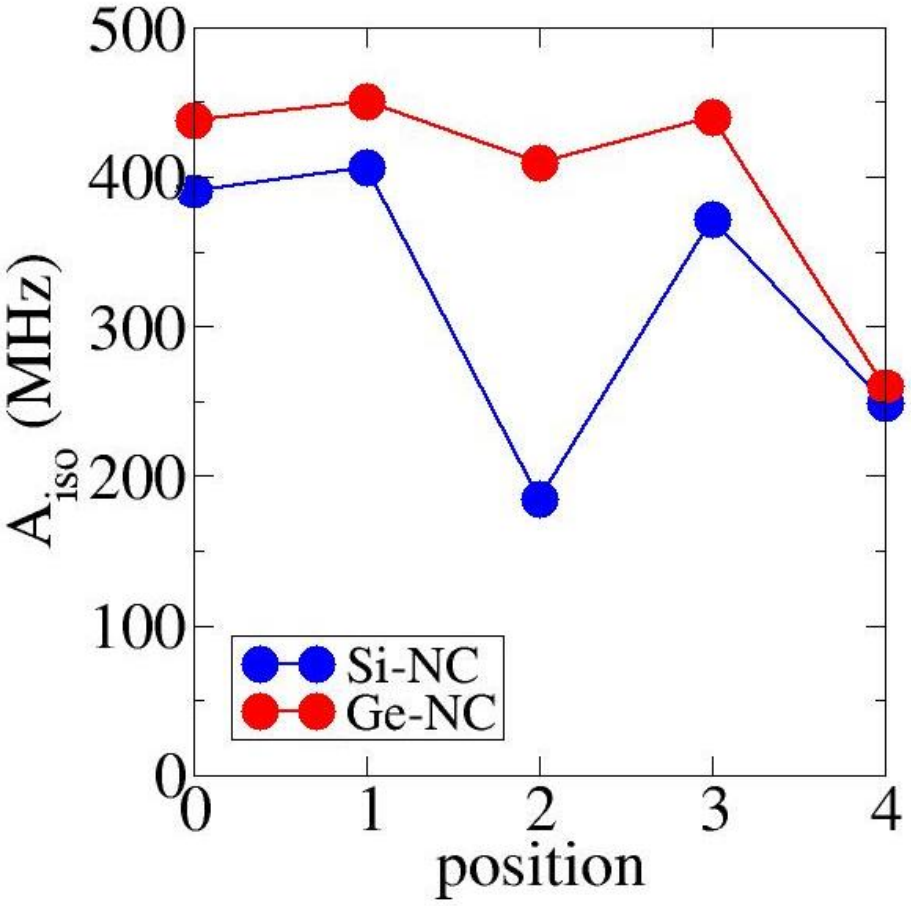


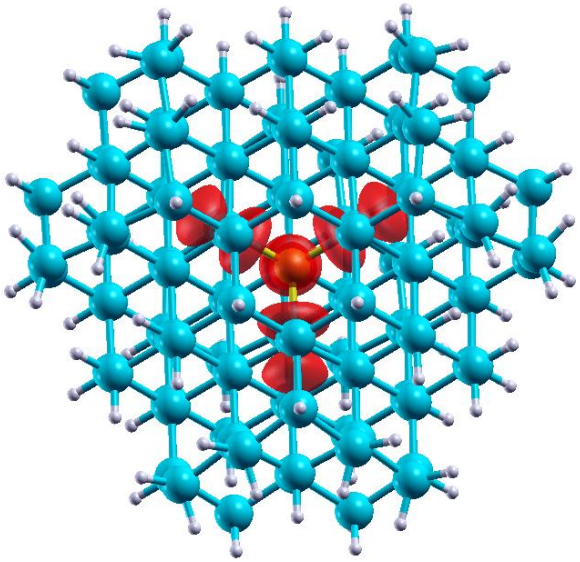
$$A_{iso} = \frac{4\pi g_e \mu_e g_N \mu_N}{3\langle S_z \rangle} \int d^3 r \; n_s(\vec{r}) \delta(\vec{r})$$

$$A_{dip}^{i,j} = \frac{g_e \mu_e g_N \mu_N}{2\langle S_z \rangle} \int d^3 r \; n_s(\vec{r}) \frac{3 r_i r_j - \delta_{i,j} r^2}{r^2}$$

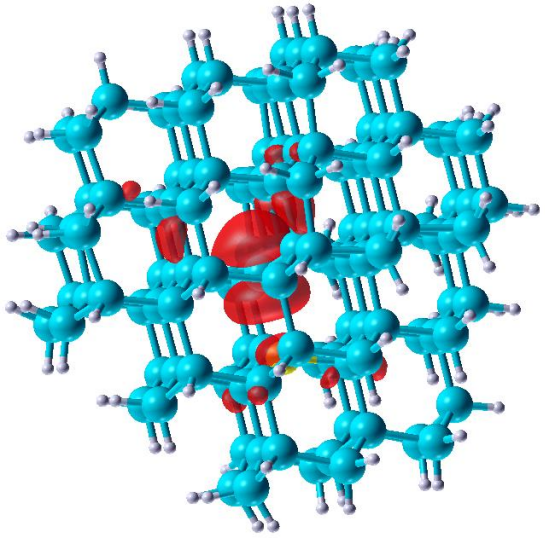
$$A_{dip} = \begin{pmatrix} -b+b' & & \\ & -b-b' & \\ & & 2b \end{pmatrix}$$

Si(Ge) dots:S^+ contact term





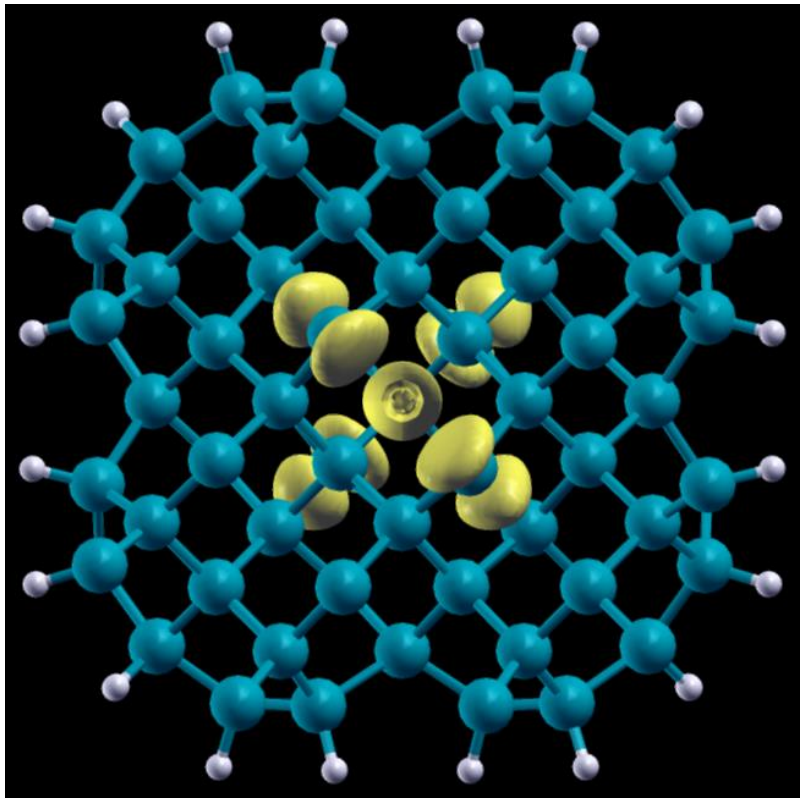
Si-NC:S^+ (1)



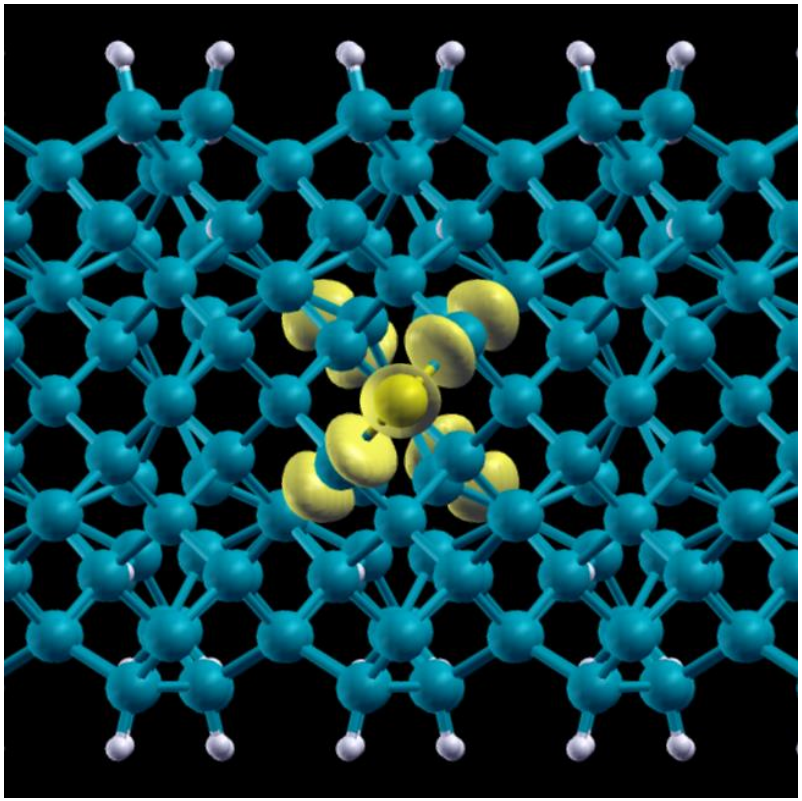
Si-NC:S^+ (2)

Single atom electronics: Se impurity

Se doped H passivated Si nanowires
(nanoelectronics, quantum computer)



front view

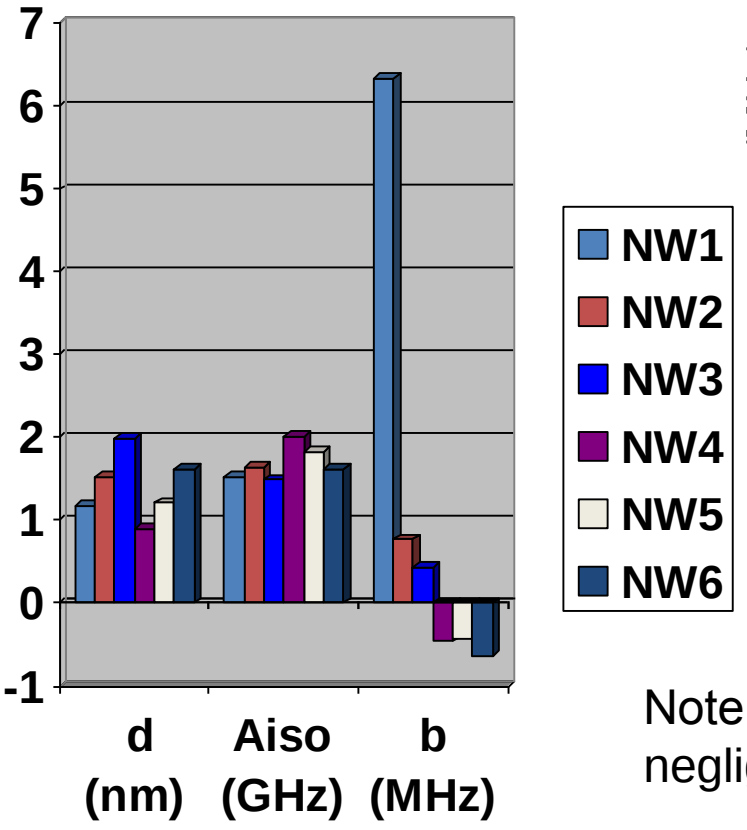


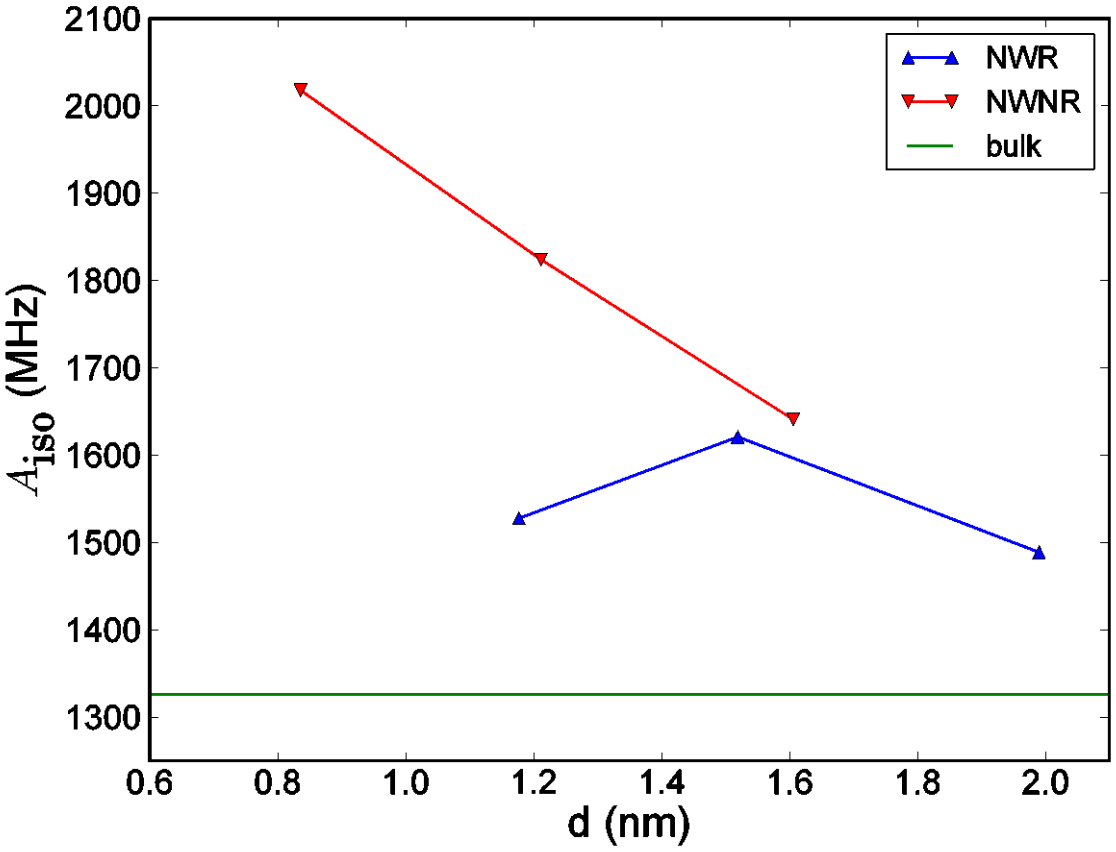
side view

Hyperfine coupling constants: axial Se

Confinement enhances the hyperfine coupling constant

Central impurity
[001]



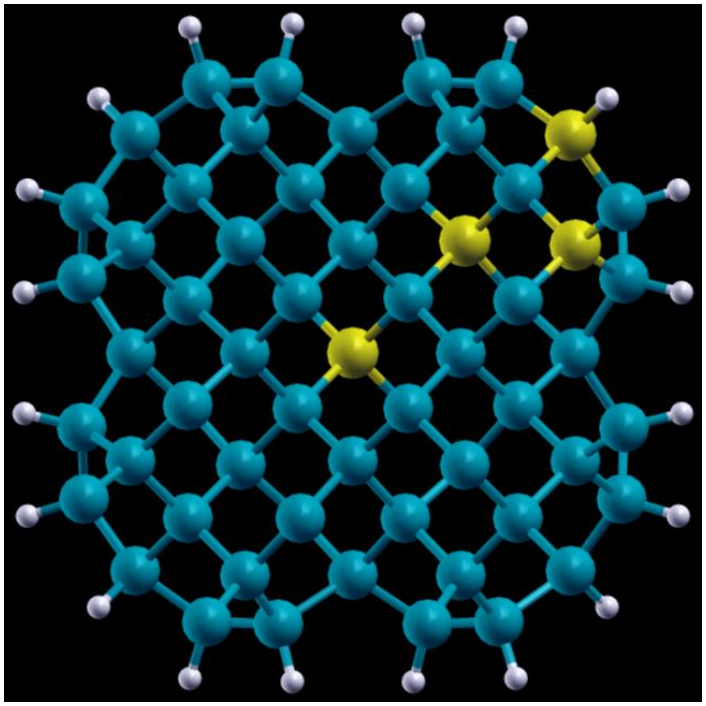


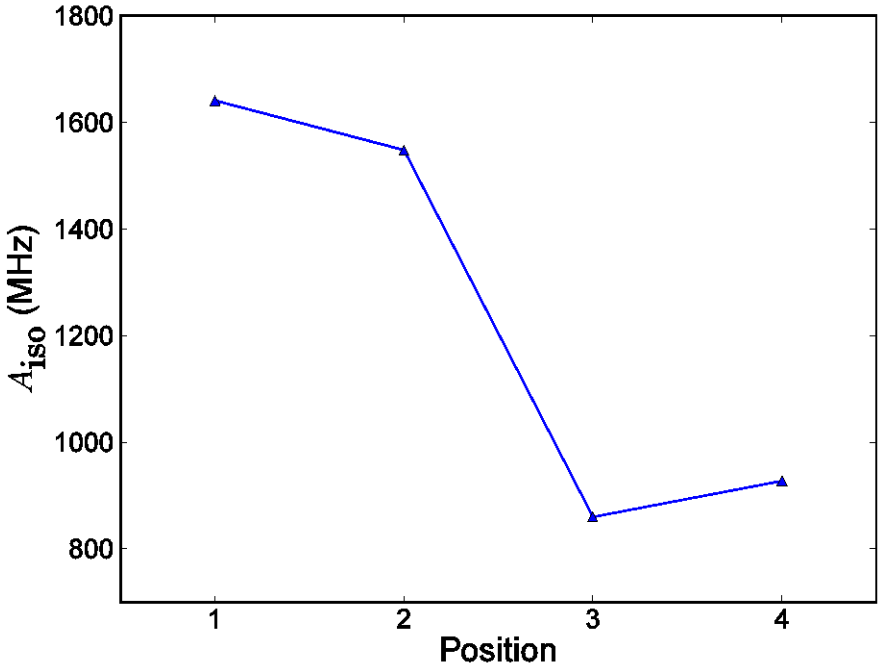
Note: b' is 18.34 MHz for NW1, and negligible (< 0.22) for all the others

Se doped Si-NW

- HFC couples nuclear and electron spin
- Quantum bits (qu-bits) are stored in the nuclear spin of Se atom

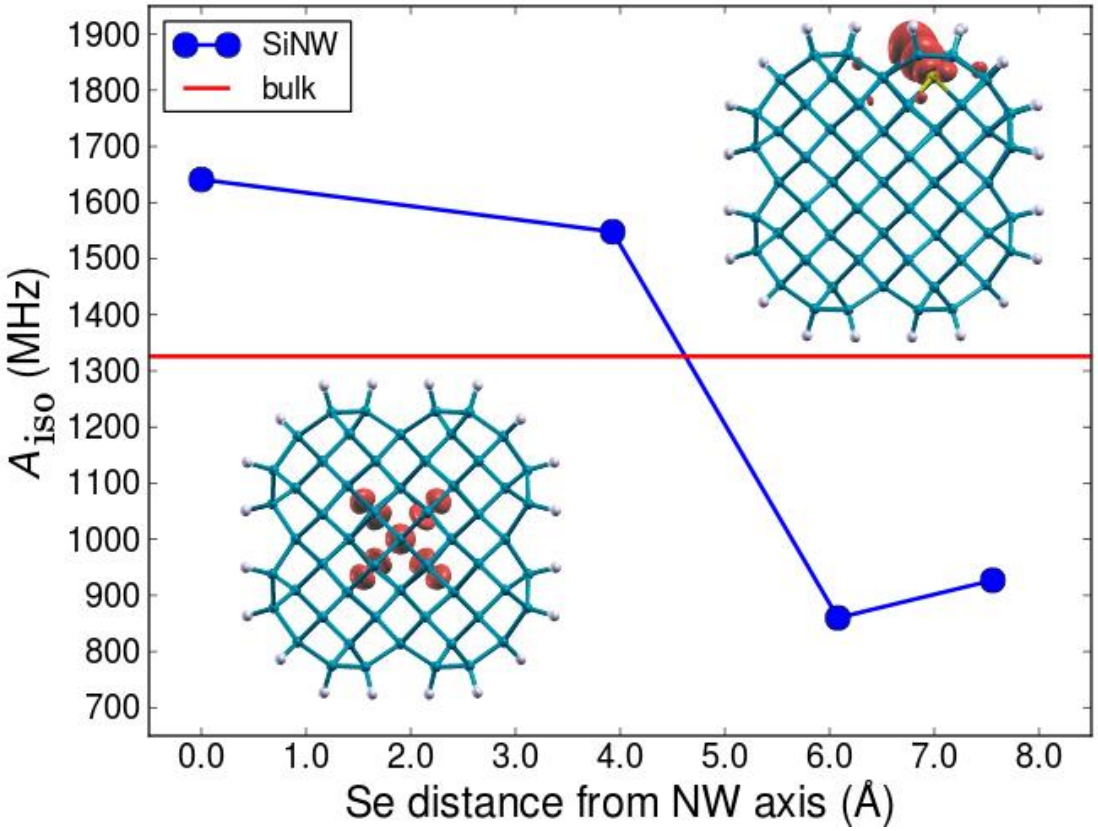
Distortion of NW for smal size is significant.
Increase of HFC of about 30% at optimum diameter





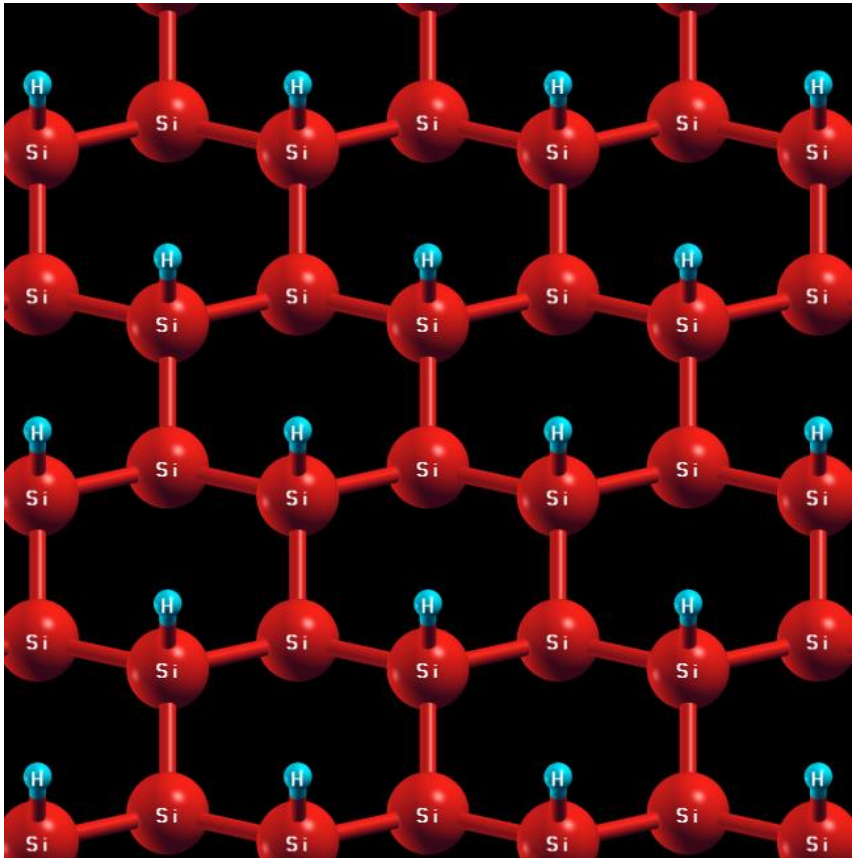
Isotropic Hyperfine Coupling

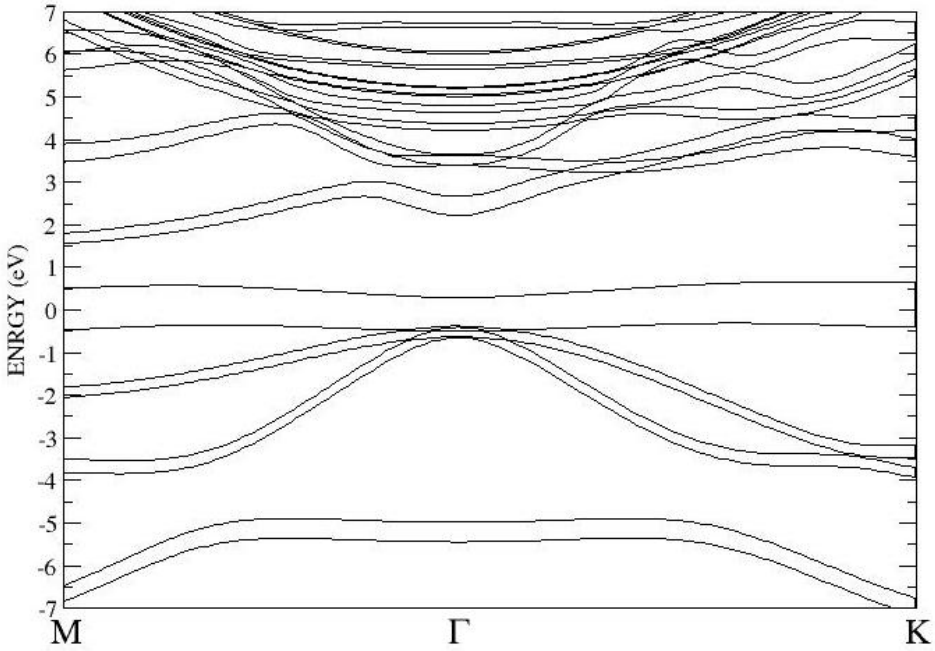
- STRONG DEPENDENCE OF HYPERFINE CONSTANT ON IMPURITY SITE
- It is possible to DETERMINE the POSITION of the impurity (Se) on the basis of EPR SPECTRA

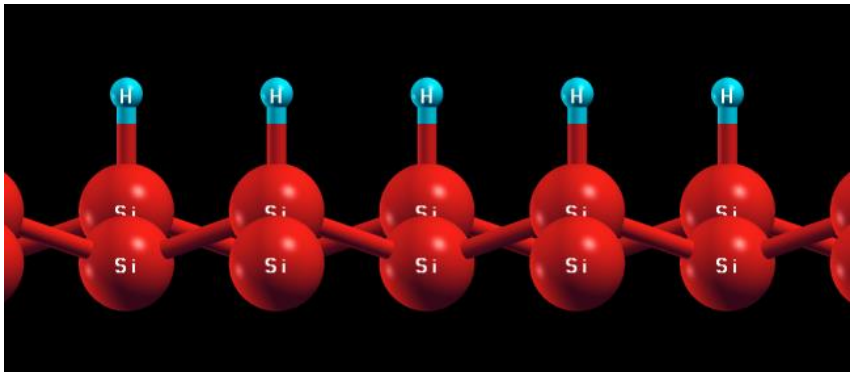


Silicane: Si@H

Magnetic Semiconductor



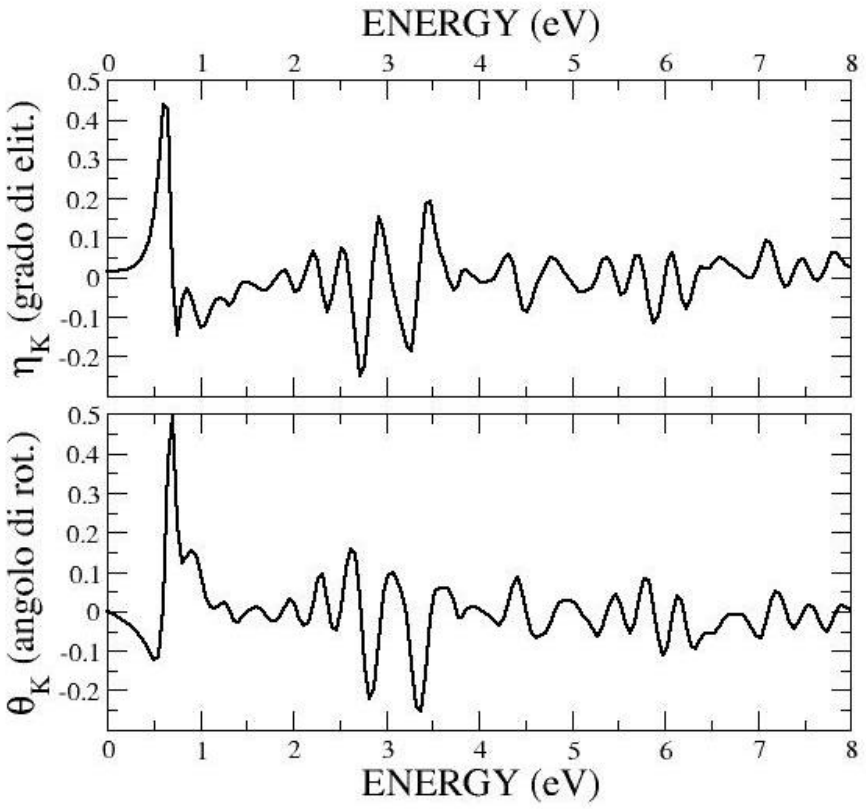


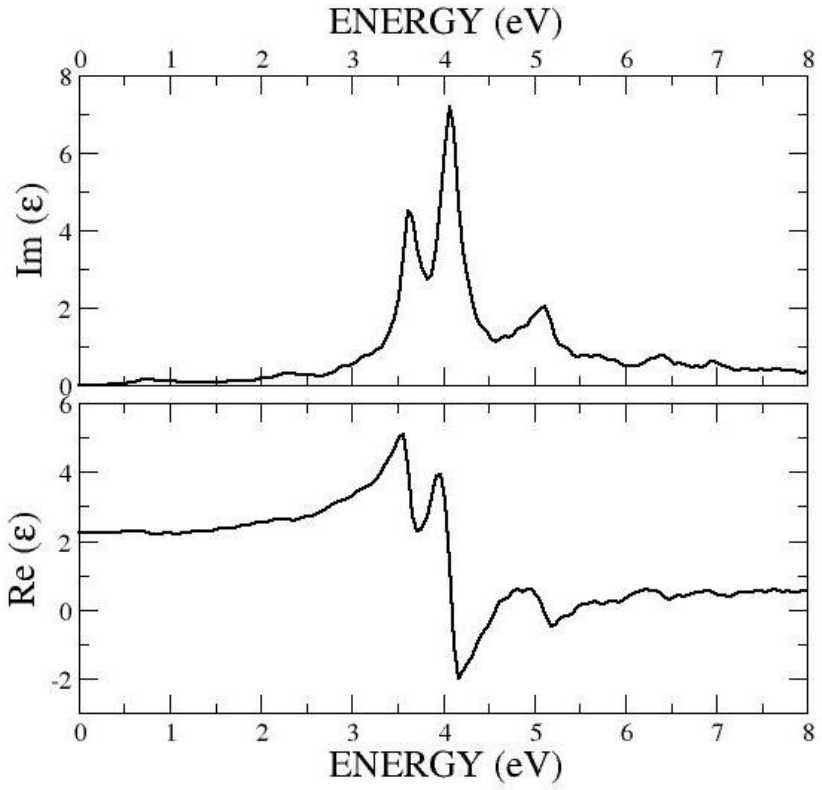


Si@H: Proprietà Ottiche

- Magneto Optical Kerr Effect
- Magnetism

Funzione dielettrica





Conclusions

- The position of the impurity can be determined by comparing EPR spectra with ab initio data
- MOKE signal in 2D for future nano-electronic devices

- La Simulazione è MOLTO più economica dell'esperimento
- Possiamo «inventare» nuovi materiali e modificarne le proprietà per una nuova elettronica.

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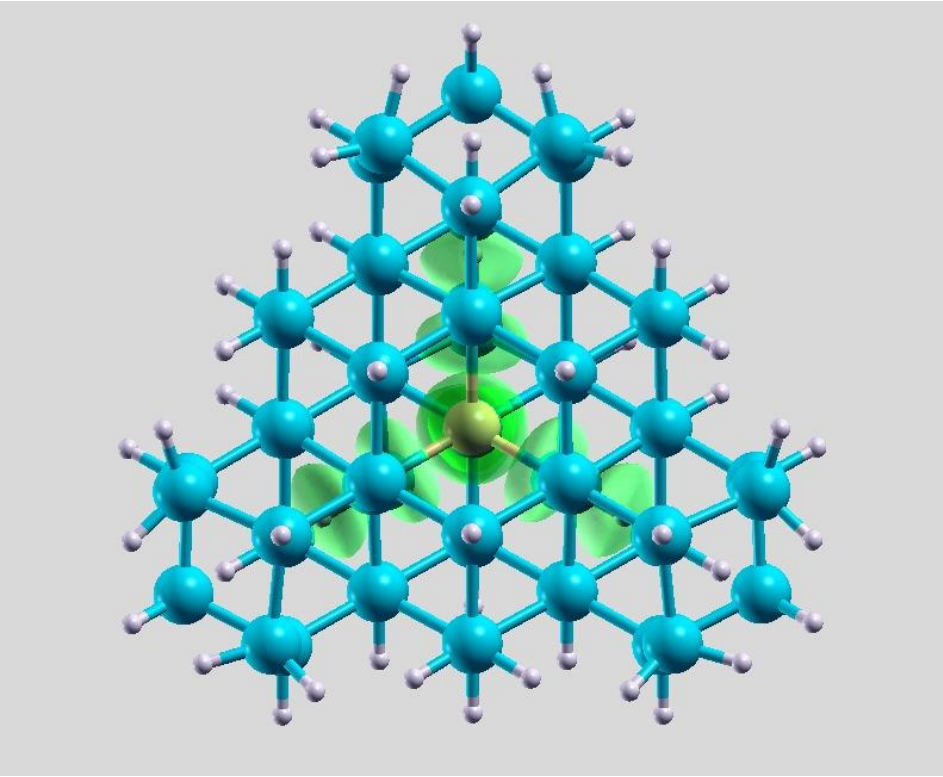
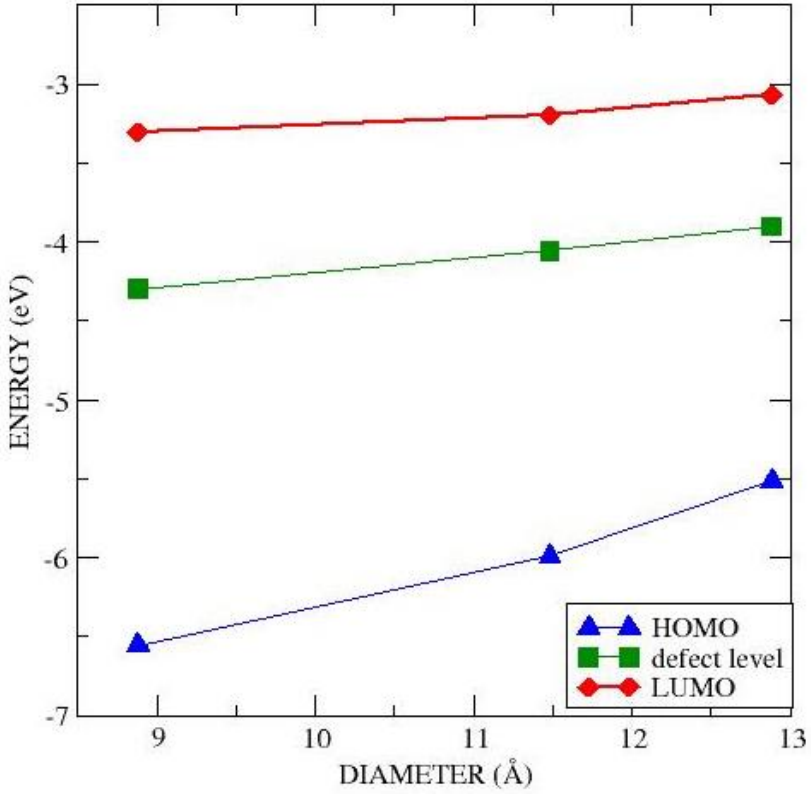
- M. Fanciulli (UNIMIB, MDM) and to all experimentalists at the MDM laboratory.
- LISA for computational resources ....

... and you for your attention !!!

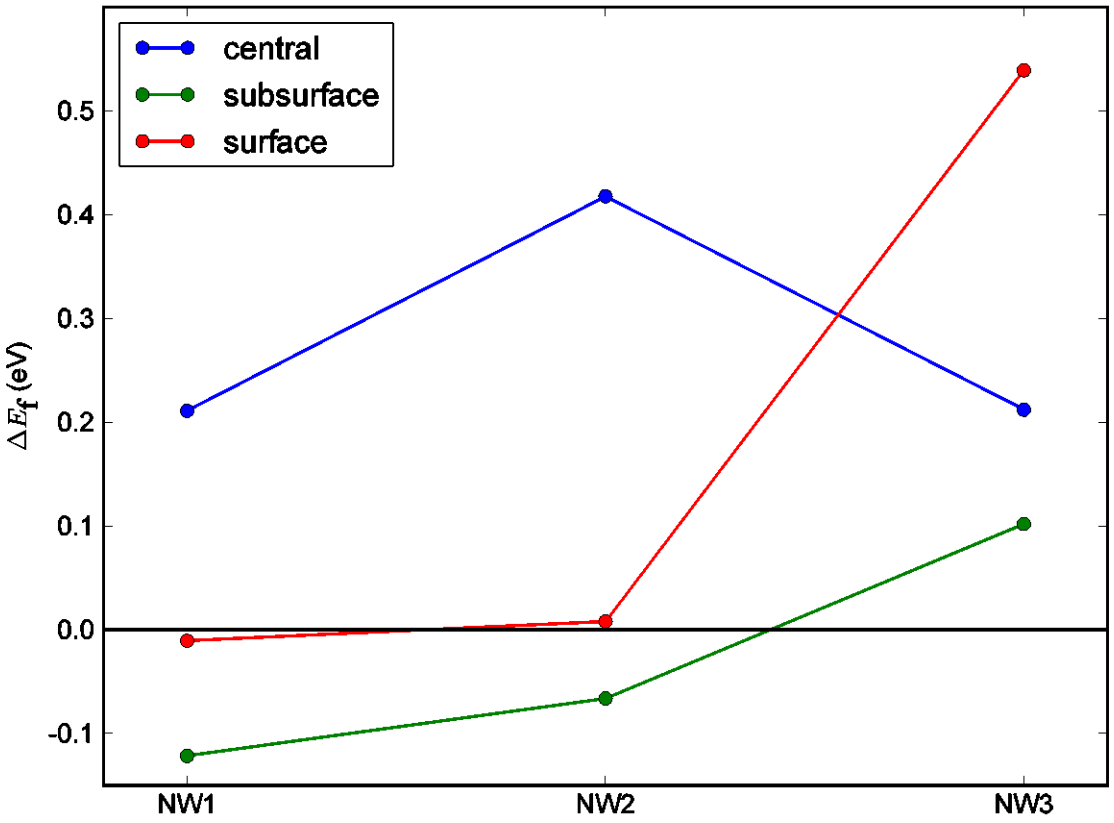
S doped Si Nano Dots





Se doped Si NW: Formation Energy

- Subsurface position is energergetic ally favoured (at least for small diameter)
- Effect of distortion for small diameters



Stability of ionized Se

- Formation energy of the defect on the axis of the nanowire as a function of the chemical potential.
- The three graphs represent the three different nanowires with diameter 1.2 nm, 1.5 nm, 2.0 nm respectively.
- The zero value is the calculated value of the formation energy of Se defect in bulk Si.