Introduction to the electronic properties of semiconductor nanostructures.

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General outline

- **Part I** :
  Introduction to semiconductor nanostructures
- **Part II** :
  Electronic structure methods
- **Part III** :
  Self-energy and excitonic corrections in nanostructures

Part I

Introduction to semiconductor nanostructures

Outline

- **I.1** :
  Electrons and holes
- **I.2** :
  Semiconductor materials and nanostructures
- **I.3** :
  Numerical simulation in nanosciences : Challenges and perspectives

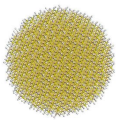
I.1 : Electrons and holes

Non-interacting systems : Ground-state (I)

- Consider N electrons moving in a one-body potential $v(\mathbf{r})$. We look for their ground-state energy $E_0(N)$ and for their ground-state wavefunction $\Psi_0(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N)$:

$$\hat{H}_N = \sum_{i=1}^{N} \hat{h}_i \quad \text{with} \quad \hat{h}_i = -\frac{\hbar^2}{2m_0}\Delta_{\mathbf{r}_i} + v(\mathbf{r}_i)$$

$$\hat{H}_N \Psi_0(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N) = E_0(N) \Psi_0(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N)$$



- **Solution** : compute the spectrum of the one-particle Hamiltonian h...

$$-\frac{\hbar^2}{2m_0}\Delta_{\mathbf{r}}\varphi_i(\mathbf{r}) + v(\mathbf{r})\varphi_i(\mathbf{r}) = \varepsilon_i \varphi_i(\mathbf{r}) \qquad [\varepsilon_i \text{ twofold spin degenerate}]$$

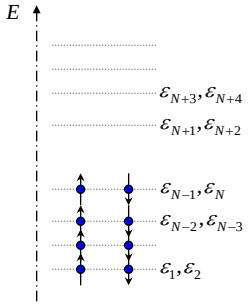
... then build a Slater determinant with the N first φ_i's :

$$\Psi_0(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N) = \begin{vmatrix} \varphi_1(\mathbf{r}_1) & \varphi_2(\mathbf{r}_1) & \cdots & \varphi_N(\mathbf{r}_1) \\ \varphi_1(\mathbf{r}_2) & \varphi_2(\mathbf{r}_2) & \cdots & \varphi_N(\mathbf{r}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \varphi_1(\mathbf{r}_N) & \varphi_2(\mathbf{r}_N) & \cdots & \varphi_N(\mathbf{r}_N) \end{vmatrix} \qquad E_0(N) = \varepsilon_1 + \varepsilon_2 + ... + \varepsilon_N$$

Non-interacting systems : Ground-state (II)

$$\Psi_0(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_{N-1}, \mathbf{r}_N) = \begin{vmatrix} \varphi_1(\mathbf{r}_1) & \varphi_2(\mathbf{r}_1) & \cdots & \varphi_{N-1}(\mathbf{r}_1) & \varphi_N(\mathbf{r}_1) \\ \varphi_1(\mathbf{r}_2) & \varphi_2(\mathbf{r}_2) & \cdots & \varphi_{N-1}(\mathbf{r}_2) & \varphi_N(\mathbf{r}_2) \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \varphi_1(\mathbf{r}_{N-1}) & \varphi_2(\mathbf{r}_{N-1}) & \cdots & \varphi_{N-1}(\mathbf{r}_{N-1}) & \varphi_N(\mathbf{r}_{N-1}) \\ \varphi_1(\mathbf{r}_N) & \varphi_2(\mathbf{r}_N) & \cdots & \varphi_{N-1}(\mathbf{r}_N) & \varphi_N(\mathbf{r}_N) \end{vmatrix}$$

Density $n_0(\mathbf{r}) = \sum_{i=1}^{N} |\varphi_i(\mathbf{r})|^2$



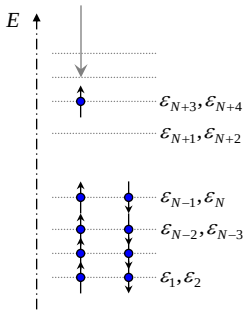
$$E_0(N) = \varepsilon_1 + \varepsilon_2 + ... + \varepsilon_{N-1} + \varepsilon_N$$

Fill the N lowest levels

Non-interacting systems : Addition energies

$$\Psi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N,\mathbf{r}_{N+1}) = \begin{vmatrix} \varphi_1(\mathbf{r}_1) & \varphi_2(\mathbf{r}_1) & \cdots & \varphi_N(\mathbf{r}_1) & \varphi_{N+3}(\mathbf{r}_1) \\ \varphi_1(\mathbf{r}_2) & \varphi_2(\mathbf{r}_2) & \cdots & \varphi_N(\mathbf{r}_2) & \varphi_{N+3}(\mathbf{r}_2) \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \varphi_1(\mathbf{r}_N) & \varphi_2(\mathbf{r}_N) & \cdots & \varphi_N(\mathbf{r}_N) & \varphi_{N+3}(\mathbf{r}_N) \\ \varphi_1(\mathbf{r}_{N+1}) & \varphi_2(\mathbf{r}_{N+1}) & \cdots & \varphi_N(\mathbf{r}_{N+1}) & \varphi_{N+3}(\mathbf{r}_{N+1}) \end{vmatrix}$$

$$n(\mathbf{r}) = \sum_{i=1}^{N} |\varphi_i(\mathbf{r})|^2 + |\varphi_{N+3}(\mathbf{r})|^2 = n_0(\mathbf{r}) + |\varphi_{N+3}(\mathbf{r})|^2$$

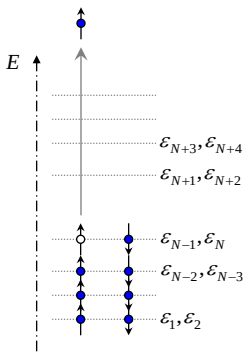


$$E = \varepsilon_1 + \varepsilon_2 + \ldots + \varepsilon_{N-1} + \varepsilon_N + \varepsilon_{N+3}$$
$$= E_0(N) + \varepsilon_{N+3}$$

Non-interacting systems : Ionization energies

$$\Psi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_{N-2},\mathbf{r}_{N-1}) = \begin{vmatrix} \varphi_1(\mathbf{r}_1) & \varphi_2(\mathbf{r}_1) & \cdots & \varphi_{N-2}(\mathbf{r}_1) & \varphi_N(\mathbf{r}_1) \\ \varphi_1(\mathbf{r}_2) & \varphi_2(\mathbf{r}_2) & \cdots & \varphi_{N-2}(\mathbf{r}_2) & \varphi_N(\mathbf{r}_2) \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \varphi_1(\mathbf{r}_{N-2}) & \varphi_2(\mathbf{r}_{N-2}) & \cdots & \varphi_{N-2}(\mathbf{r}_{N-2}) & \varphi_N(\mathbf{r}_{N-2}) \\ \varphi_1(\mathbf{r}_{N-1}) & \varphi_2(\mathbf{r}_{N-1}) & \cdots & \varphi_{N-2}(\mathbf{r}_{N-1}) & \varphi_N(\mathbf{r}_{N-1}) \end{vmatrix}$$

$$n(\mathbf{r}) = \sum_{i=1}^{N-2} |\varphi_i(\mathbf{r})|^2 + |\varphi_N(\mathbf{r})|^2 = n_0(\mathbf{r}) - |\varphi_{N-1}(\mathbf{r})|^2$$

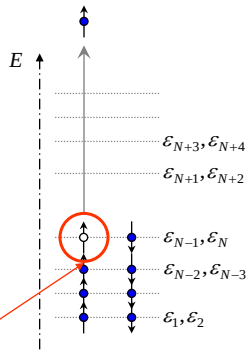


$$E = \varepsilon_1 + \varepsilon_2 + \ldots + \varepsilon_{N-2} + \varepsilon_N$$
$$= E_0(N) - \varepsilon_{N-1}$$

Non-interacting systems : Ionization energies

$$\Psi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_{N-2},\mathbf{r}_{N-1}) = \begin{vmatrix} \varphi_1(\mathbf{r}_1) & \varphi_2(\mathbf{r}_1) & \cdots & \varphi_{N-2}(\mathbf{r}_1) & \varphi_N(\mathbf{r}_1) \\ \varphi_1(\mathbf{r}_2) & \varphi_2(\mathbf{r}_2) & \cdots & \varphi_{N-2}(\mathbf{r}_2) & \varphi_N(\mathbf{r}_2) \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \varphi_1(\mathbf{r}_{N-2}) & \varphi_2(\mathbf{r}_{N-2}) & \cdots & \varphi_{N-2}(\mathbf{r}_{N-2}) & \varphi_N(\mathbf{r}_{N-2}) \\ \varphi_1(\mathbf{r}_{N-1}) & \varphi_2(\mathbf{r}_{N-1}) & \cdots & \varphi_{N-2}(\mathbf{r}_{N-1}) & \varphi_N(\mathbf{r}_{N-1}) \end{vmatrix}$$

$$n(\mathbf{r}) = \sum_{i=1}^{N-2} |\varphi_i(\mathbf{r})|^2 + |\varphi_N(\mathbf{r})|^2 = n_0(\mathbf{r}) - |\varphi_{N-1}(\mathbf{r})|^2$$



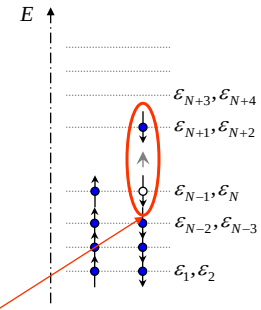
$$E = \varepsilon_1 + \varepsilon_2 + \ldots + \varepsilon_{N-2} + \varepsilon_N = E_0(N) - \varepsilon_{N-1}$$

Hole wavefunction and energy

Non-interacting systems : Excitation energies

$$\Psi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_{N-1},\mathbf{r}_N) = \begin{vmatrix} \varphi_1(\mathbf{r}_1) & \varphi_2(\mathbf{r}_1) & \cdots & \varphi_{N-1}(\mathbf{r}_1) & \varphi_{N+1}(\mathbf{r}_1) \\ \varphi_1(\mathbf{r}_2) & \varphi_2(\mathbf{r}_2) & \cdots & \varphi_{N-1}(\mathbf{r}_2) & \varphi_{N+1}(\mathbf{r}_2) \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \varphi_1(\mathbf{r}_{N-1}) & \varphi_2(\mathbf{r}_{N-1}) & \cdots & \varphi_{N-1}(\mathbf{r}_{N-1}) & \varphi_{N+1}(\mathbf{r}_{N-1}) \\ \varphi_1(\mathbf{r}_N) & \varphi_2(\mathbf{r}_N) & \cdots & \varphi_{N-1}(\mathbf{r}_N) & \varphi_{N+1}(\mathbf{r}_N) \end{vmatrix}$$

$$n(\mathbf{r}) = \sum_{i=1}^{N-1} |\varphi_i(\mathbf{r})|^2 + |\varphi_{N+1}(\mathbf{r})|^2 = n_0(\mathbf{r}) - |\varphi_N(\mathbf{r})|^2 + |\varphi_{N+1}(\mathbf{r})|^2$$

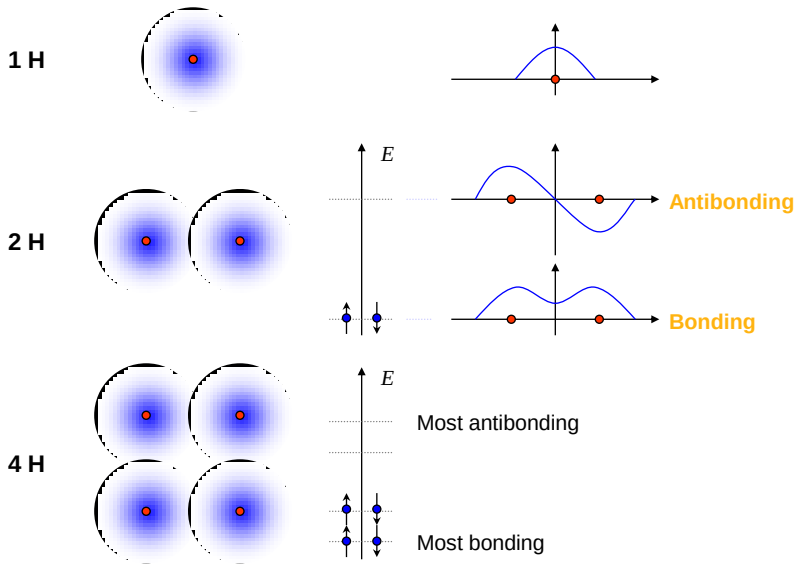


$$E = \varepsilon_1 + \varepsilon_2 + \ldots + \varepsilon_{N-1} + \varepsilon_{N+1} = E_0(N) - \varepsilon_N + \varepsilon_{N+1}$$

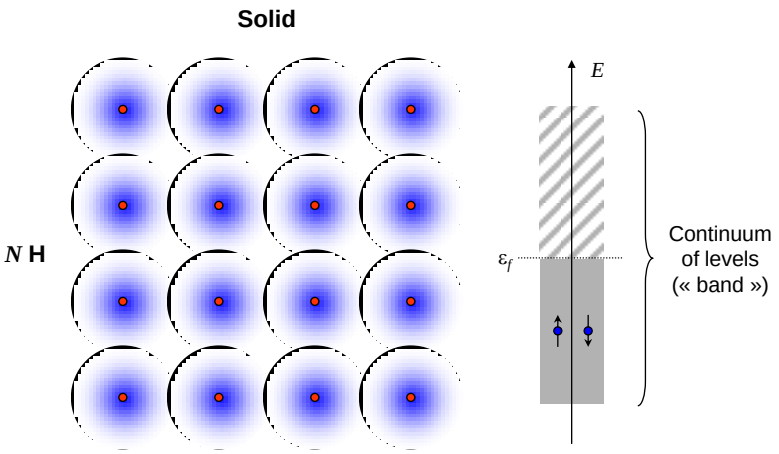
« Electron-hole pair »

I.2 : Semiconductor materials and nanostructures

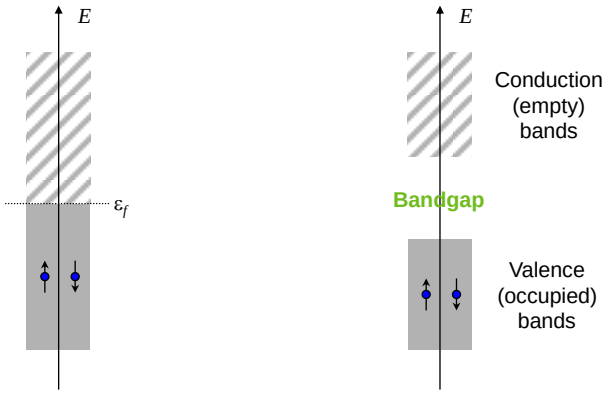
From the atom to the solid (I)



From the atom to the solid (II)



Bulk metals, insulators, and semiconductors

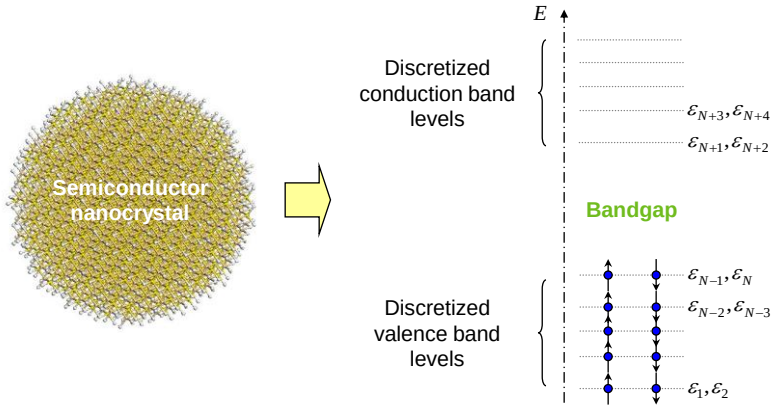


Metals

Semiconductors (low bandgap)
Insulators (large bandgap)

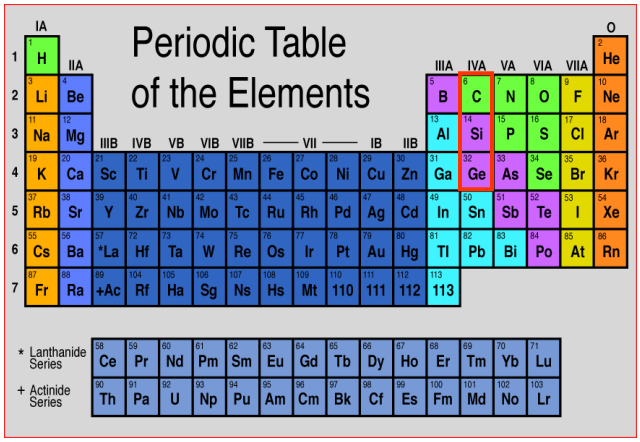
No low energy electronic excitations

Semiconductor nanostructures



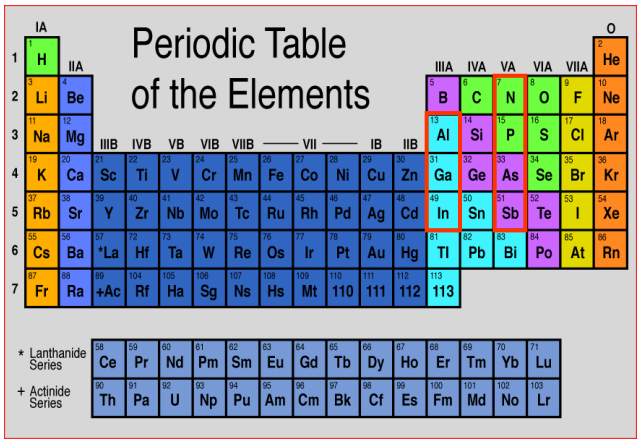
- The bandgap is actually larger than in bulk materials due to « quantum confinement » (see later examples on nanocrystals).

Usual semiconductors (I)



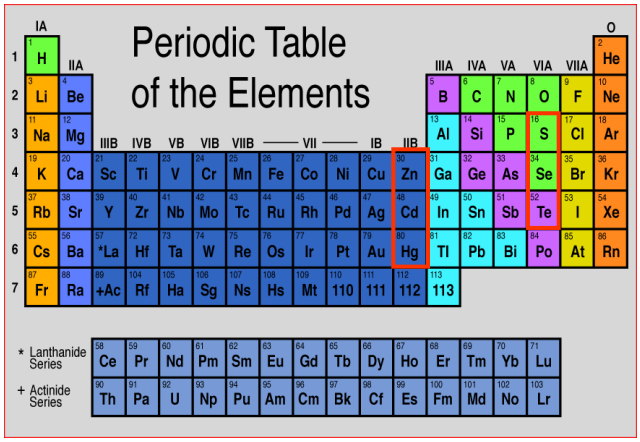
- **Group IV elements** : Si, Ge, C (Diamond). Covalent systems.

Usual semiconductors (II)



- **III-V semiconductors** : GaAs, InAs, InSb…
  Slightly ionic bonds (« $Ga^{+}As^{-}$ »).

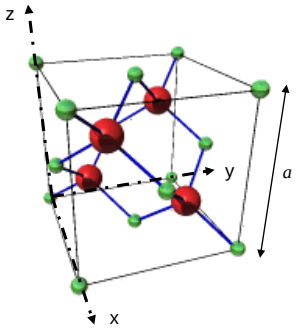
Usual semiconductors (III)



- **II-VI semiconductors** : CdTe, ZnSe…

Crystal structure

- Most usual semiconductors crystallize in the cubic **Diamond/Zinc-Blende** structure.



It is a **face-centered cubic** (FCC) lattice with a two atom unit cell :
- one at (0,0,0).
- the other at $a(1,1,1)/4$.

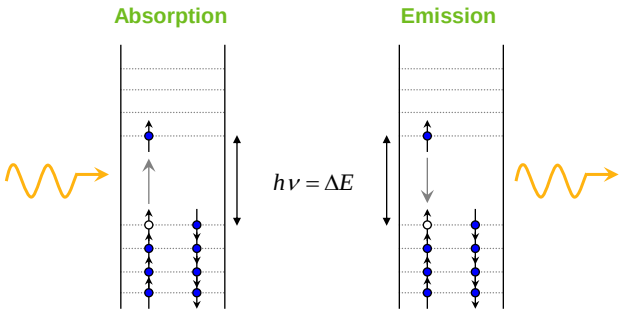
In the **Zinc-Blende** structure, each FCC sublattice is occupied by a different atom (e.g. Ga/As, In/P).

In the **Diamond** structure, the two sublattices are occupied by the same atom (e.g. Si, Ge, C).

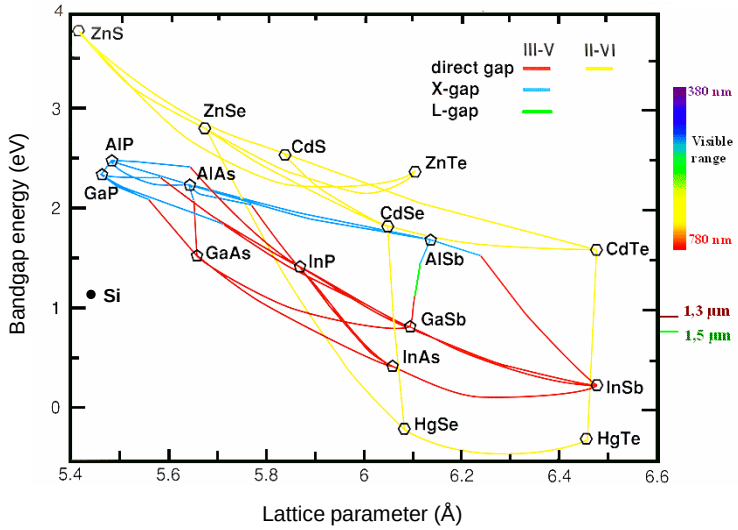
- Alloys can also be synthetized, e.g. $In_{0.8}Ga_{0.2}As$.
  One FCC sublattice is occupied by the In/Ga atoms (80% In+20% Ga ~ randomly distributed), the other by the As atoms.

Optical applications of semiconductors

- Well defined bandgap energy :
  - **Light emission** : LEDs, lasers, …
  - **Light absoption/detection** : Photovoltaics, …



Bandgap vs lattice parameter



Semiconductors for microelectronics

- **Semiconductors** *vs* **metals** :
  - **Semiconductors** have no low-energy electronic excitations :
    - Highly resistive. ☹
    - Incomplete screening of the electric fields :

$$V(r) = \frac{q}{\varepsilon r}$$

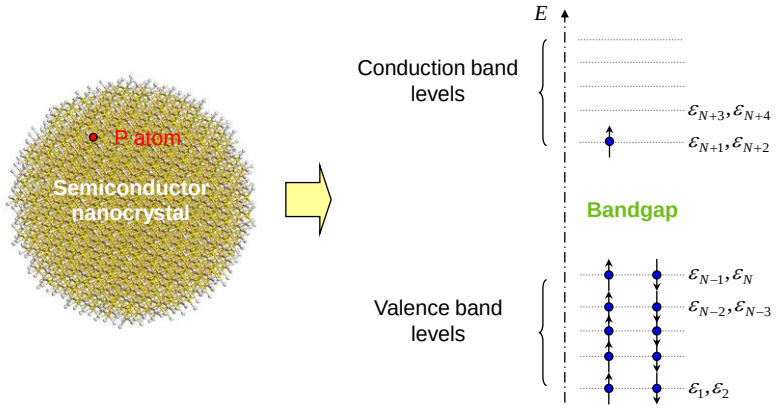
      Electric fields can be applied deep inside a semiconductor !.. ☺
  - **Metals** have a large density of « free » electrons :
    - Highly conductive. ☺

    But :
    - Almost complete screening of the electric fields ⇒ Metals are just equipotentials. They can hardly be controlled by external electric fields ! ☹
- **« Doped semiconductors » combine the best of the two worlds** !

Doping the semiconductors (I)

- Example : ***n*-type doping** of silicon.

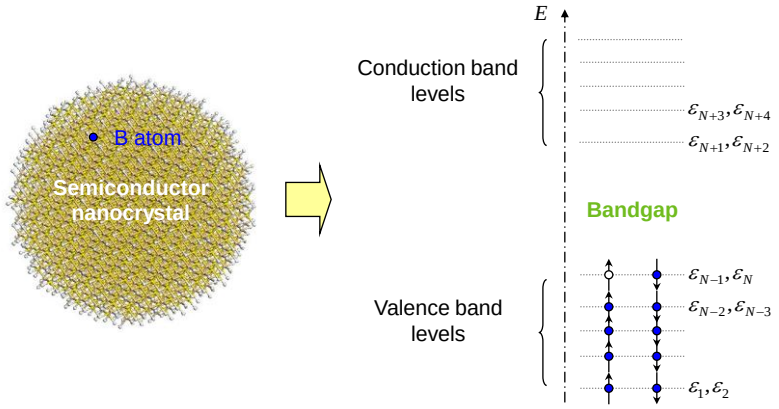
Replace a few silicon atoms with phosphorous (one more electron) :



Doping the semiconductors (II)

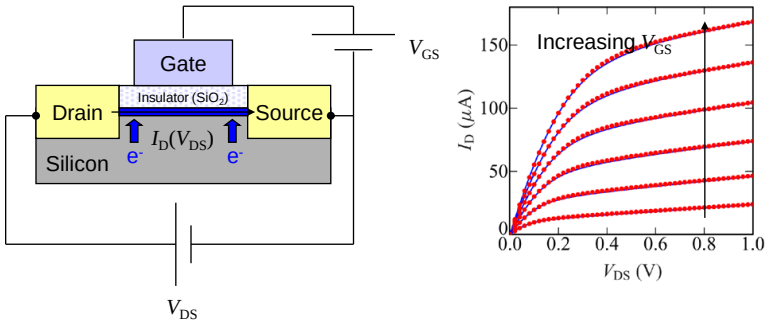
- Example : ***p*-type doping** of silicon.

Replace a few silicon atoms with boron (one less electron) :



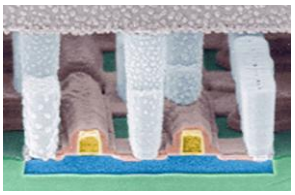
Application : the field effect transistor

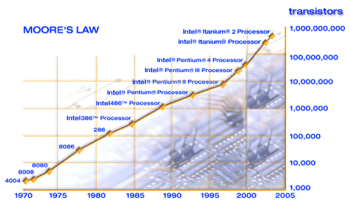
- Doped semiconductors :
  - Are reasonnably **conductive**.
  - Can be **controlled by external electric fields**.
- Example : The field-effect transistor – Millions of them in this computer !!



Towards nanoelectronics

- Continuous reduction in the characteristic size of the transistors (Moore's law). The number of transistors on a chip **doubles ~ every two years** !





Production : 65 & 45 nm « nodes ».
Research : 32 nm (2010), 22 nm, 16 nm (?)...

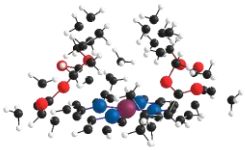
⇒ **Technological and physical limitations ?** ⇐

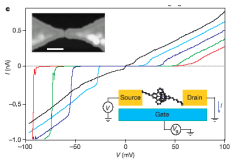
- « Beyond CMOS » : « Bottom-up » approaches based on the assembly of nanometer-scale building blocks.

⇒ **New devices** ⇐

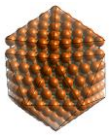
Some building blocks in nanosciences

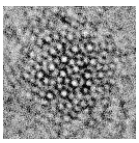
- **Molecules** :

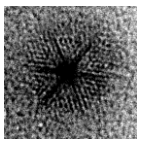




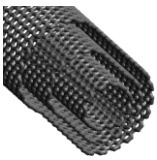
- **Nanocrystals** :

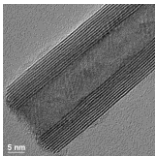


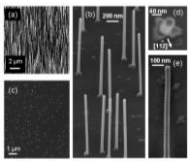


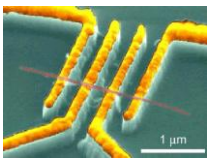


- **Carbon nanotubes, semiconductor nanowires** :



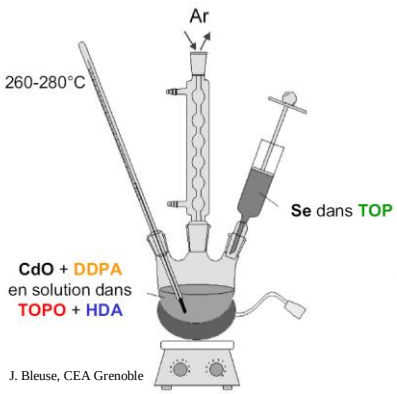


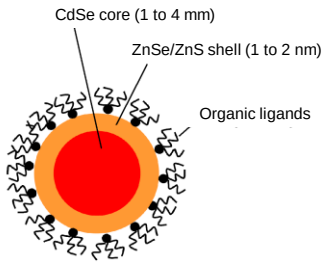


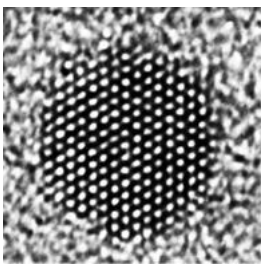


Semiconductor nanostructures : Nanocrystals (I)

- Colloidal (liquid phase) synthesis of semiconductor **nanocrystals** (CdS, CdSe, ZnSe, InAs, InP…) :

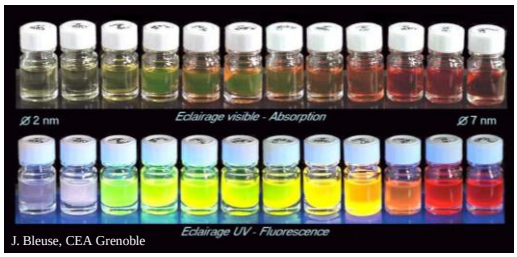






A. P. Alivisatos, J. Phys. Chem. **100**, 13226 (1996).

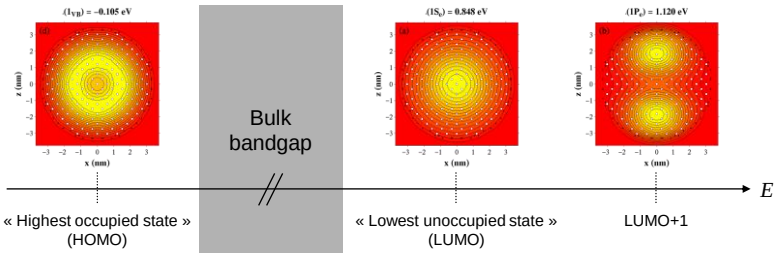
Semiconductor nanostructures : Nanocrystals (II)



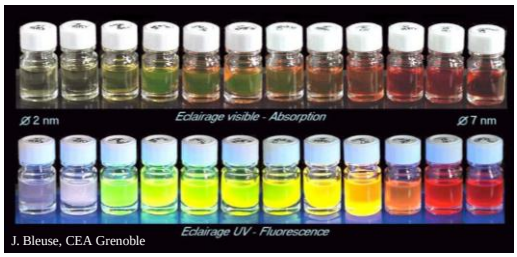
- **Quantum confinement** :

  The bandgap energy increases with decreasing diameter. The absorption & emission shift from red to blue.

- Discrete, atomic-like set of states (« Artificial atoms ») :



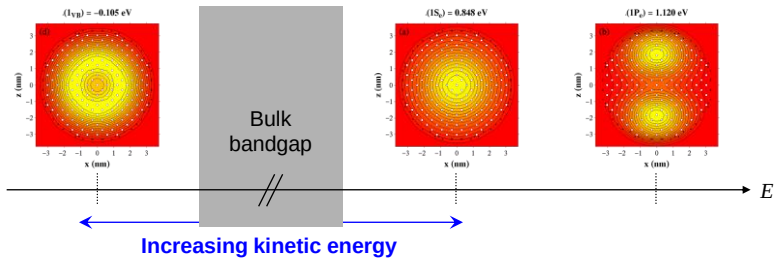
Semiconductor nanostructures : Nanocrystals (III)



- **Quantum confinement** :

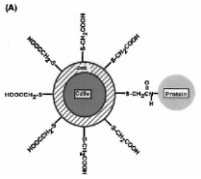
  The bandgap energy increases with decreasing diameter. The absorption & emission shift from red to blue.

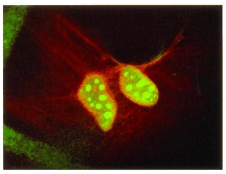
- The confinement increases the kinetic energy of the electrons and holes :



Semiconductor nanostructures : Nanocrystals (IV)

- **Applications** (examples) :
  - Fluorescent labels for biology :

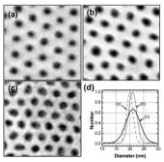


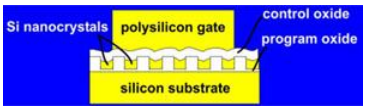


The nanocrystals are capped with molecules that bind to specific targets, such as tumor cells for example.

M. Bruchez Jr. et al., Science **281**, 2013 (1998) ; W. C. W. Chan and S. Nie, Science **281**, 2016 (1998)

  - Few-electron memories (Si nanocrystals) :



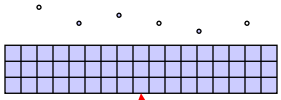


Electrons are stored in the nanocrystals.

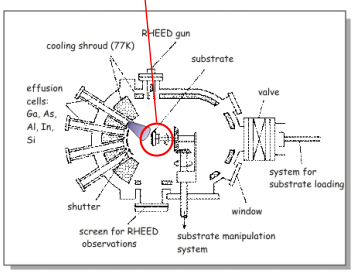
IBM research

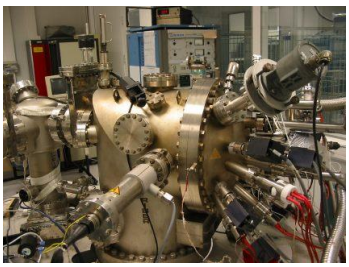
Semiconductor nanostructures : InAs/GaAs dots (I)

- Stransky-Krastanov growth :



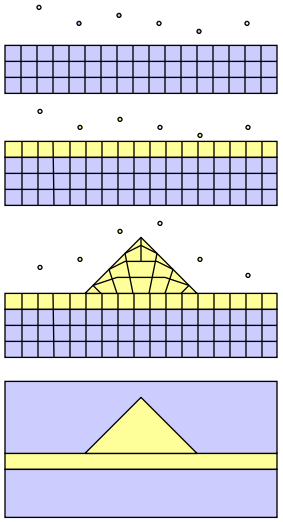
Semiconductor structures can be grown layer by layer using « molecular beam epitaxy ».





Semiconductor nanostructures : InAs/GaAs dots (I)

- Stransky-Krastanov growth :



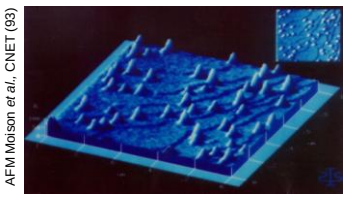
Semiconductor structures can be grown layer by layer using « molecular beam epitaxy ».

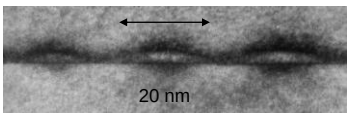
The bond length is 6.7% larger in InAs than in GaAs. The InAs layer is thus compressed by the thick GaAs substrate…

InAs pyramids finally grow onto the thin InAs « wetting layer ». The surfaces of the pyramids indeed help relaxing strains.

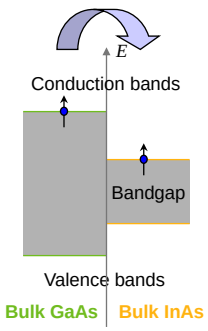
The pyramids can last be embedded in a thick, overgrown GaAs layer.

Semiconductor nanostructures : InAs/GaAs dots (II)





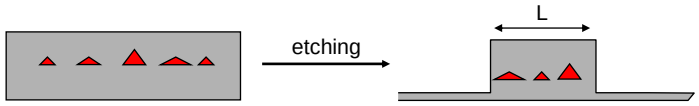
TEM A. Ponchet CNRS (95)



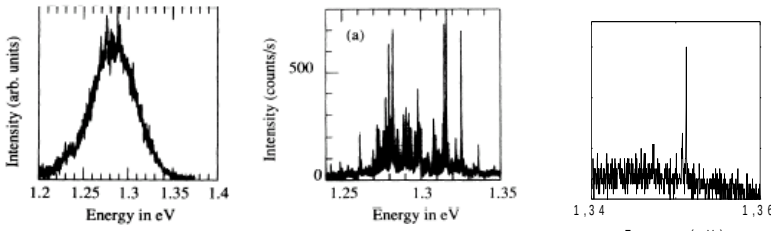
- The bandgap energy is lower in InAs (~0.5 eV) than in GaAs (~1.5 eV). The electrons and holes are thus confined in the InAs « quantum dots ».

Semiconductor nanostructures : InAs/GaAs dots (III)

J.Y. Marzin *et al.*, Phys. Rev. Lett. **73**, 716 (1994)



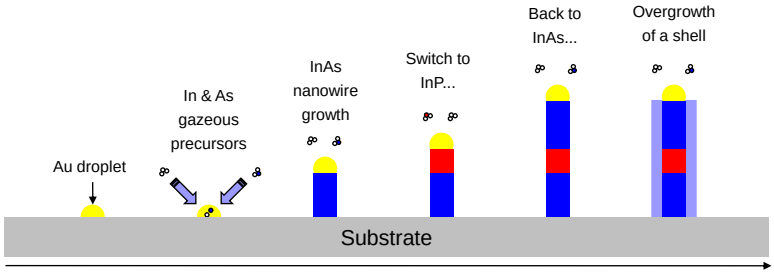
L = 5 µm : **10000** QDs | L = 0.5 µm : **100** QDs | L ~ 50 nm : **1** QD



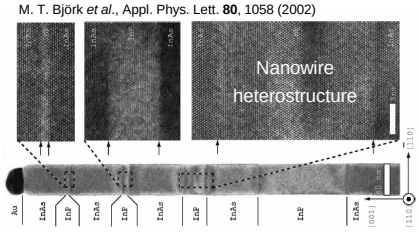
- Very sharp emission from a single InAs quantum dot (QD).
  Applications : Quantum dots lasers…

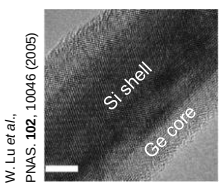
Semiconductor nanostructures : Nanowires (I)

- Vapor-Liquid-Solid (VLS) growth :



M. T. Björk *et al.*, Appl. Phys. Lett. **80**, 1058 (2002)

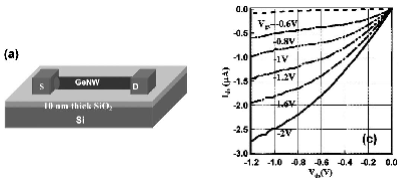




Semiconductor nanostructures : Nanowires (II)

- **Applications** (examples) :

  - Nanowire field effect transistor :

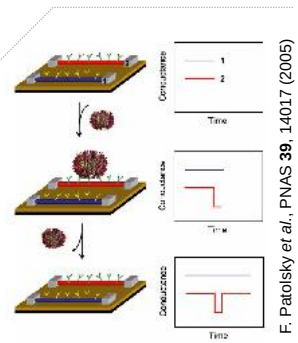


The current between the drain and source is controlled by the gate voltage.

D. Wang *et al*., Appl. Phys. Lett. **83**, 2432 (2003)

  - Detection of single molecules/viruses :

The surface of the nanowire is capped with molecules that bind to specific targets (DNA, viruses). The conductance of the nanowire changes each time the target binds to the wire.



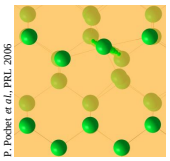
F. Patolsky *et al*., PNAS **39**, 14017 (2005)

I.3 : Numerical simulation in nanosciences : Challenges and perspectives

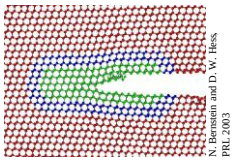
Numerical simulation in nanosciences : Challenges

- **Atomistic simulation** is needed at the nanometer scale.

- Two challenges :
  - Modelize the structural and electronic properties of the **materials** at the atomic scale, to :
    - Improve our understanding of the physics of present devices.
    - Anticipate the merits and limits of emerging technologies.



How do vacancies migrate in silicon ?



Fracture proapgation in silicon…

Numerical simulation in nanosciences : Challenges

- **Atomistic simulation** needed at the nanometer scale.

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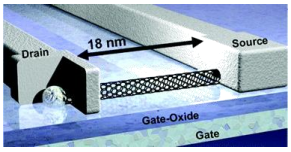
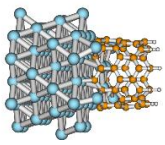
  - Modelize **nano-objects** to understand and optimize their :
    - Structural,
    - Optical, [Light sources, photovoltaics, …]
    - Transport properties. [Nanoelectronics]





Numerical simulation in nanosciences : Challenges

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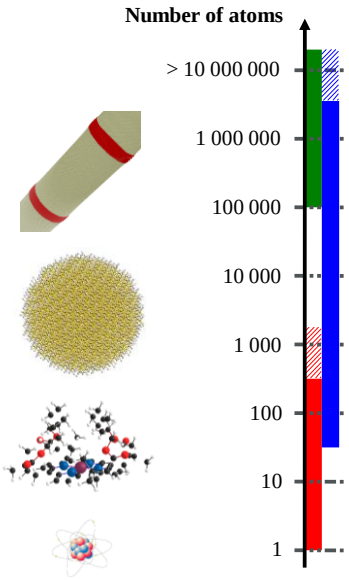
  - Modelize **nano-objects** to understand and optimize their :
    - Structural,
    - Optical, [Light sources, photovoltaics, …]
    - Transport properties. [Nanoelectronics]

Towards a numerical "nanoscope/nanospectrometer" able to compute properties that are hardly accessible experimentally.

Methods



« Multi-scale » approaches

Continuous medium (non atomistic)

Examples : Continuum elasticity, effective mass

« Semi-empirical » methods

Simplified and parametrized hamiltonians
Classical/quantum mechanics

Examples : Inter-atomic potentials (structure)
Tight-binding (electronic props.)
Monte-Carlo (statistics)

« *Ab initio* » methods (« first principles »)

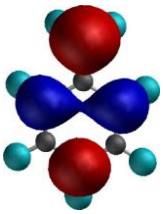
No « adjustable parameters »
(≠ « no approximations »)
Quantum mechanics

Example : Density Functional Theory (DFT).

Ab initio methods

- **No adjustable parameters (≠ no approximations)**.

- Example : Density Functional Theory (DFT).
  - The DFT allows the calculation of the **ground-state energy and properties of solids and molecules** (Hohenberg & Kohn 1964, Kohn & Sham 1965). It consists in replacing the system of interacting electrons with a fictious system of non-interacting electrons moving in an effective potential v_{hxc}.



$$-\frac{\hbar^2}{2m_0}\Delta_{\mathbf{r}}\psi(\mathbf{r})+v(\mathbf{r})\psi(\mathbf{r})+v_{hxc}[\psi](\mathbf{r})\psi(\mathbf{r})=\varepsilon\psi(\mathbf{r})$$

Hartree/Exchange/Correlation potential
(accounts for the effects of the electronic interactions)
Approximations ! (LDA, GGA, ...)
Depends on the ψ's (« self-consistency ») !

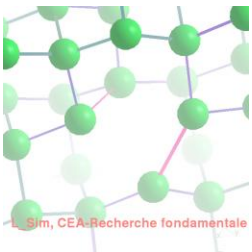
- **Numerically intensive** (10 to ~1 000 atomes depending on the computer).

Application : Vacancy diffusion in silicon (I)

- **Vacancy** = **Missing atom**.

- Semiconductors used in microelectronics are doped : Some silicon atoms have been replaced with e.g., boron or phosphorous to introduce extra electrons or holes.

- These dopants are usually "implanted" in very specific locations on the chip.



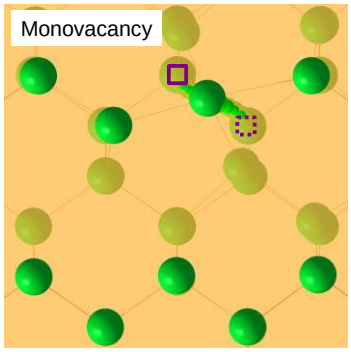
- **Vacancy diffusion induces the migration of dopants**
  ⇒ Dispersion of device characteristics.

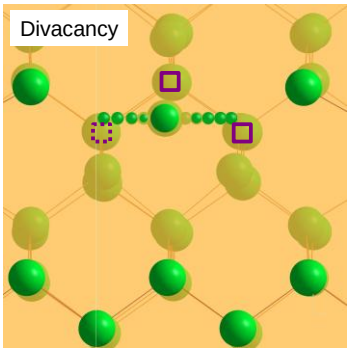
- **The diffusivity of vacancies (related to the "migration energy" E_m) is controversial :**
  - **Watkins 1964 : E_m = 0.45 eV.**
  - **Bracht 2003 : E_m = 1.80 eV...**

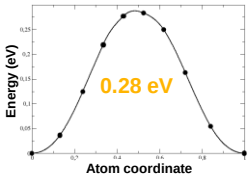
Can atomistic simulation answer to this controversy ?

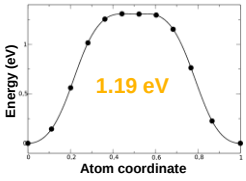
Application : Vacancy diffusion in silicon (II)

- *Ab initio* calculations (216 atoms) :







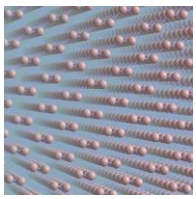


Application : Vacancy diffusion in silicon (III)

- The *ab initio* calculations only provide a hint… What is indeed the exact dynamics of the vacancies ?

- Kinetic Monte-Carlo :

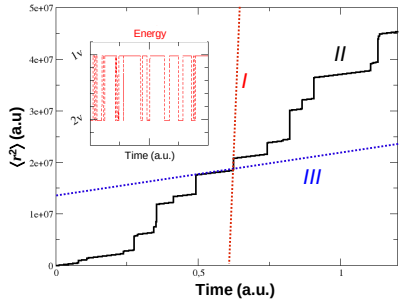
  - **Two vacancies in a > 10 millions Si atoms box**.
    The vacancies can “jump” between neighboring sites.
    The configuration of the system is characterized by the position of the vacancies.

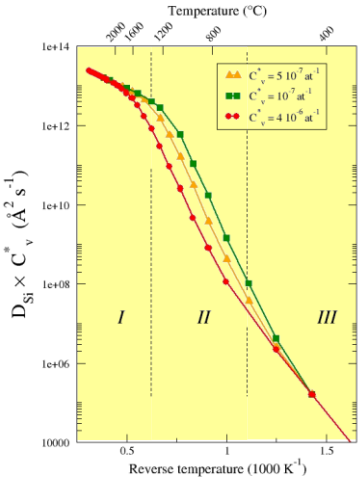


  - **A simplified model for the transition energies**, parametrized on *ab initio* calculations.

  - **An efficient sampling of the configurations space**
    (« Monte-Carlo » algorithms), that allows a fast calculation of the most probable trajectories of the vacancies.

Application : Vacancy diffusion in silicon (IV)



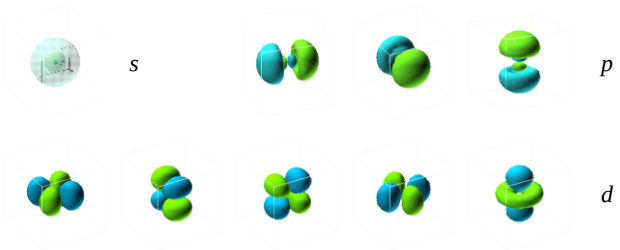


- Three regimes :
  - Low temperature (*III*) :
    Slow divacancy diffusion.
  - High temperature (*I*) :
    Complete divacancy dissociation.
    Fast monovacancy diffusion.
  - Intermediate temperature (*II*) :
    Partial dissociation of divacancies ⇒ **Average diffusivity**.

D. Caliste et P. Pochet, *Vacancy-Assisted Diffusion in Silicon: A Three-Temperature-Regime Model*, Phys. Rev. Lett. **97**, 135901 (2006).

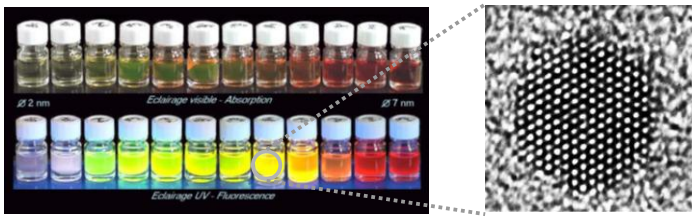
Semi-empirical methods

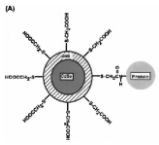
- Example : The tight-binding method.

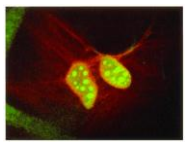


- Principle : **Write the wavefunctions as linear combination of atomic orbitals**.
  - The **range** of the model is limited to 1st, 2nd or 3rd nearest-neighbor atoms.
  - The matrix elements of the hamiltonian are considered as adjustable parameters usually fitted to the bulk band structures then **transferred** to the nanostructures.
  - **The computation time scales linearly with the number of atoms** (up to a few millions of atoms today).

Application : Optical properties of nanocrystals

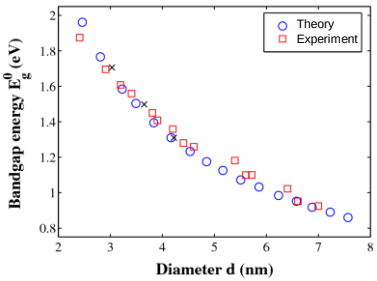




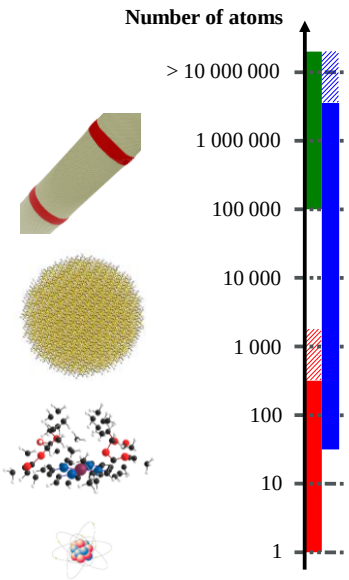


Application : Fluorescent labels in biology

M. Bruchez Jr. *et al.*, Science 1998
W. C. W. Chan and S. Nie, Science 1998



Methods



« Multi-scale » approaches

Continuous medium (non atomistic)

Examples : Continuum elasticity, effective mass

« Semi-empirical » methods

Simplified and parametrized hamiltonians
Classical/quantum mechanics

Examples : Inter-atomic potential (structure)
Tight-binding (electronic props.)
Monte-Carlo (statistics)

« *Ab initio* » methods (« first principles »)

No « adjustable parameters »
(≠ « no approximations »)
Quantum mechanics

Example : Density Functional Theory (DFT).