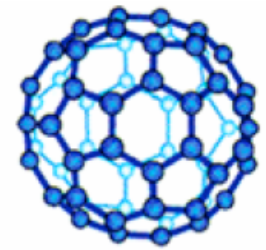
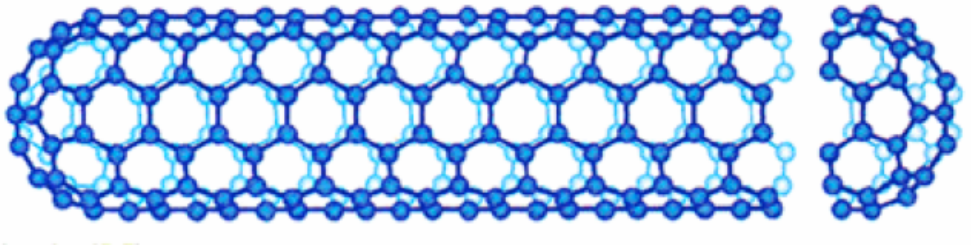
Quantum transport in carbon nanotubes

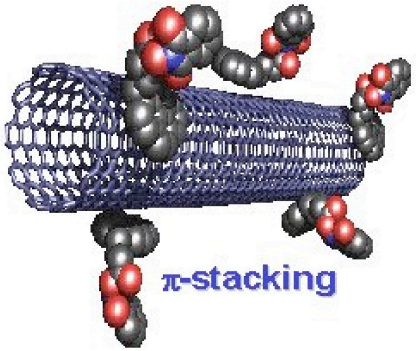
Jean-Christophe Charlier

UNIVERSITY OF LOUVAIN, BELGIUM

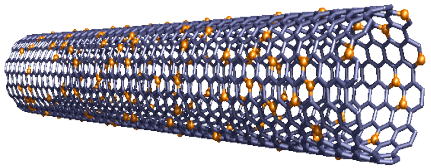
Jean-Christophe.Charlier@uclouvain.be



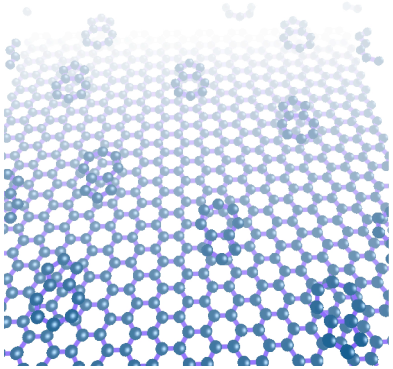




OUTLINE

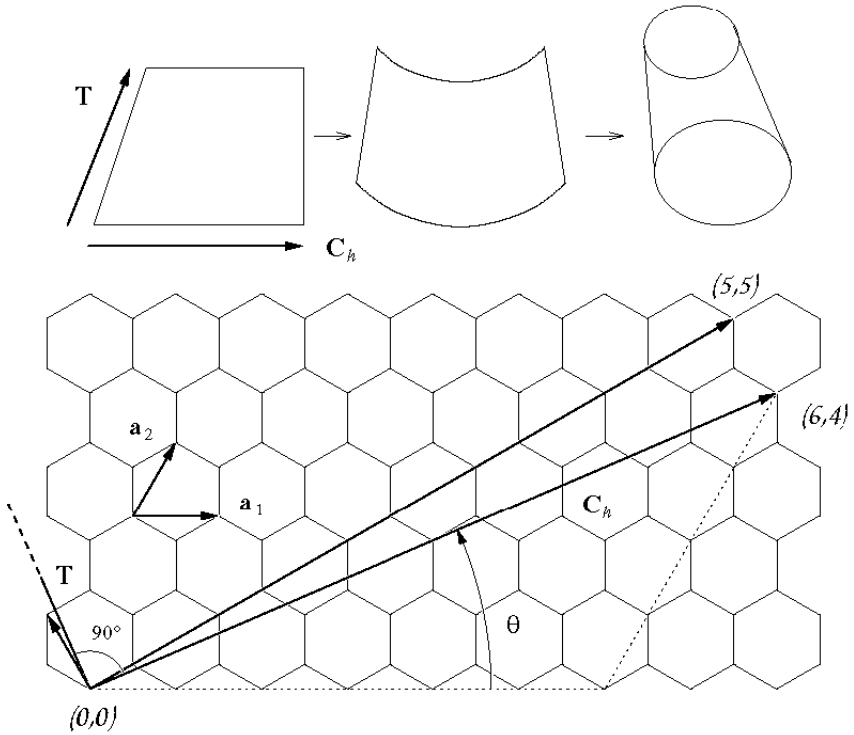


- Quantum transport in ideal carbon nanotubes
  1D ballistic conductor !
- Doping in carbon nanotubes *(boron & nitrogen)*
- Adsorption of organic molecules on carbon nanotubes (*non-covalent functionalisation*)
- Defects in carbon nanotubes *(spintronics)*



Carbon nanotubes

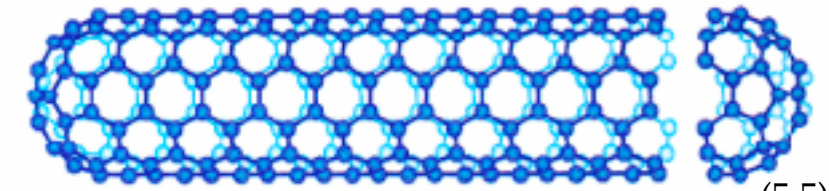
CNT as “rolled” graphene sheet:



Chiral vector: $\mathbf{C}_h = n\mathbf{a}_1 + m\mathbf{a}_2$

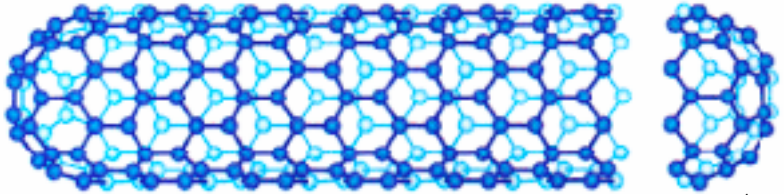
Translational vector: $\mathbf{T} = t_1\mathbf{a}_1 + t_2\mathbf{a}_2$

Armchair: (n,n)



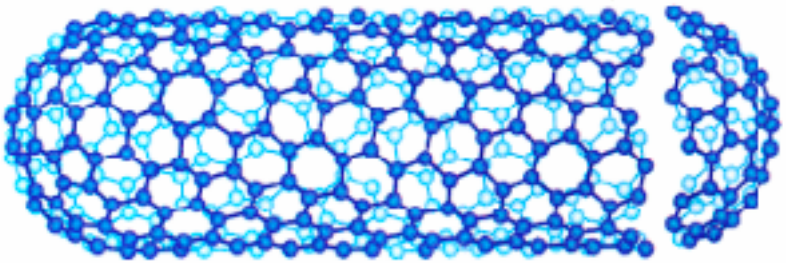
(5,5)

ZigZag: (n,0)



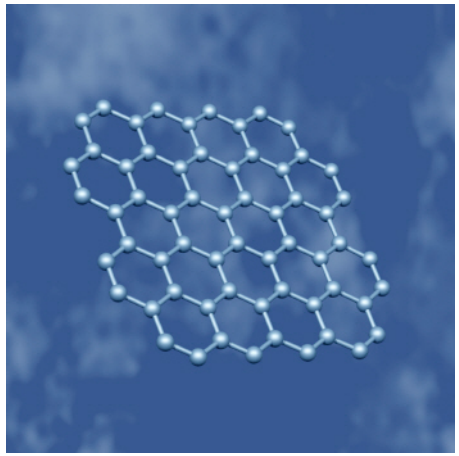
(9,0)

Chiral: (n,m)

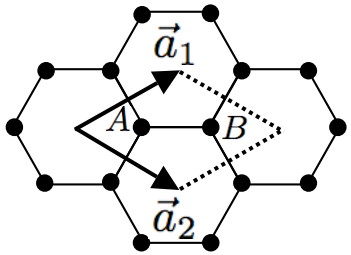


(10,5)

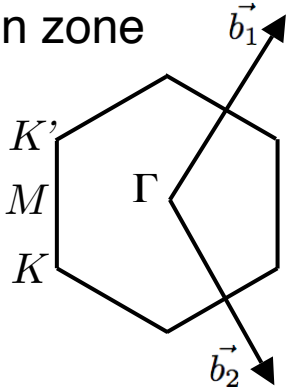
Graphene : electronic structure

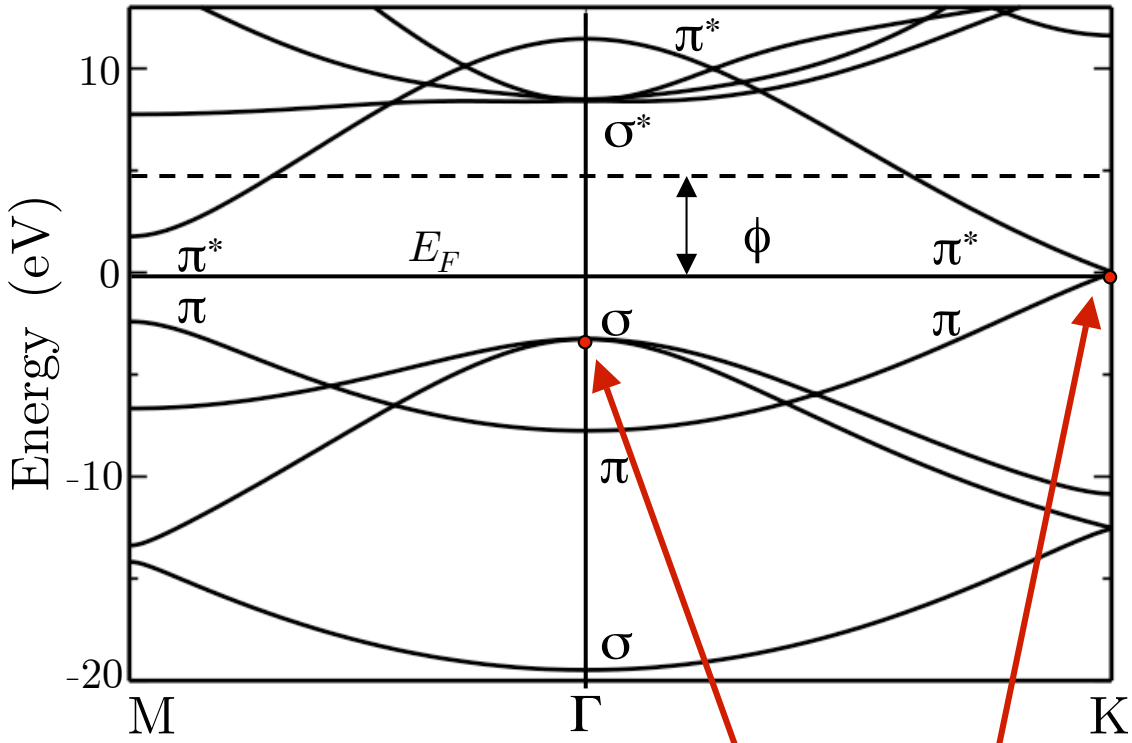


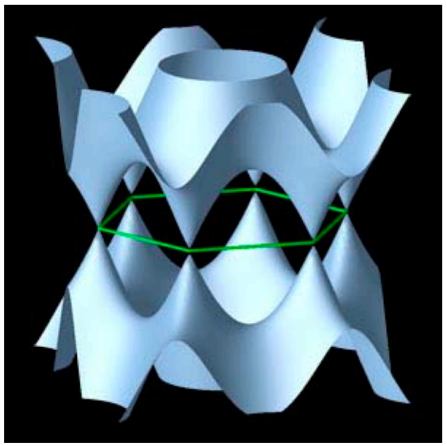
Primitive cell

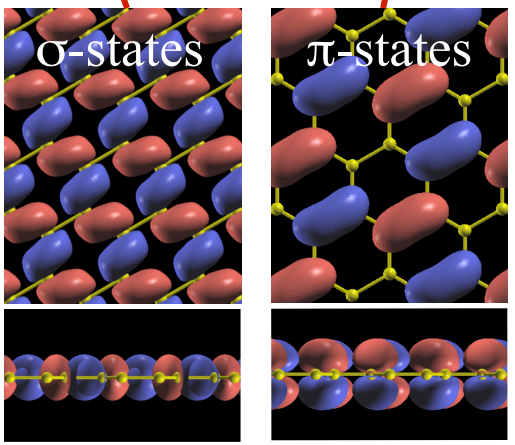


Brillouin zone







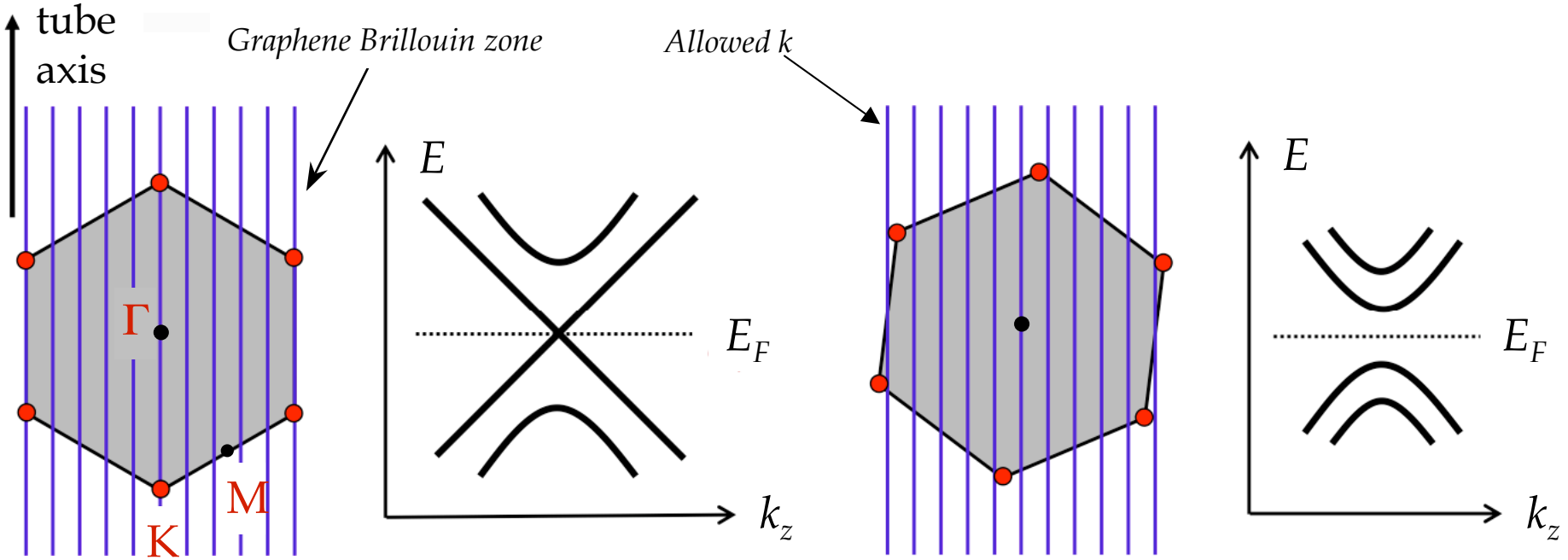


J.-C. Charlier, X. *Blase, S. Roche.*, Rev. Mod. Phys. 2007

Electronic properties

Periodic boundary conditions along the circumference: $\mathbf{C} \cdot \mathbf{k}_{//} = 2\pi q$ → k_x and k_y quantized →

$n - m = 3l$: metal
$n - m = 3l \pm 1$: semiconductor
$l = 0, 1, 2, \ldots$

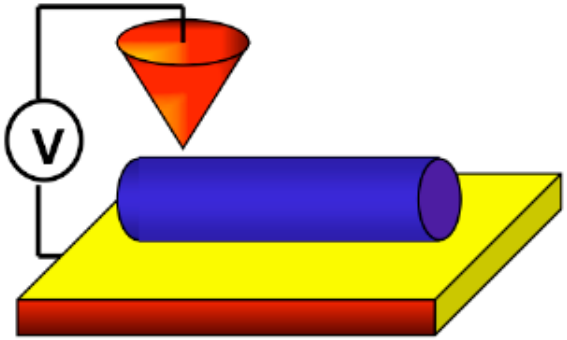


1D Metal
i.e. arm(5,5), zigzag(12,0)

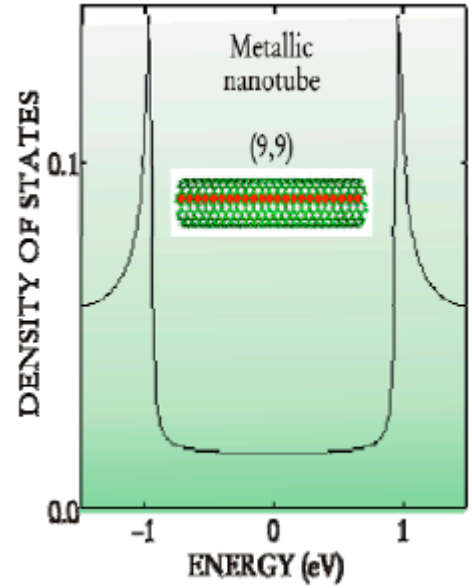
1D Semiconductor
i.e. zigzag(8,0)

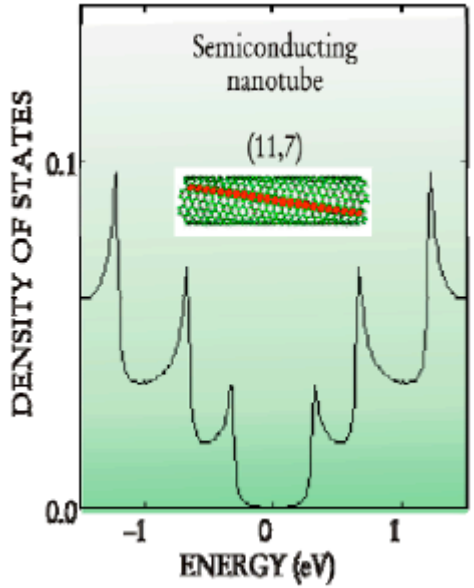
CNT : electronic properties

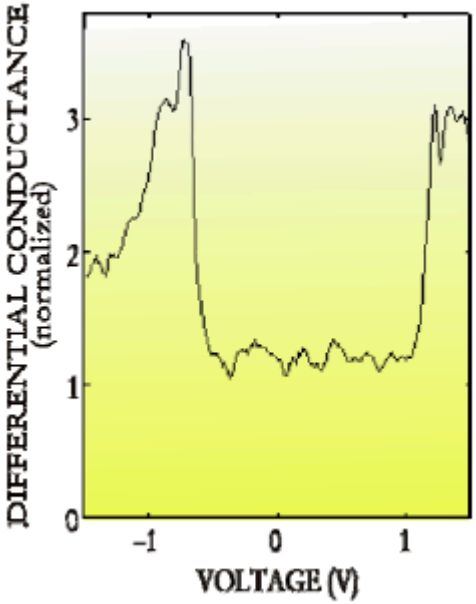
STMicroscopy and
STSpectroscopy

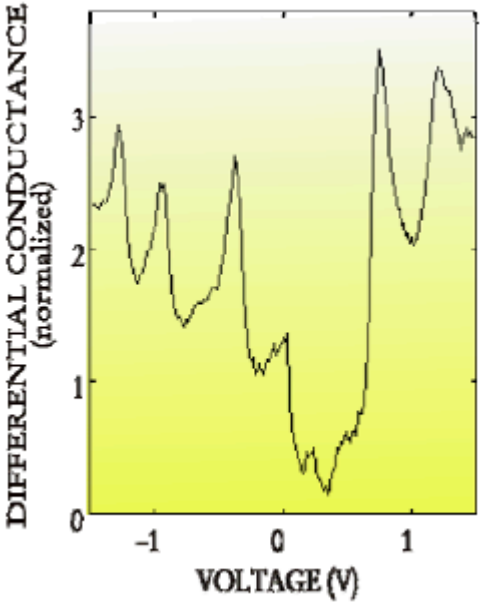


- ϕ, d --> n, m
- E_{gap}
- IV
- dI/dV $\propto$ DOS







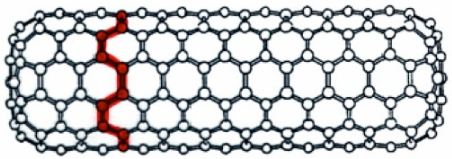


Wildöer, Venema, Rinzler, Smalley, Dekke
Nature **391**, 59 (1998)

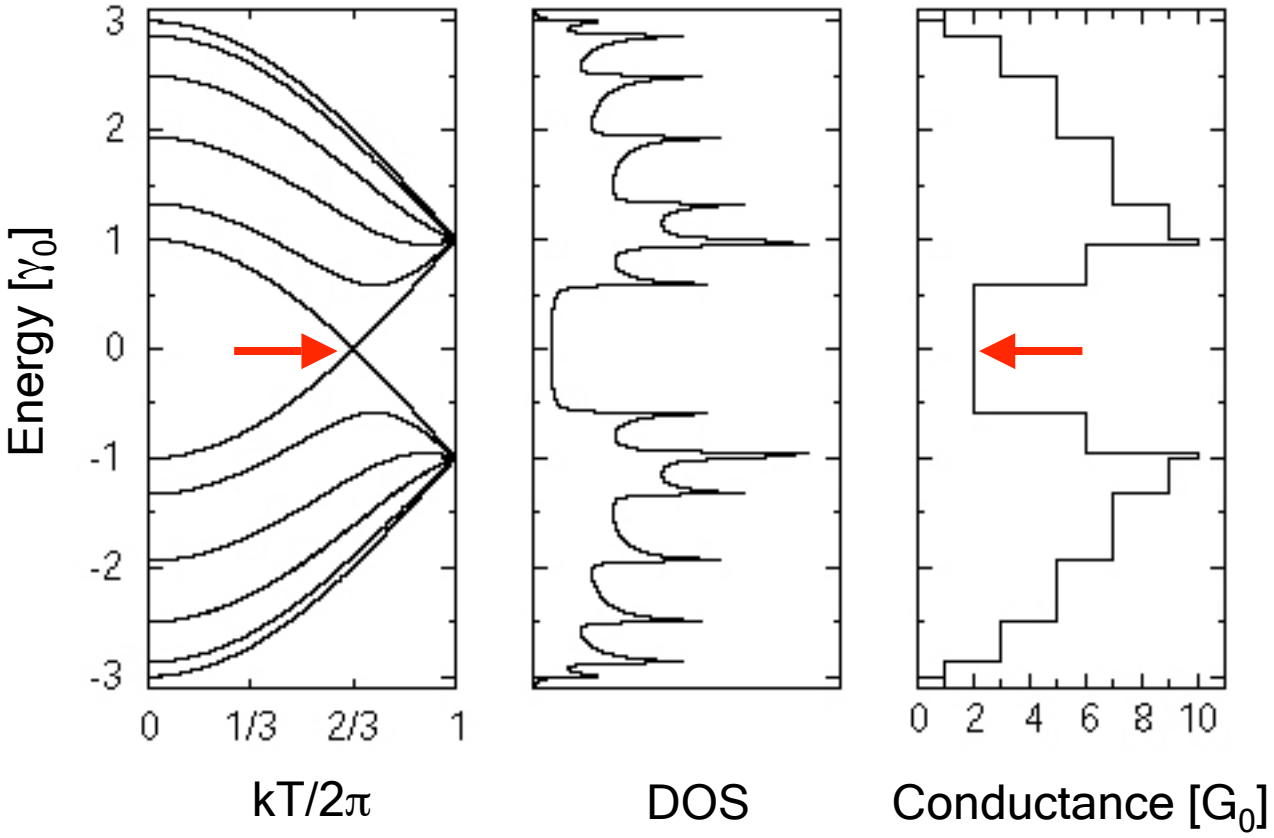
Odom, Huang, Kim, Lieber
Nature **391**, 62 (1998)

CNT : ballistic conductor

Example : an ideal armchair carbon nanotube



arm(5,5), π-π* tight-binding



Landauer-Büttiker [PRB **31**, 6207 (1985)] equilibrium transport @ 0K and V=0 :

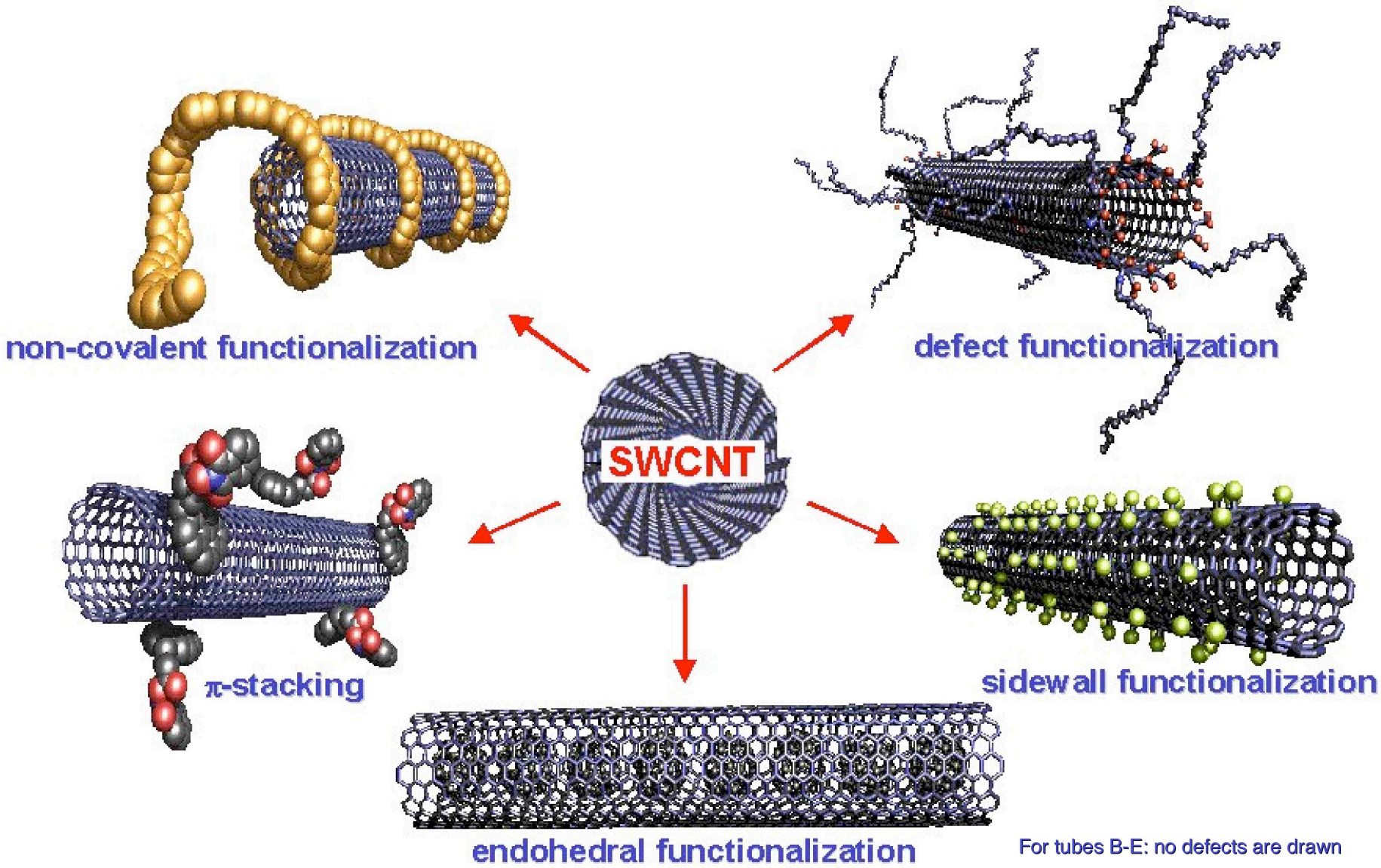
$G(E) = T(E).G_0$

Where $G_0 = 2e^2/h$ = quantum of conduct.
T(E) = transmission coefficient of scattering theory
T(E) ~ # conduction channels @E

$v_F \sim 10^6$ m/s
$\lambda_e \sim 1$ μm

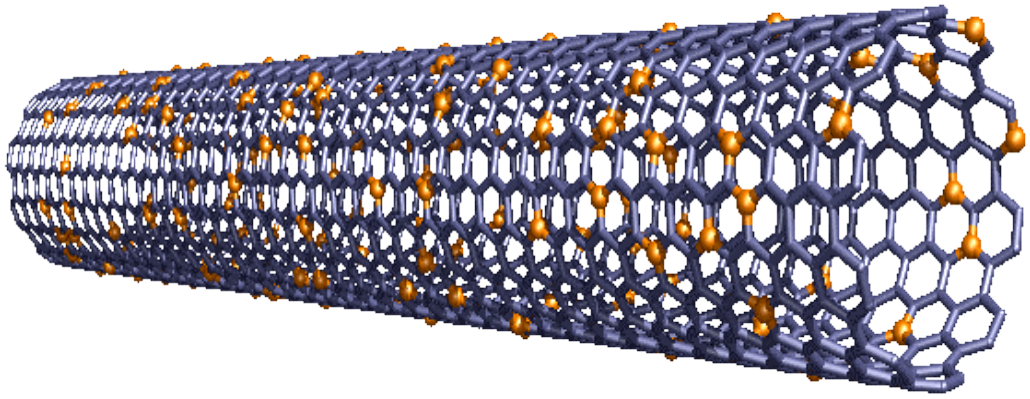
$G(E_F) = T(E_F).G_0 = 2$ units of $2e^2/h$
$\sim (12.9\ k\Omega)^{-1}$

CNT : functionalization



For tubes B-E: no defects are drawn

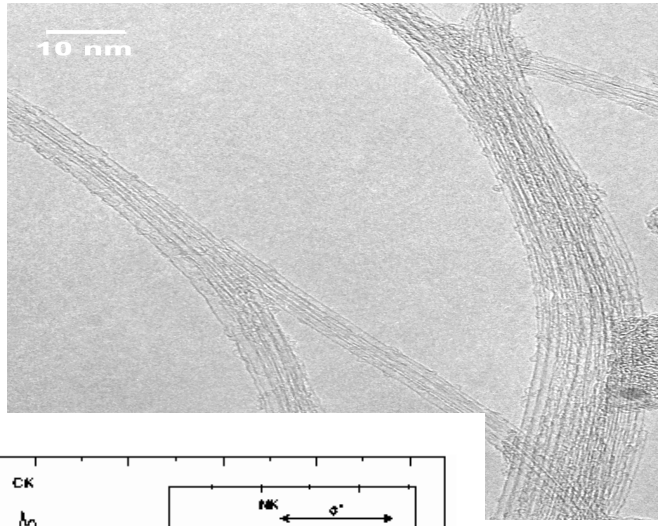
1. DOPING

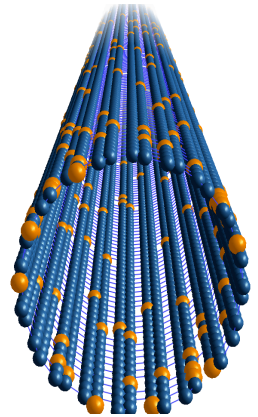


Doping carbon nanotubes

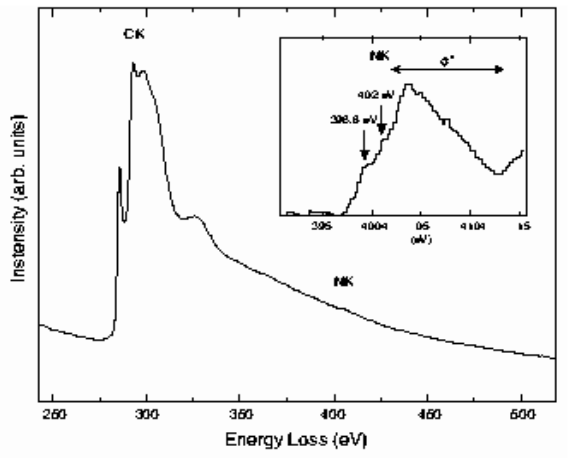
Incorporation of N_2(gas) during the synthesis

Bundles of Nitrogen-doped Single-wall nanotubes



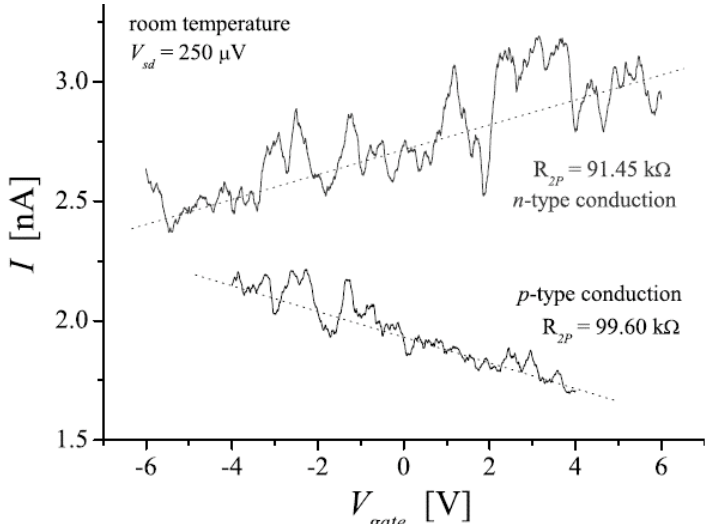


M. Glerup *et al.*
Chem. Phys. Lett.
387, 193 (2004)



EELS spectrum

Fig. 3. EEL core electron K-shell spectra of CN_x nanotube bundles (sample 4). The nanotubes are doped with around 1 at.% nitrogen. For the C-K edge well defined π^* and σ^* fine structure features are observed which are evidences of sp^2-hybridisation in graphitic structures. The inset is a magnification of the N-K edge.

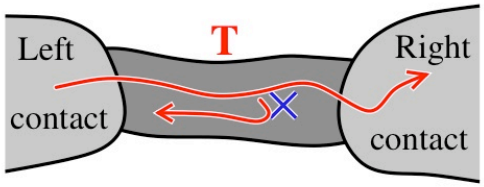


V. Krstic *et al.*
Europhys. Lett. 77, 37001 (2007)

Computation of the transport properties

Landauer

Computation of the *transfert probability* from the left lead to the right lead.



Conductance from transmission:

$$G(E) = G_0 . \sum_{p \in \mathrm{L}} \sum_{q \in \mathrm{R}} \mathrm{T}_{p \to q}$$

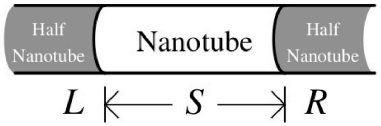
Conductance from Green function

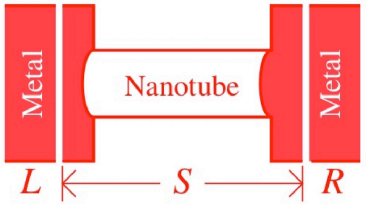
$$T = \mathrm{Tr}\left[\Gamma_L G_S^{(r)} \Gamma_R G_S^{(a)}\right]$$

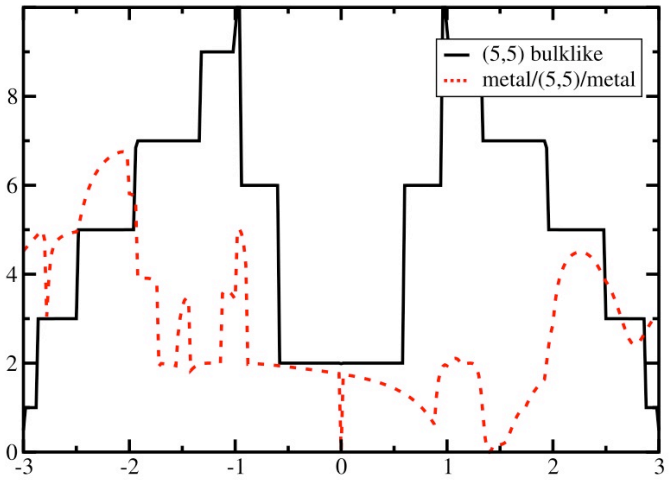
with $\Gamma_{L,R} = i\left[\Sigma_{L,R}^{(r)} - \Sigma_{L,R}^{(a)}\right]$

and $G_S^{(r,a)} . \left[E - \hat{H}_S - \Sigma_L^{(r,a)} - \Sigma_R^{(r,a)}\right] = \hat{1}$

Discussion on the leads







Elastic scattering only?

- No exange without any reservoir (like phonons e.g.)
- No electron-electron interactions are taken into account

S. Datta, *Quantum transport : Atom to transistor*, Cambridge University Press 2006

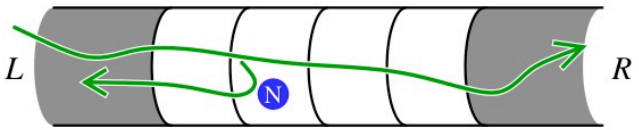
B and N: one substitution

ab initio study (DFT-LDA)

Model:

The system is a (10,10) nanotube containing a single substitution.

The leads are made from two half-infinite perfect nanotubes

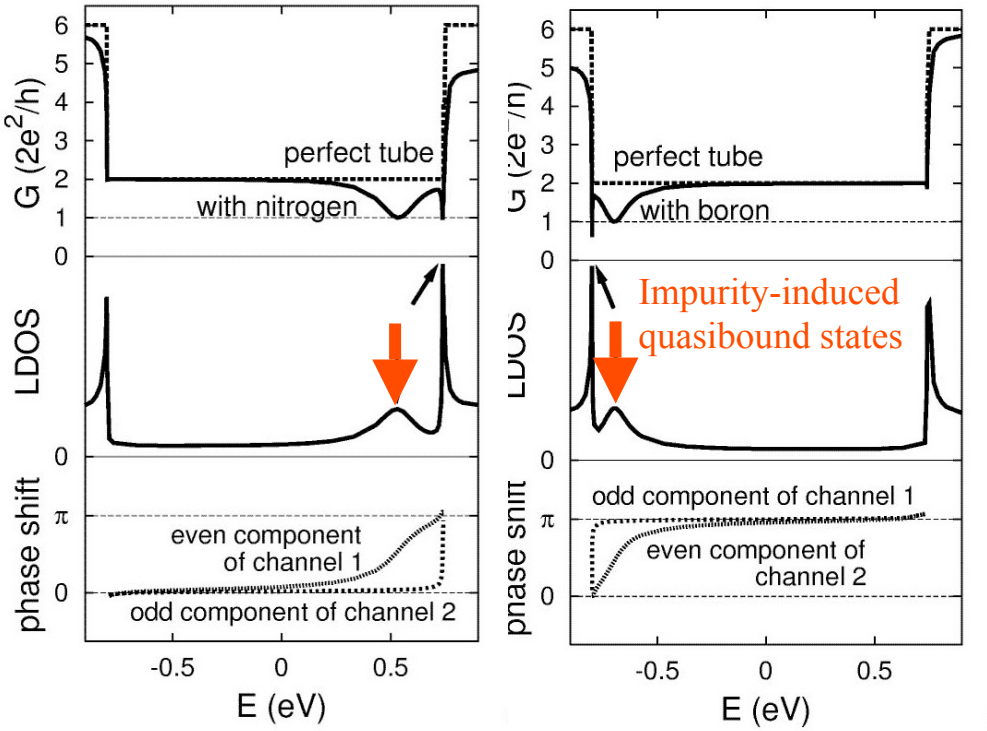


H. J. Choi *et al*,

Phys. Rev. Lett. **84**, 2917 (2000)

Nitrogen

Boron

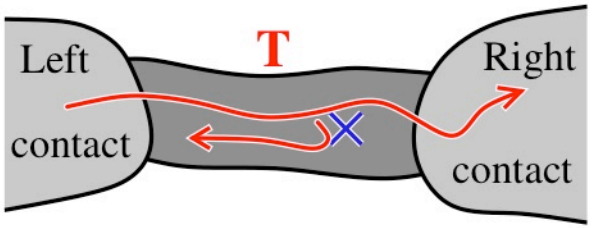


1 atomic substitution within an 8 cells long carbon nanotube

Computation of the transport properties

Landauer

Computation of the *transfert probability* from the left lead to the right lead.

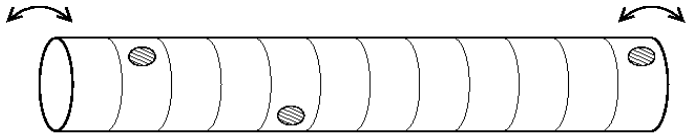


Conductance from transmission:

$$G(E) = G_0 . \sum_{p \in \mathrm{L}} \sum_{q \in \mathrm{R}} \mathrm{T}_{p \to q}$$

“Device”

Kubo



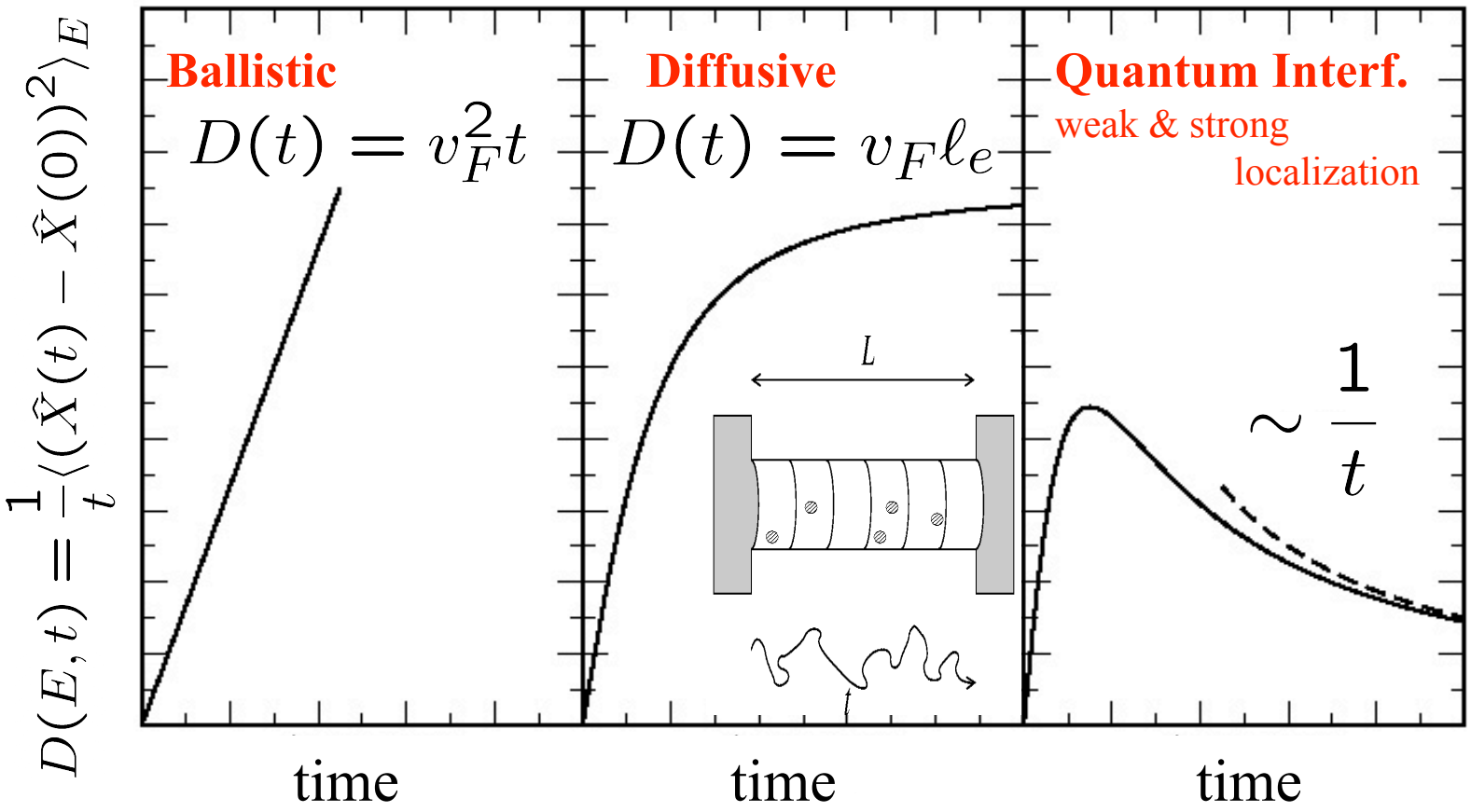
Electronic conductivity is a measure of the correlation function of charge carriers

$$\sigma_{\mathrm{DC}}(E) = \frac{2e^2\hbar}{\Omega} f(E)$$

$$f(E) = \frac{n(E)}{2\pi\hbar} \lim_{t \to \infty} D_E(t)$$

“Material”

Quantum transport regimes and conductance scaling



$$G(E) = \frac{2e^2}{h} N(E)$$

$$G(E) = \frac{2e^2}{h} \frac{\ell_e}{L_{syst}}$$

$$G(E) = \frac{2e^2}{h} \left(\frac{\ell_e}{L_{syst}} - \delta\sigma\right)$$

$$G(E) = \frac{2e^2}{h} exp\left(-\frac{\ell_e}{L_{syst}}\right)$$

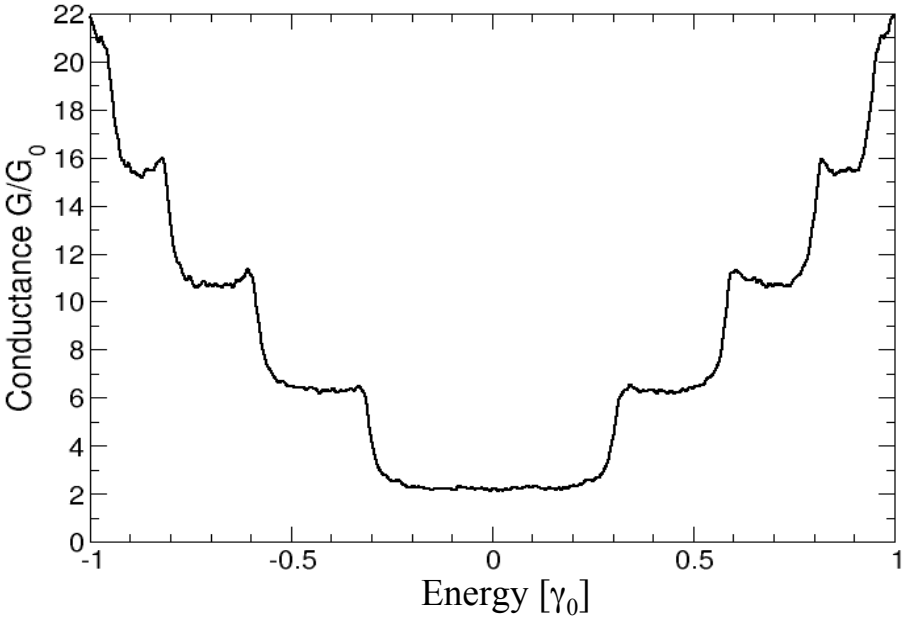
➡ conductance quantification !

ℓ_e : *electronic mean free path*

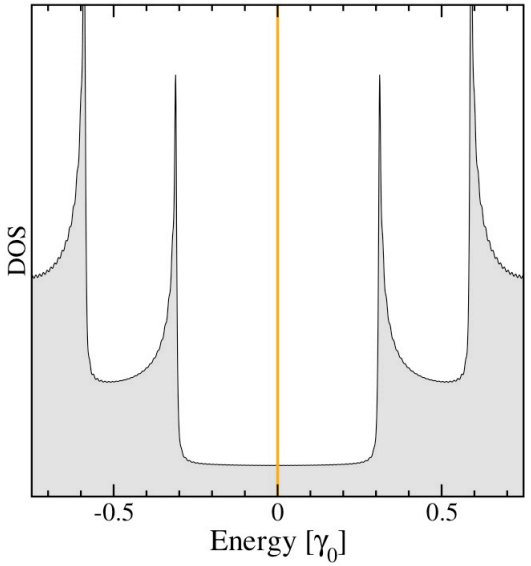
S. Roche et al., Phys. Rev. Lett. **79**, 2518 (1997).

Pristine (10,10) carbon nanotube

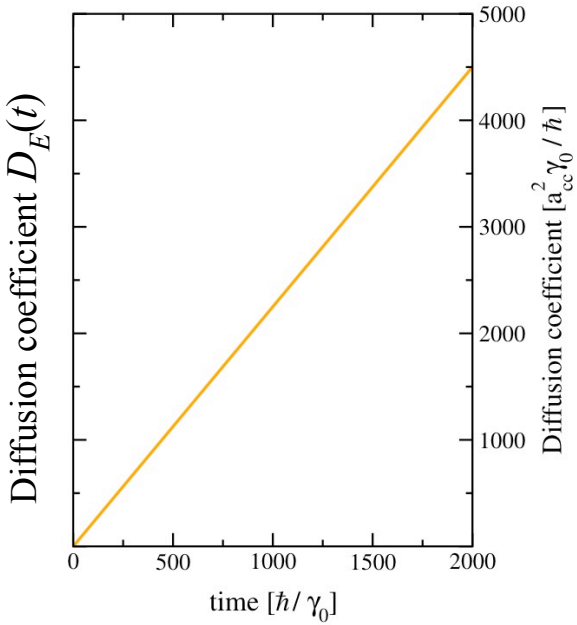
Conductance :



DOS :



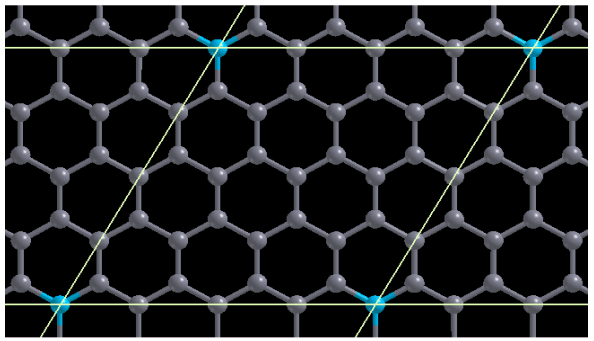
Ballistic regime !

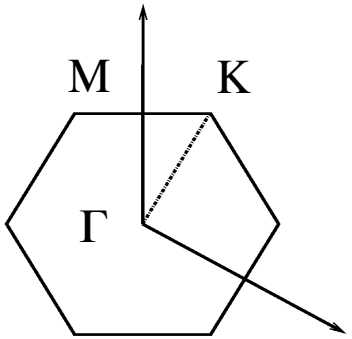


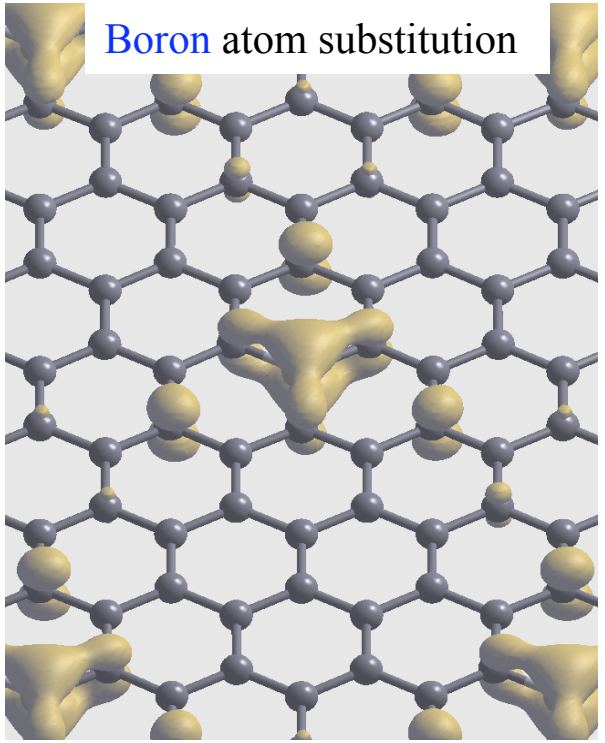
B- or N-doped (10,10) carbon nanotube

How to treat accurately the charge transfer ?

http://www.abinit.org





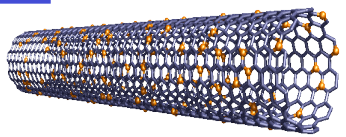


First-principles calculations

- Density Functional Theory (DFT)
- Local Density Approximation (LDA)
- Pseudopotentials
- Supercell geometry (10Å vacuum between tubes)
- Plane wave expansion (30 Ha)
- Code : abinit

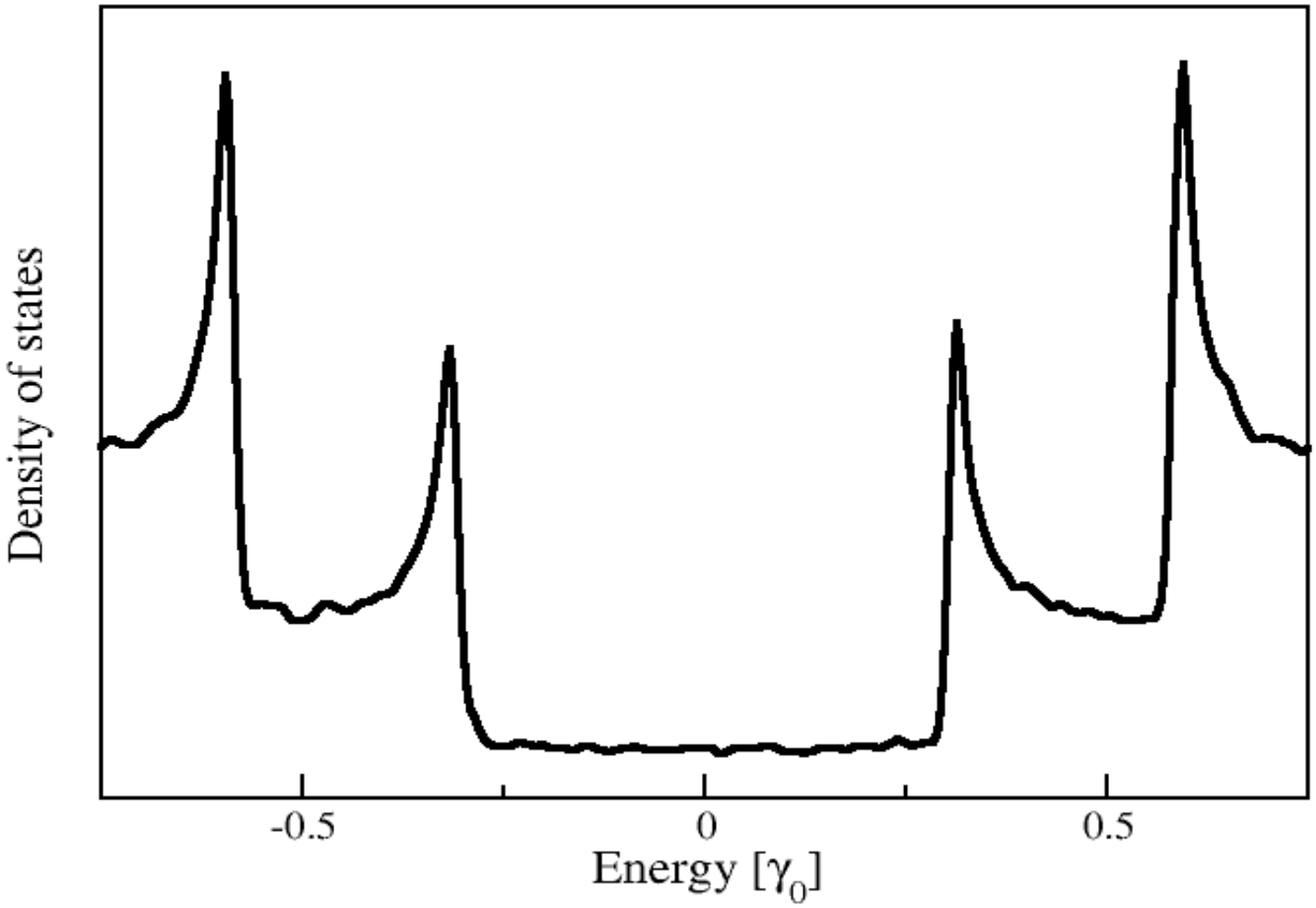
S. Latil, S. Roche, D. Mayou and J.-C. Charlier
Phys. Rev. Lett. 92, 256805 (2004).

Boron-doped nanotubes: Density of States

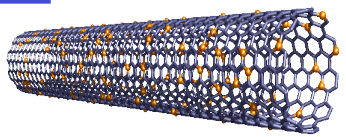


Nanotube (10,10)

BORON: 0.01 %

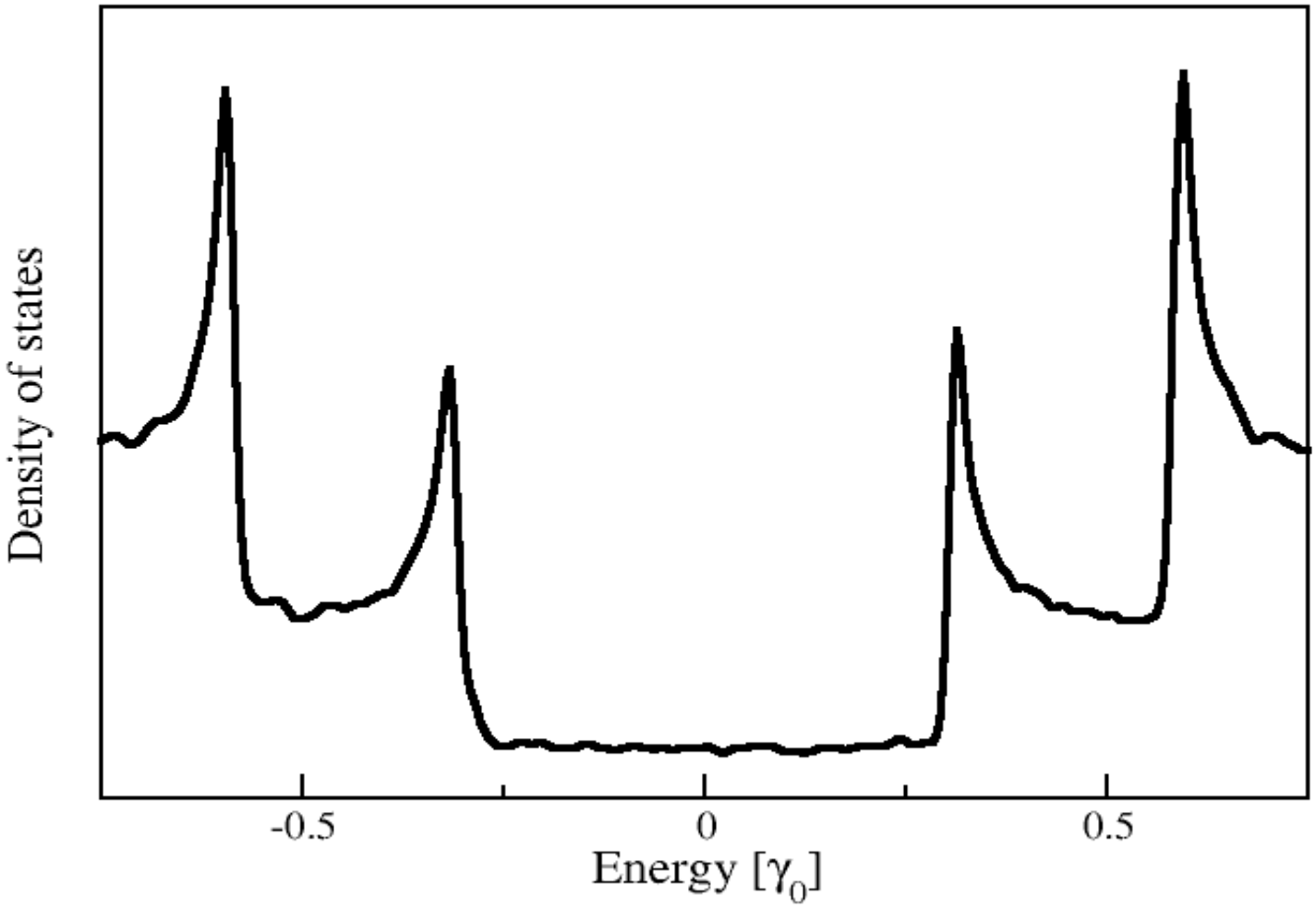


Boron-doped nanotubes: Density of States

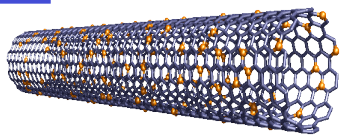


Nanotube (10,10)

BORON: 0.02 %

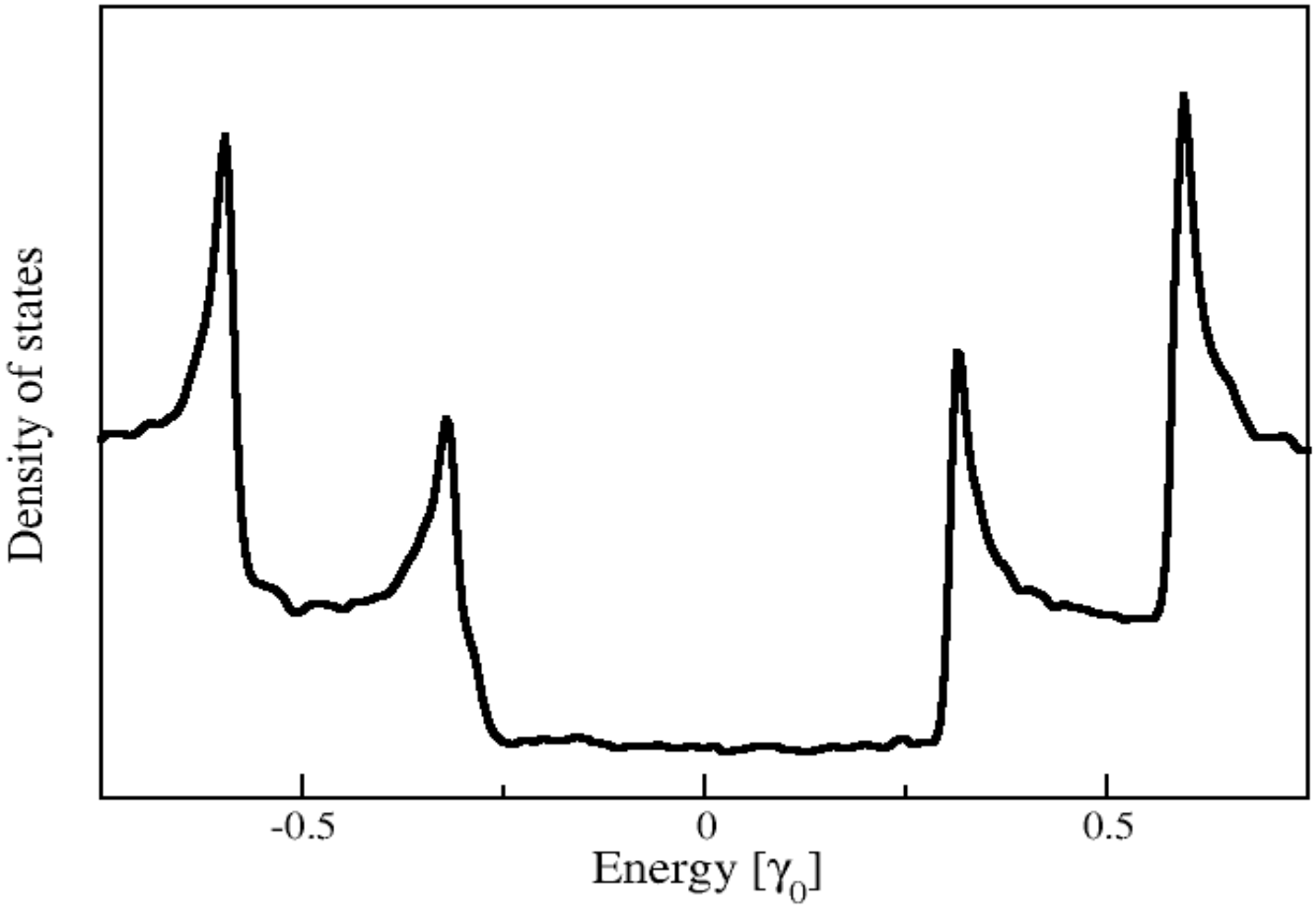


Boron-doped nanotubes: Density of States

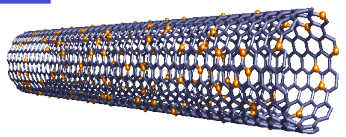


Nanotube (10,10)

BORON: 0.05 %

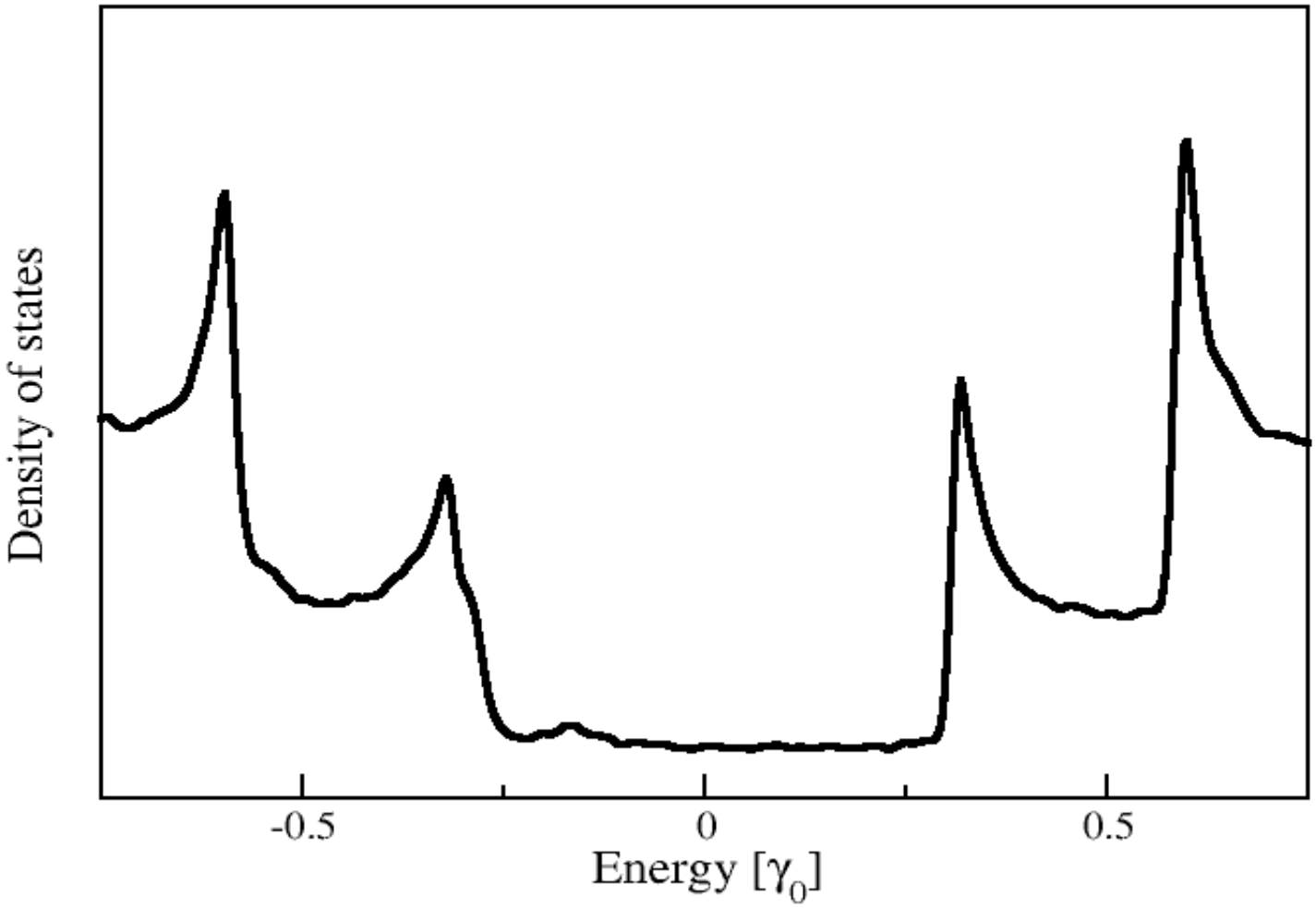


Boron-doped nanotubes: Density of States

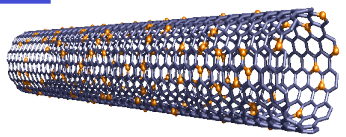


Nanotube (10,10)

BORON: 0.1 %

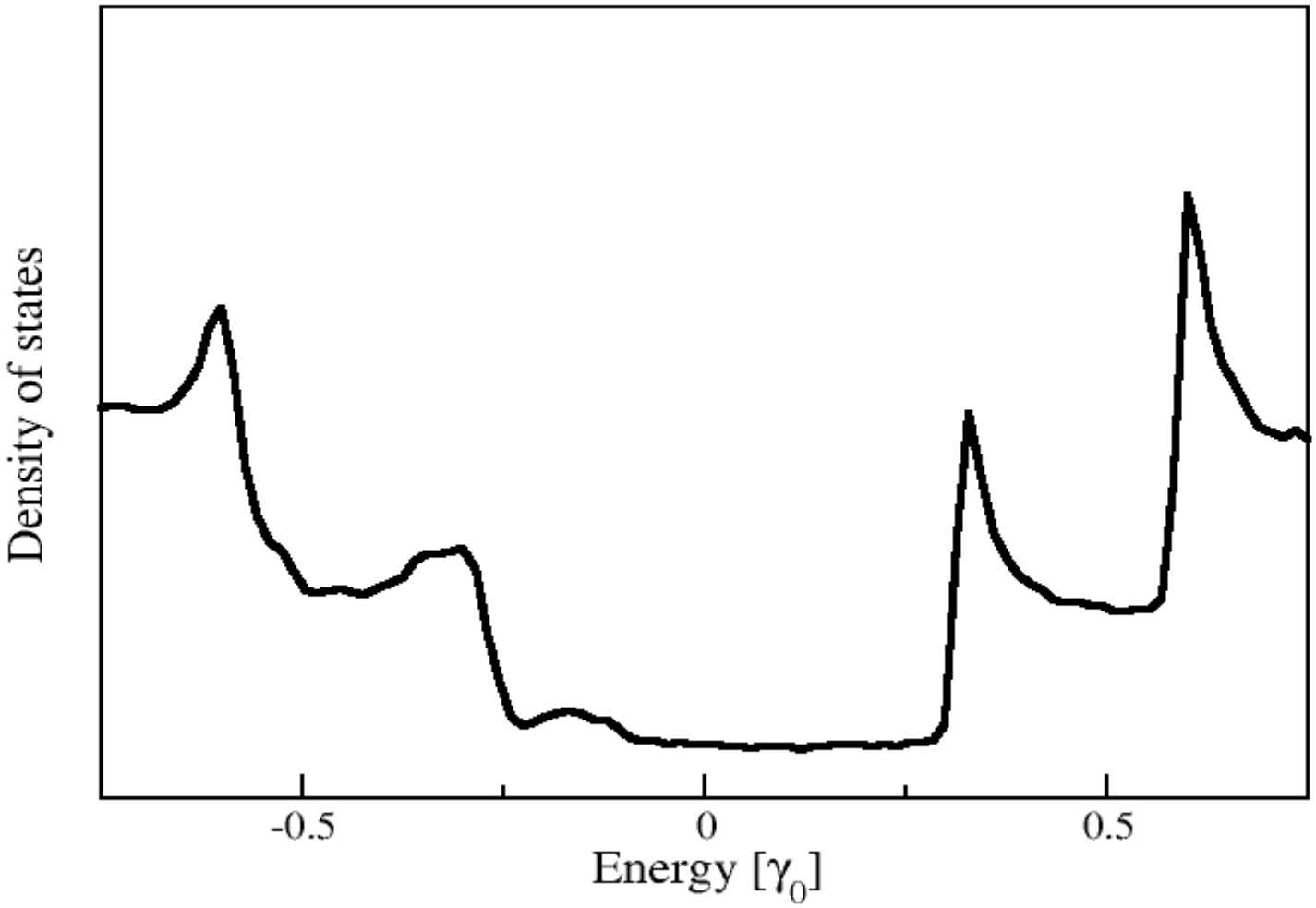


Boron-doped nanotubes: Density of States

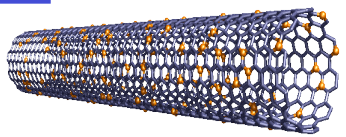


Nanotube (10,10)

BORON: 0.2 %

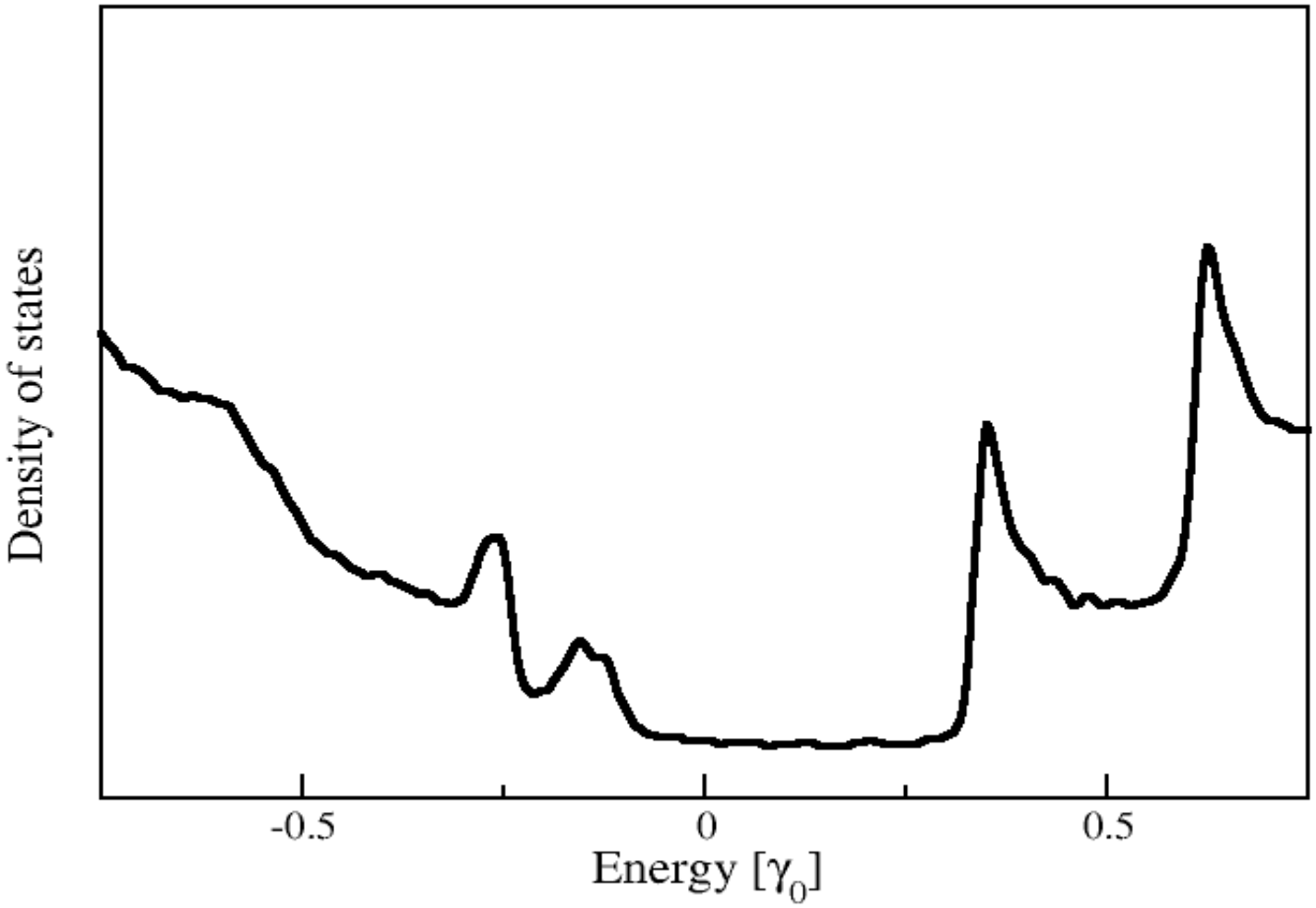


Boron-doped nanotubes: Density of States



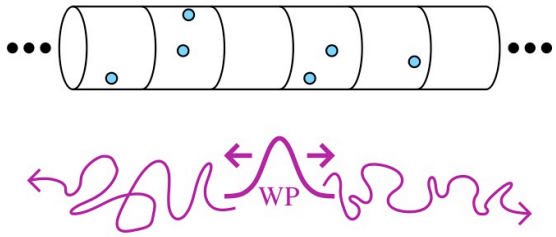
Nanotube (10,10)

BORON: 0.5 %

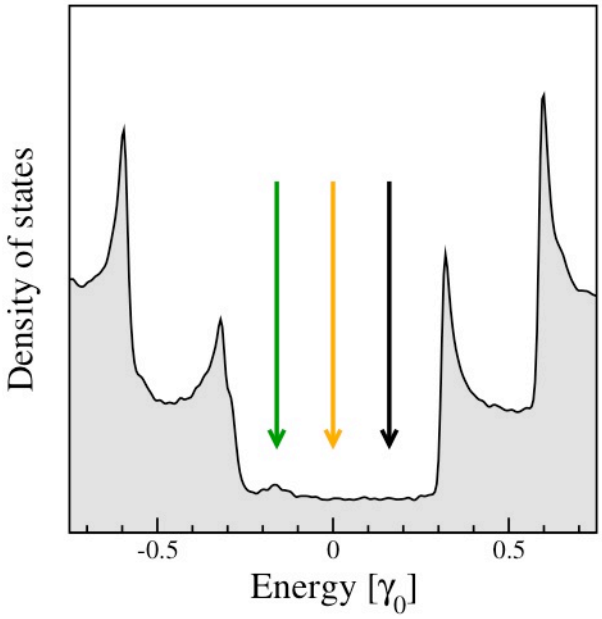


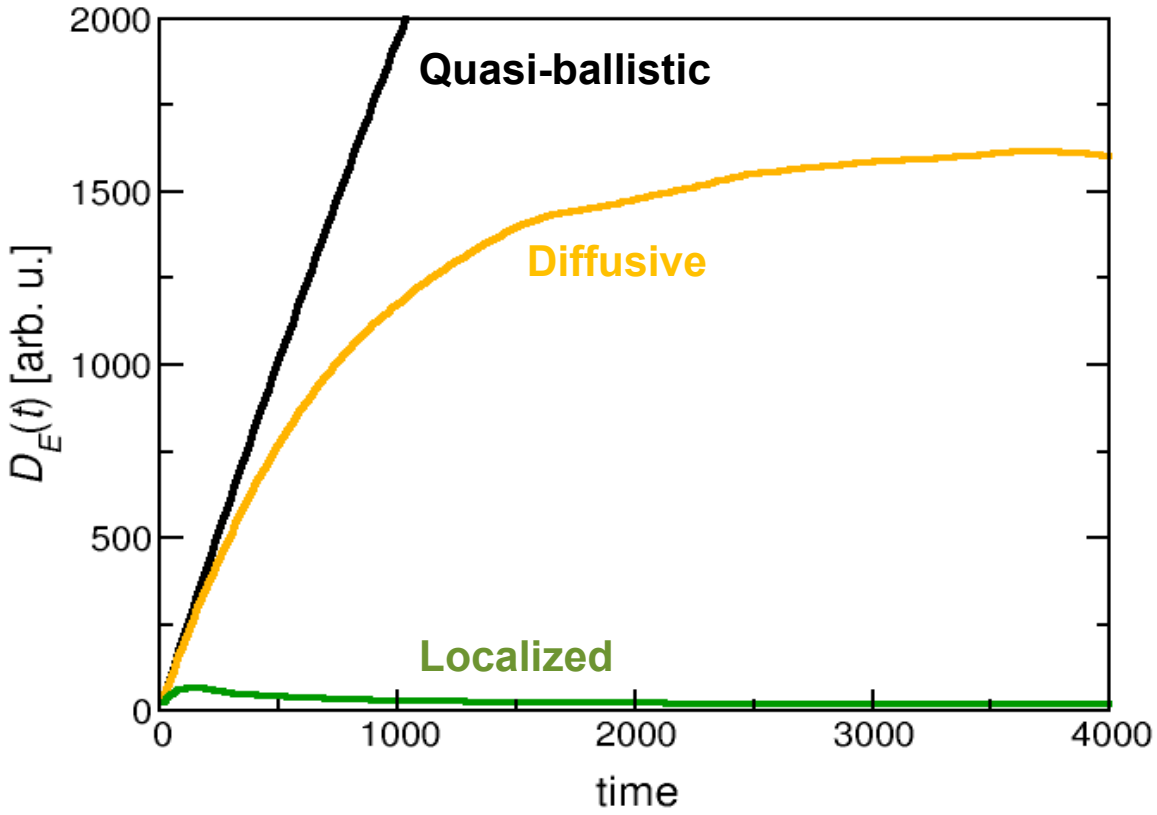
Boron-doped nanotubes: Quantum diffusion

Determination of the conduction regime :



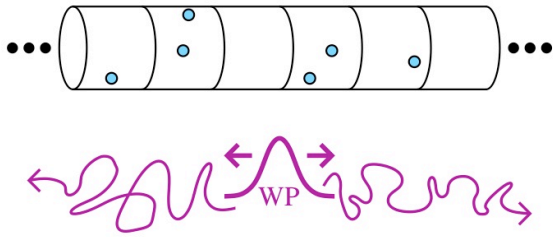
(10,10) - CNT containing 0.1% of boron impurities, located randomly.



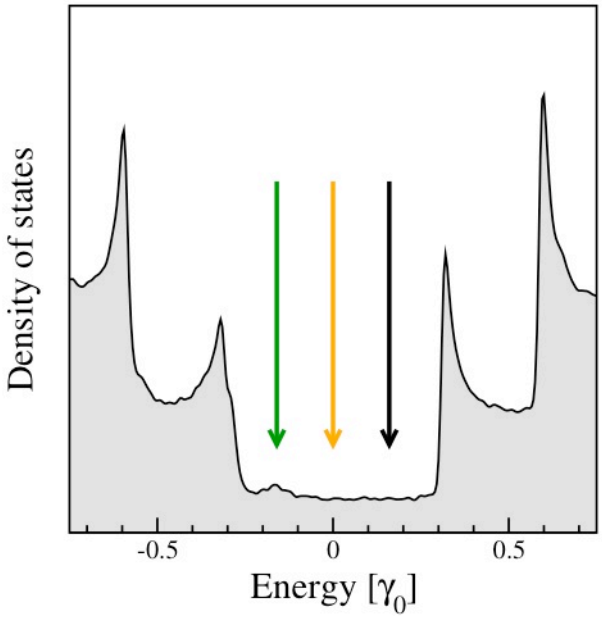


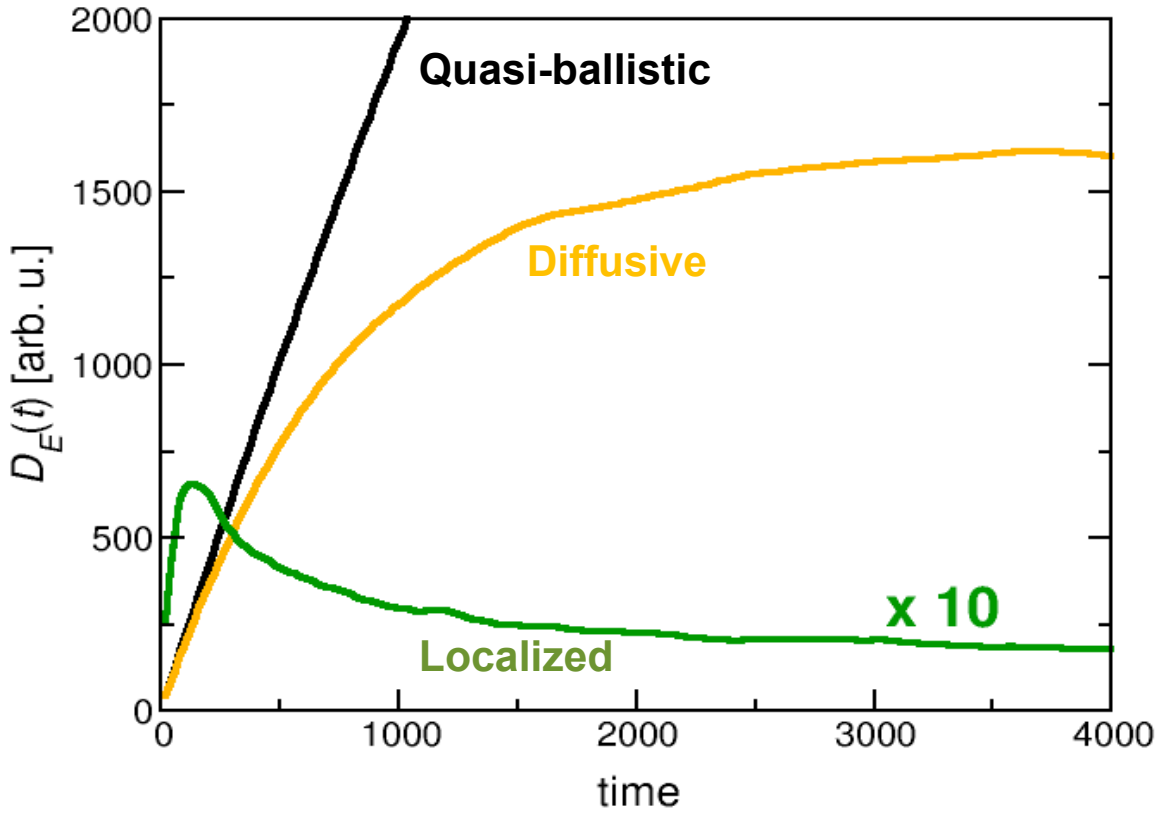
Boron-doped nanotubes: Quantum diffusion

Determination of the conduction regime :



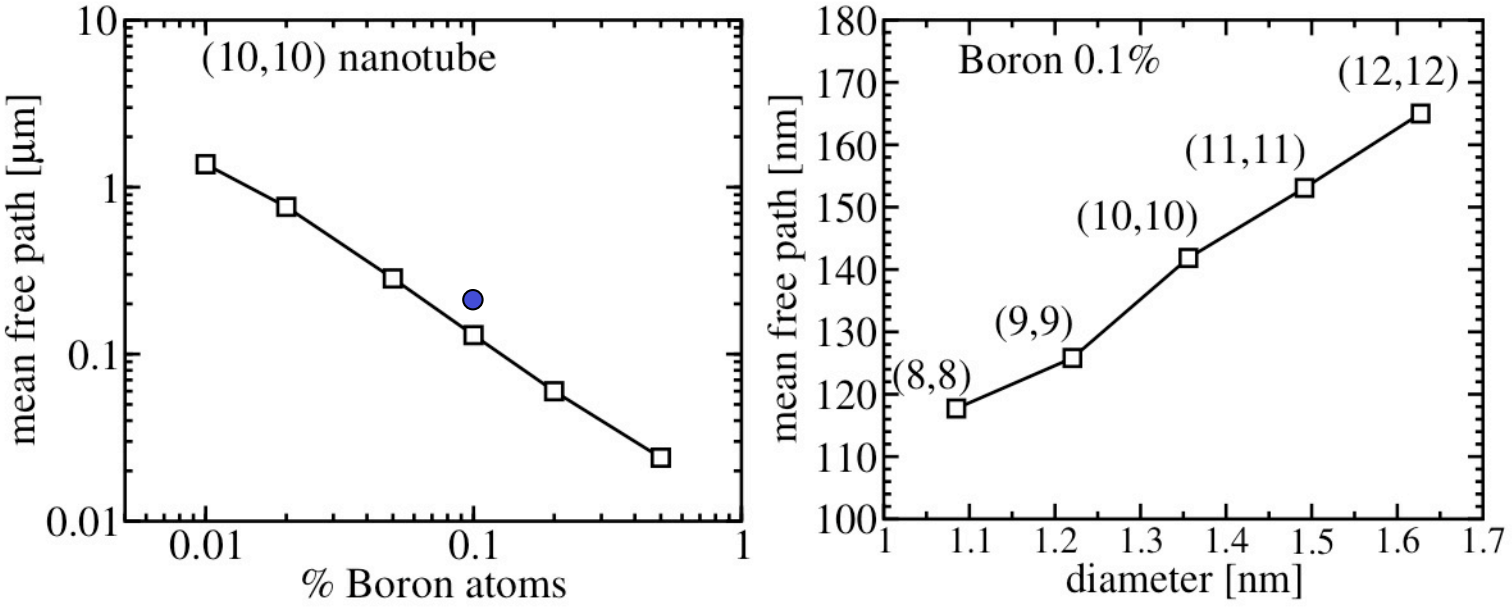
(10,10) - CNT containing 0.1% of boron impurities, located randomly.





B doped nanotubes

Scaling of the mean free path at $E = E_F$



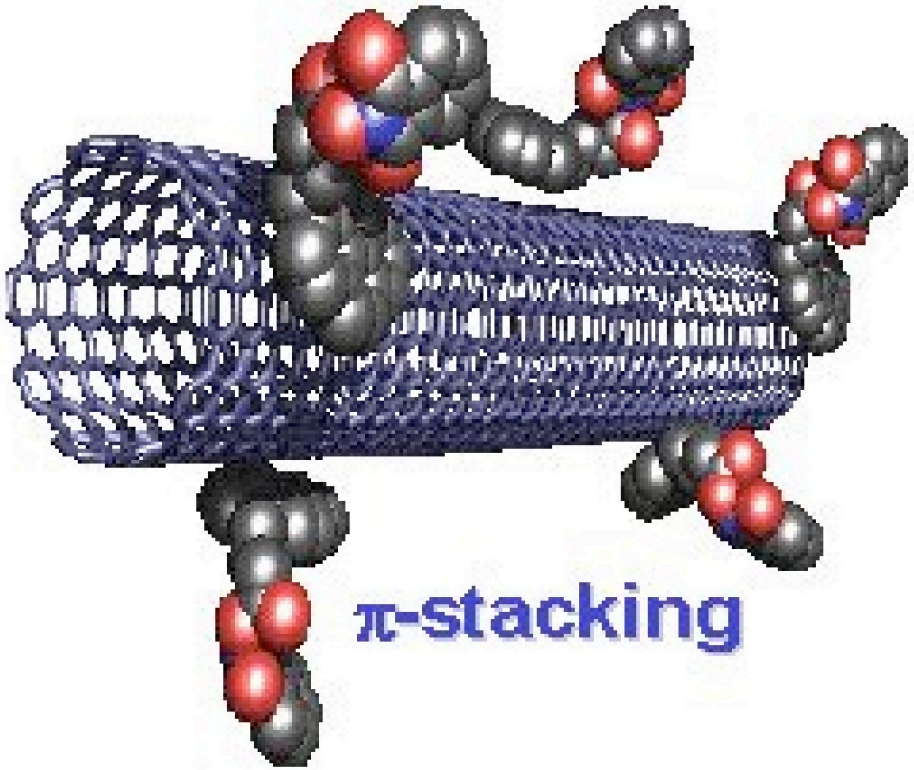
- $\ell_e(E_F)$ scales inversely with disorder "strength" → $\left(\ell_e \simeq \frac{1}{\rho_B}\right)$
- $\ell_e(E_F)$ scales linearly with nanotube radius

In agreement with experimental data [0.1% B, 20nm diam.] :

PRB 63, 161404 (2002) ; PRB 67, 041401 (2003)

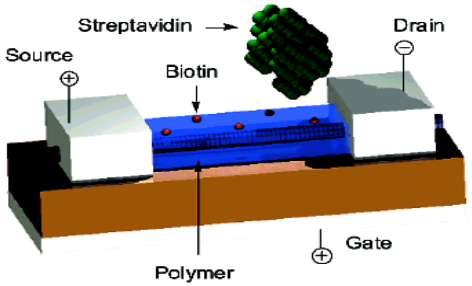
- $\ell_e \simeq 220 - 250nm$

2. NON-COVALENT FUNCTIONALIZATION



Non-covalent functionalization of carbon nanotubes

Motivations:



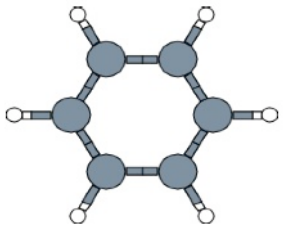
- Bundles of carbon nanotubes (CNT)

  ⇒ Spread them into a matrix

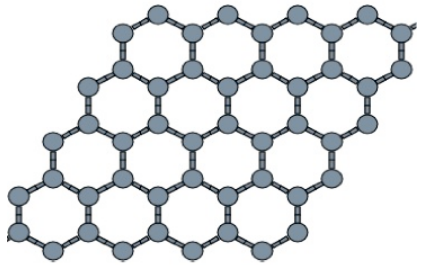
- Functionalize the CNTs and keep their conduction properties

  ⇒ "Soft" functionalization, non-covalent

- Fundamental study, reactivity with organic molecules (gas sensors)



π-stacking interaction between π-conjugated systems...

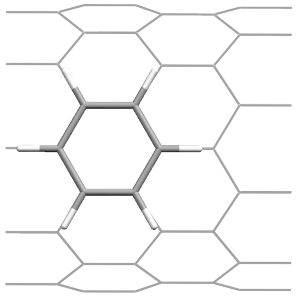


⇒
- Weak interactions (including Van der Waals forces) between two systems with π electrons
- Low binding energy (small overlap), but may modify the electronic properties

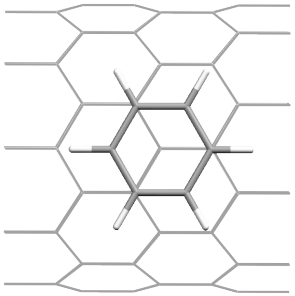
Benzene on NANOTUBE

- Perfect tubes, frozen system, large enough supercells (> 10Å vac.)
- Various adsorption sites considered

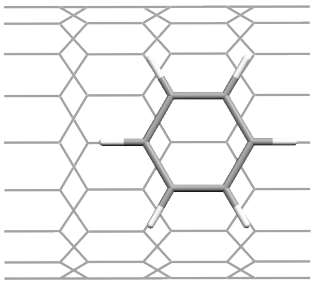
abinit



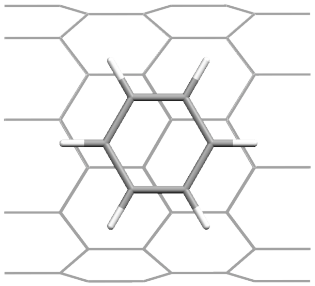
Hexagon



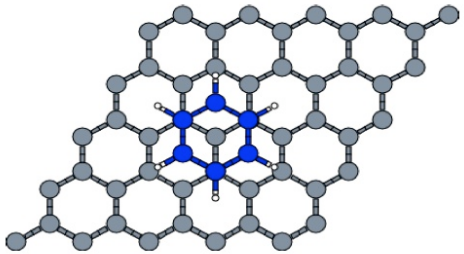
Stack



Bridge

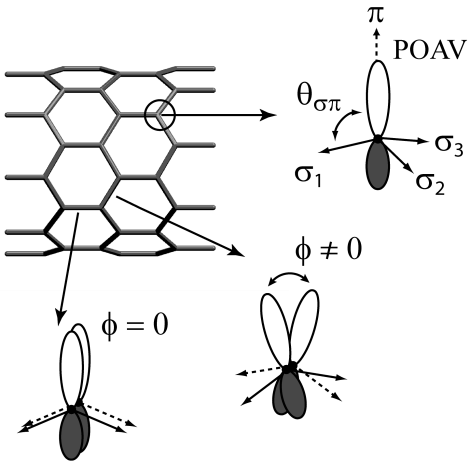


Bridge-bis



F. Tournus, *et al.*, PRB 71, 165421 (2005)
F. Tournus *et al.*, PRB 72, 075431 (2005)

"The smaller the POAV misalignment angle is, the more favorable the benzene adsorption is."

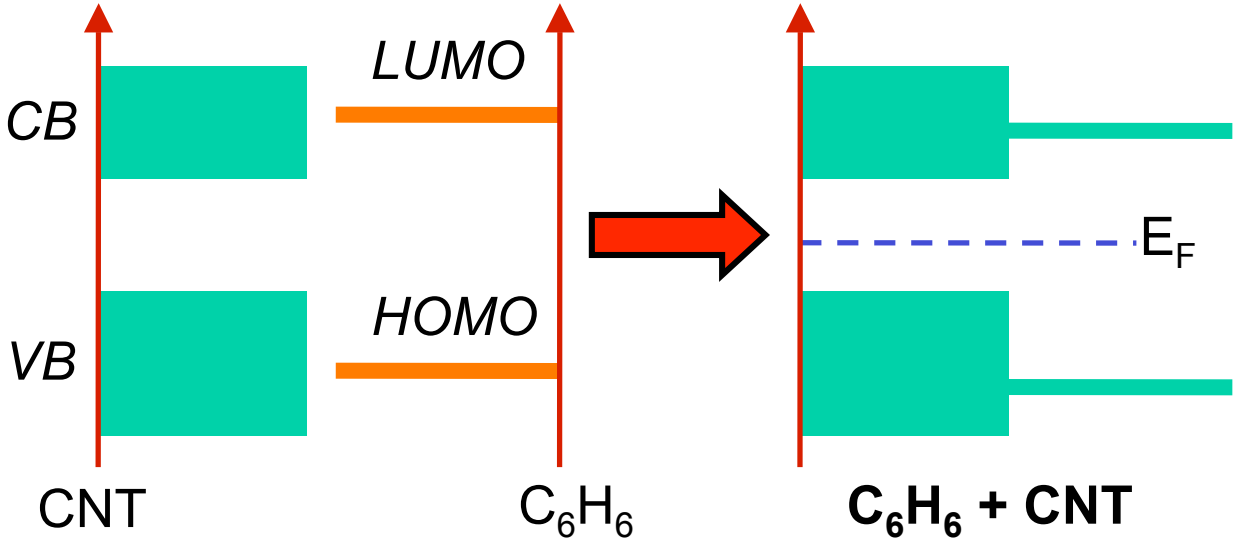


Why is the adsorption more favorable on one type of bond ?

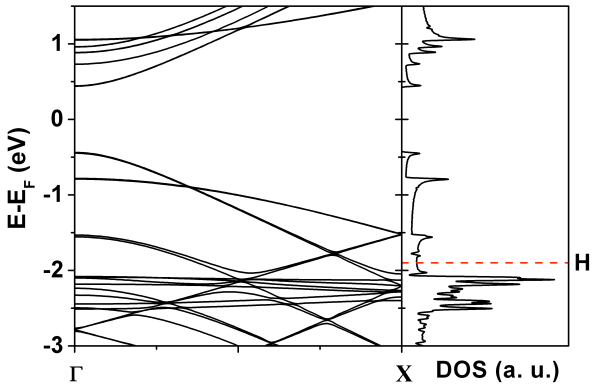
⇒ POAV misalignment angle ϕ

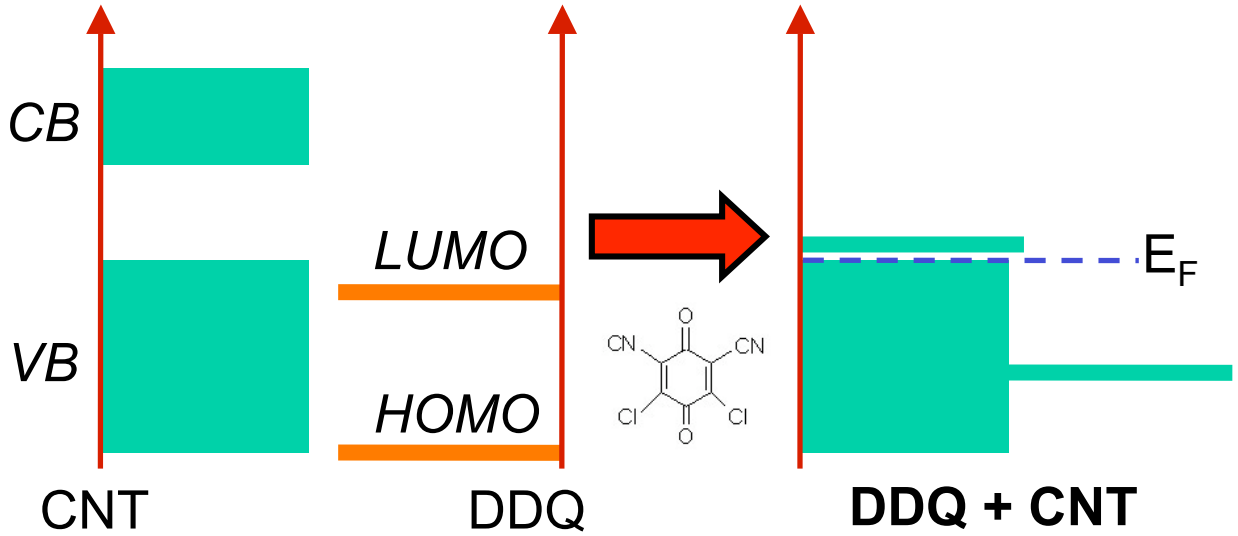
Electronic changes upon molecule adsorption

The behavior is dictated by the relative position of the HOMO and LUMO of the molecule, with respect to the valence and conduction bands of the tube.

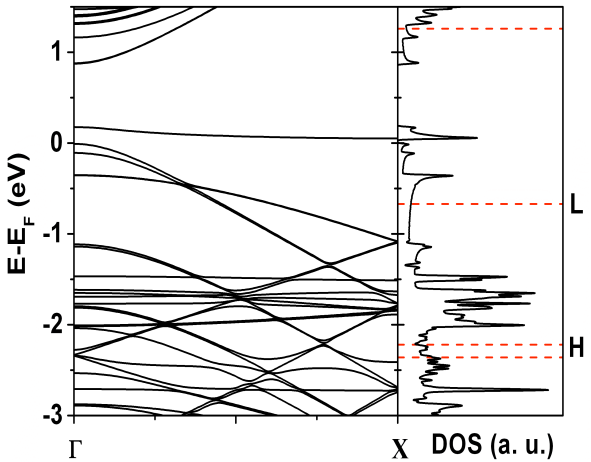


Superposition of DOS:
the gap is unchanged



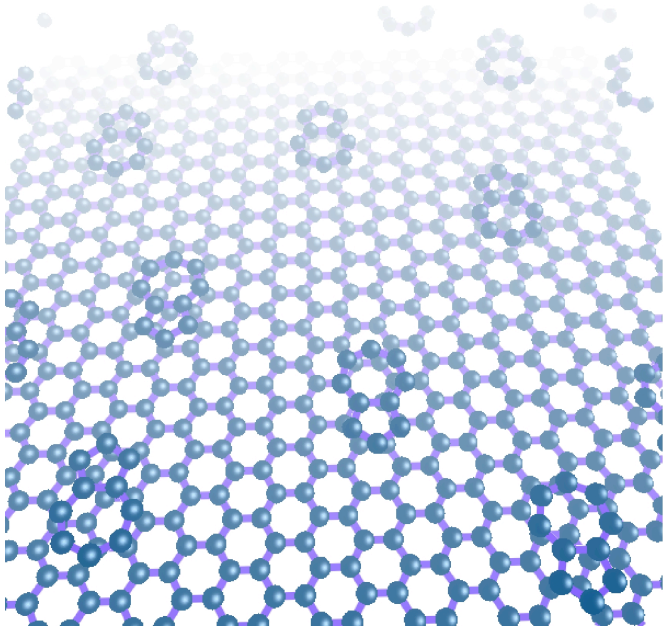


Metallisation of the CNT
+ charge transfer (~0.2 e$^-$)

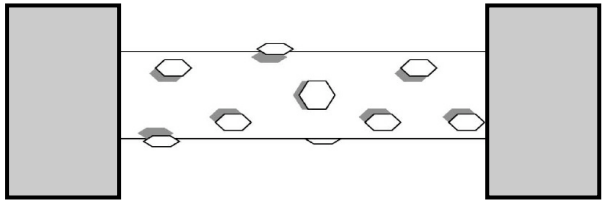


The quantum transport in CNTs with random coverage of physisorbed molecules

- π-conjugated hydrocarbon molecule : benzene (C_6H_6) and azulene molecule ($C_{10}H_{18}$).
- Questions :



How random coverage of physisorbed molecules may act as scattering centers for the propagating electrons at the Fermi energy ?



Is physisorption able to affect the generic transport length scales

(such as mean free path) ?

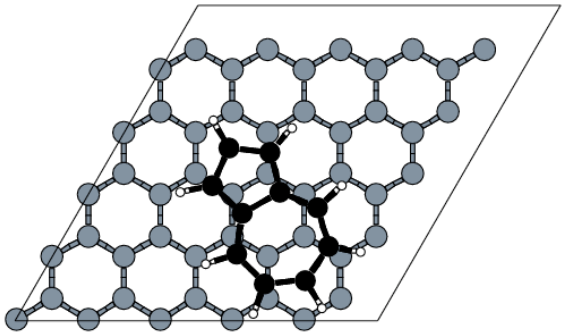
- Recent thermopower measurements have shown the effect of physisorption of small membered ring molecules (C_6H_{2n} with n=3,4,6).

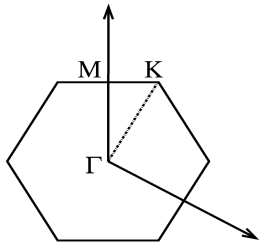
variation of the conductance close to the Fermi energy !

The π-stacking interaction

- MULTISCALE METHOD : ABINITIO + TB approach

Ab initio (DFT)





Effective model

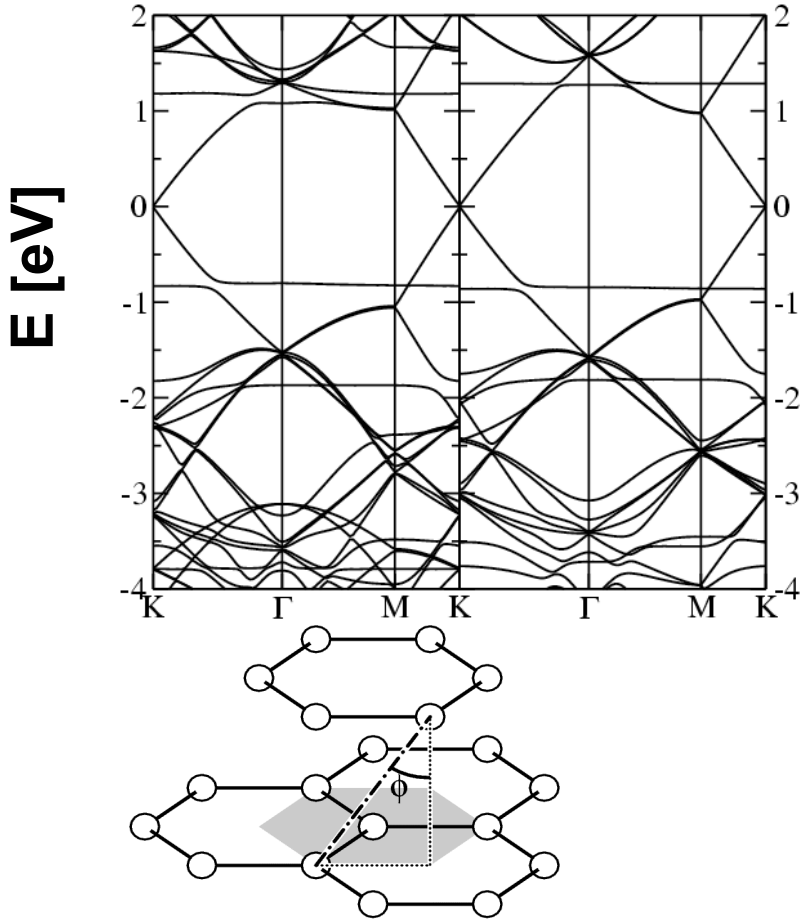
$|\pi_i\rangle =$ orbital on site i

$\varepsilon_i =$ on-site energy at i

$$H = \sum_{\langle i,j \rangle} \varepsilon_i |\pi_i\rangle\langle\pi_i| - \gamma_0 \sum_{\langle i,j \rangle} |\pi_j\rangle\langle\pi_i| - \sum_{\langle i,j \rangle} \beta_{ij} |\pi_j^{mol}\rangle\langle\pi_i^{CNT}| + C.C$$

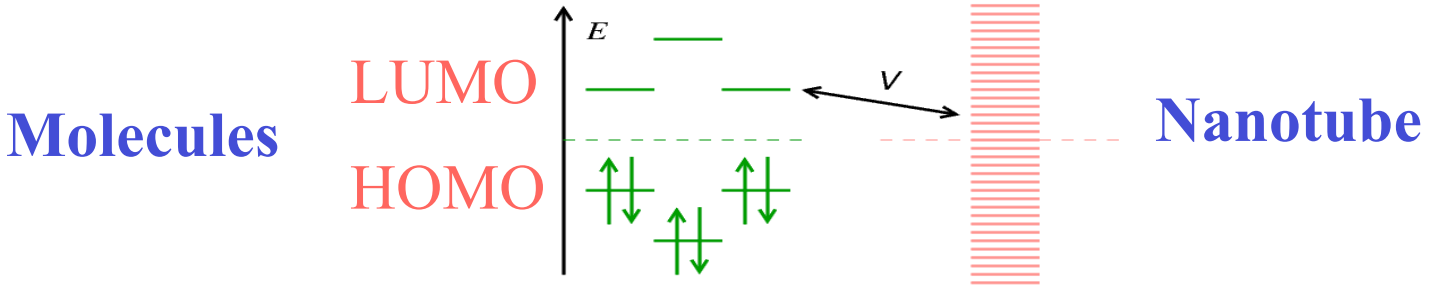
DFT

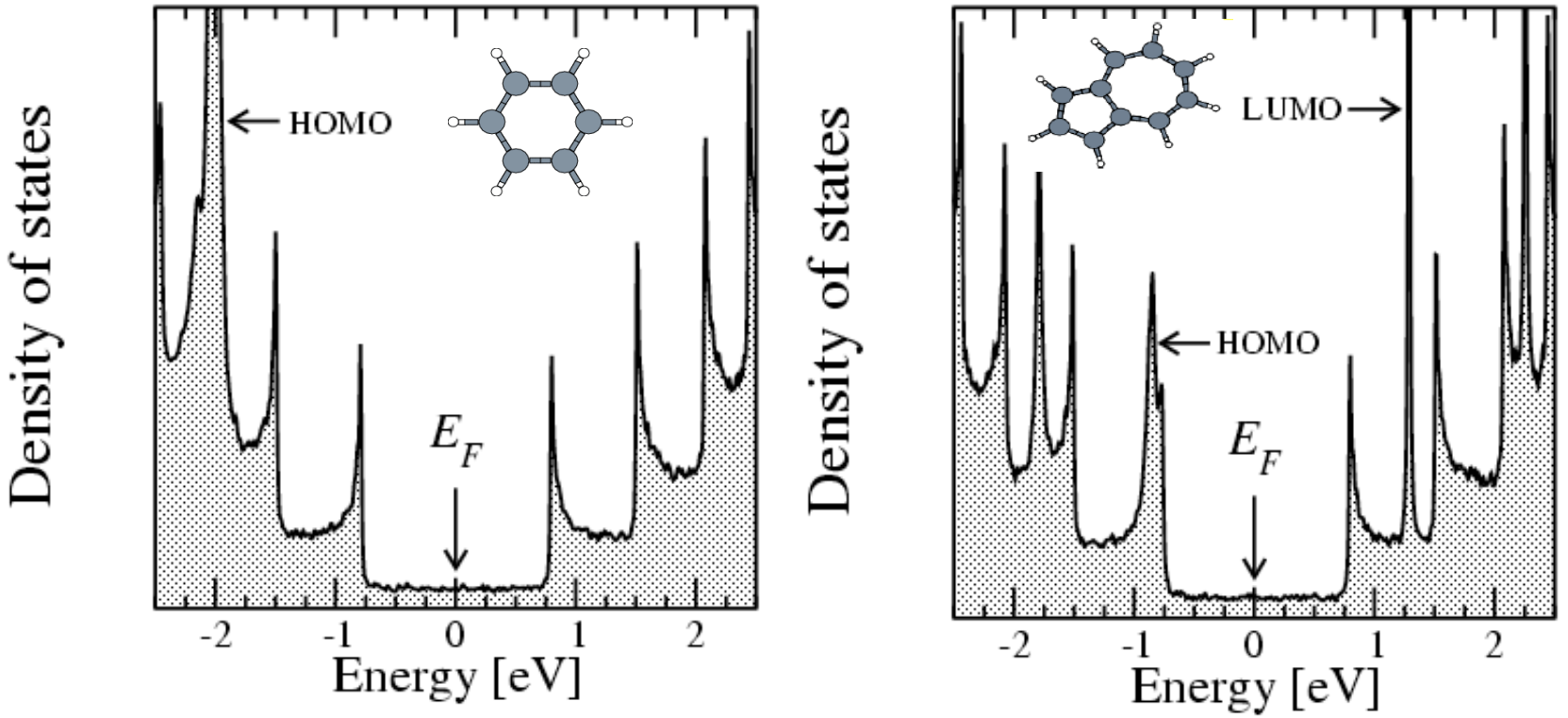
tight-binding parametrization



$$\beta_{ij} = \gamma_0 \cos(\phi_{ij}) e^{-(d_{ij}-\delta)/L}$$

Density of states



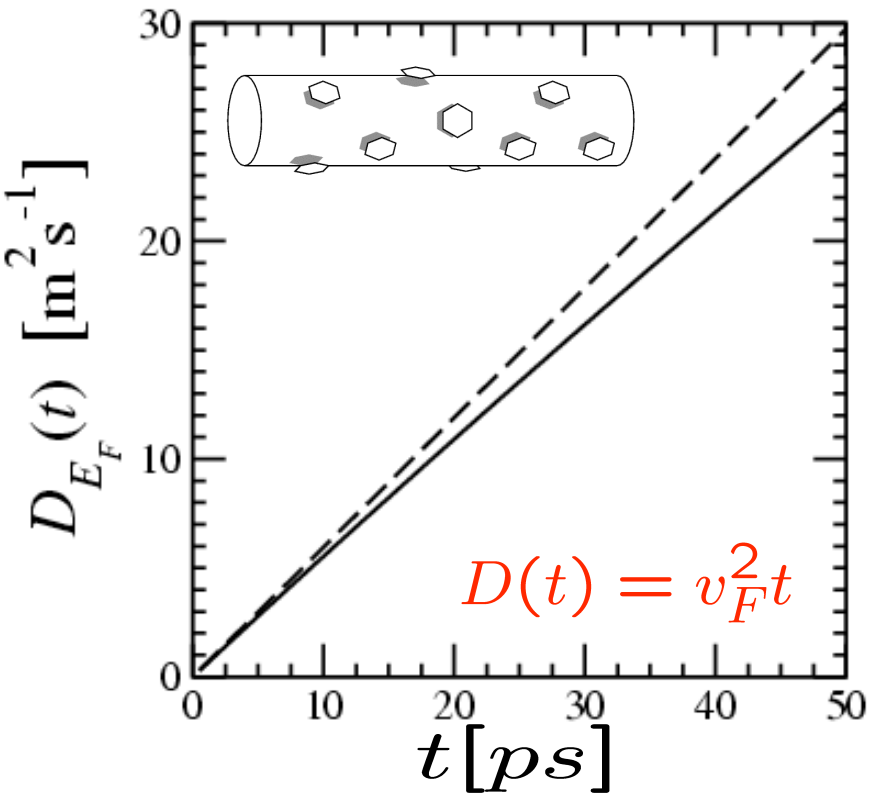


Quantum diffusion

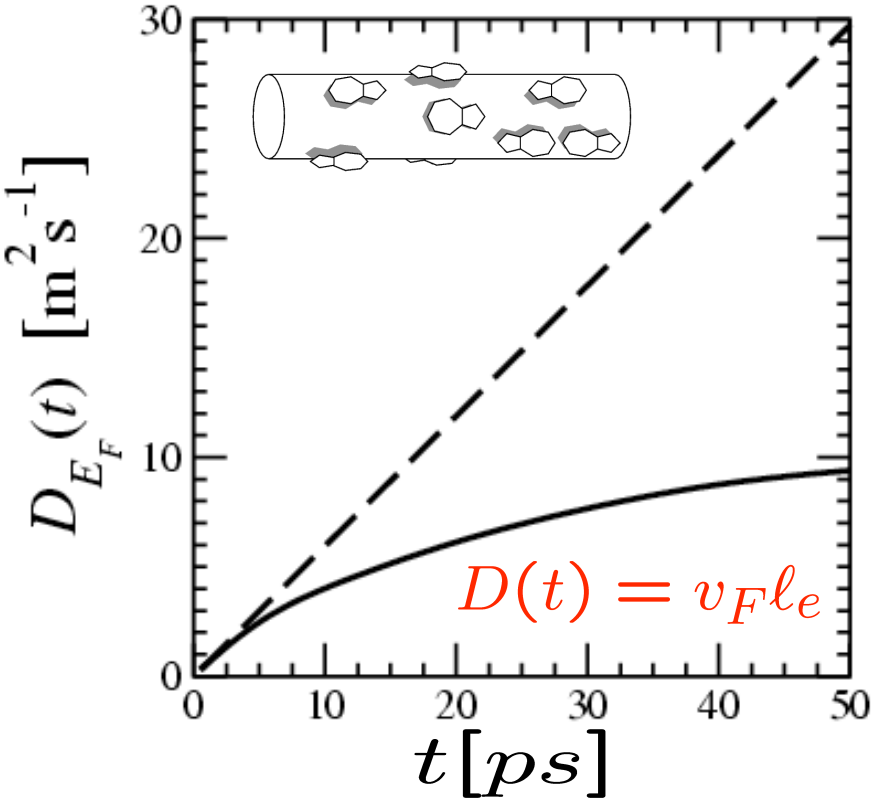
Density coverage
~ 10-15 %

Random coverage of physisorbed molecules C_6H_6 et de $C_{10}H_8$

Ballistic conduction

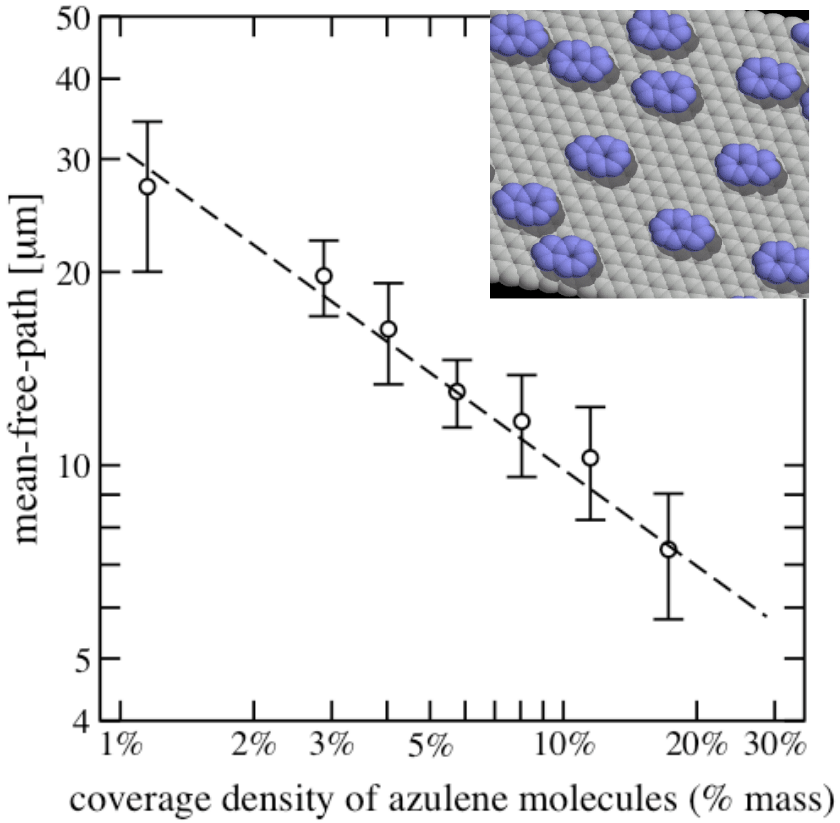


Diffusive conduction



Molecule-dependent conduction regime !

Evolution of the mean free path vs. the azulene coverage density



$$D_E(t) \sim v_F \ell_e$$

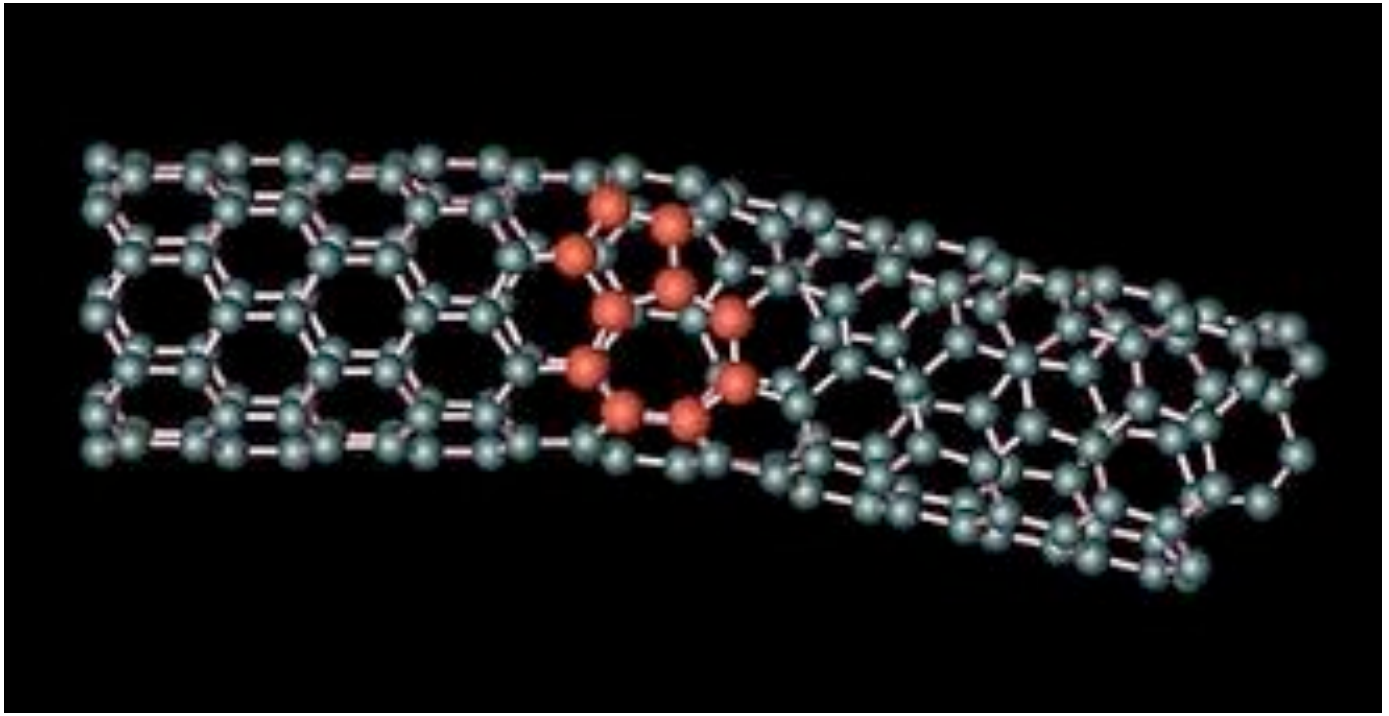
- In contrast with the chemical doping, where : $\ell_e \sim 1/\rho_{dopant}$
- The mean free path associated to the azulene physisorption manifests a weaker dependence on the density of grafted molecules.

$$\ell_e \sim 1/\sqrt{\rho_{mol}}$$

Conclusion : π-interactions via molecular physisorption can produce substantial backscattering in the CNT, modifying its electronic mean free path and its conductance that downscales with the coverage density. Strong dependence on the molecular nature...

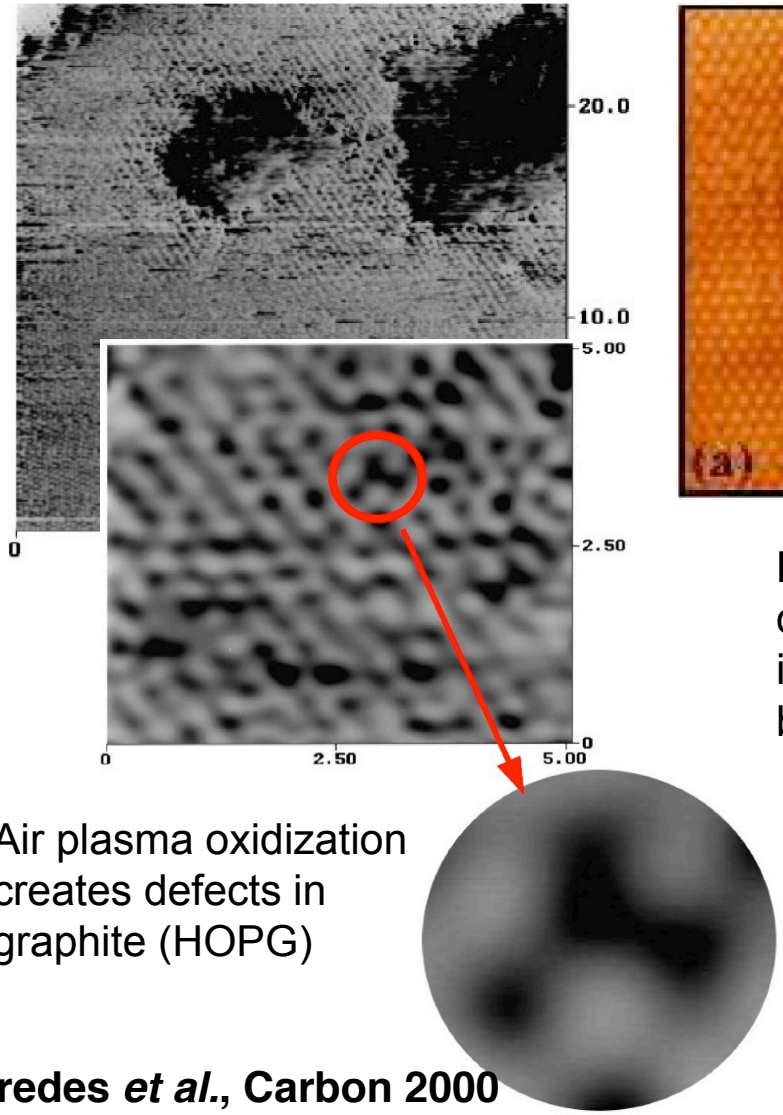
S. Latil, S. Roche, J.-C. Charlier, Nano Lett. 5, 2216 (2005).

3. TOPOLOGICAL DEFECTS



Experimental evidences...

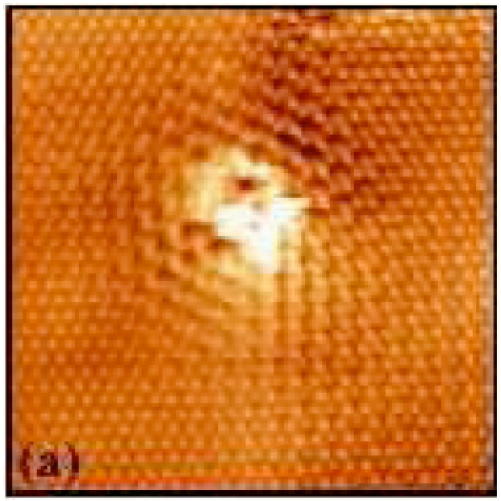
in Graphite



Air plasma oxidization creates defects in graphite (HOPG)

Paredes *et al.*, Carbon 2000

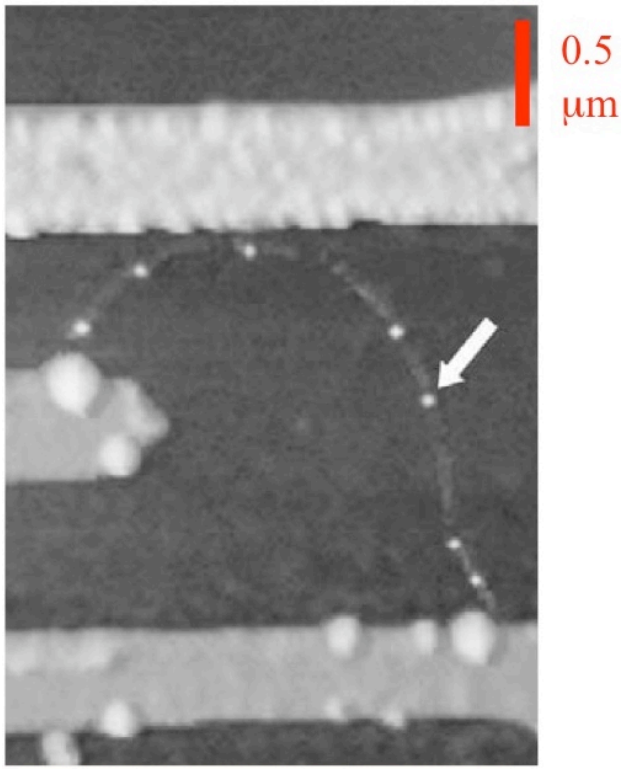
in Graphene



Defect-induced quantum interferences in bilayer graphite

Mallet *et al.*, PRL 2007

in SWNT

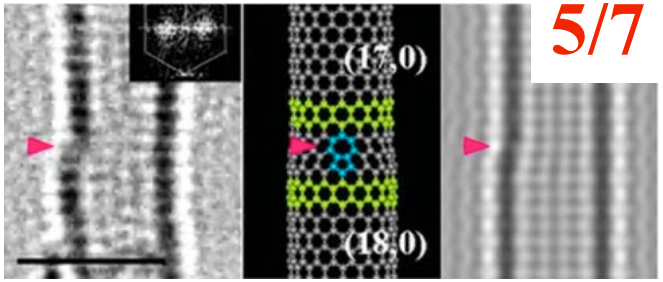


Reactivity of defects in SWNT using electrochemical treatment (Ni atoms)

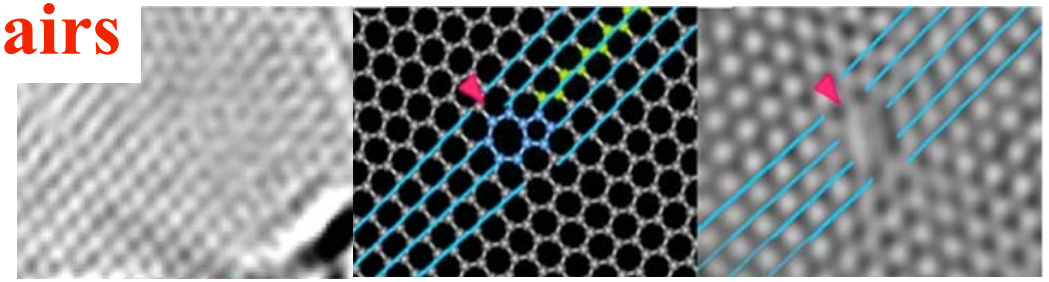
Fan *et al.*, Nat. Mat. 2005

Direct evidences for atomic defects

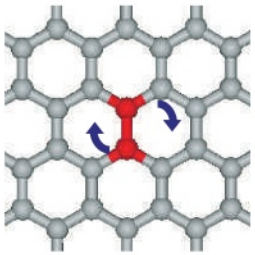
(1) Direct experimental approach : HRTEM

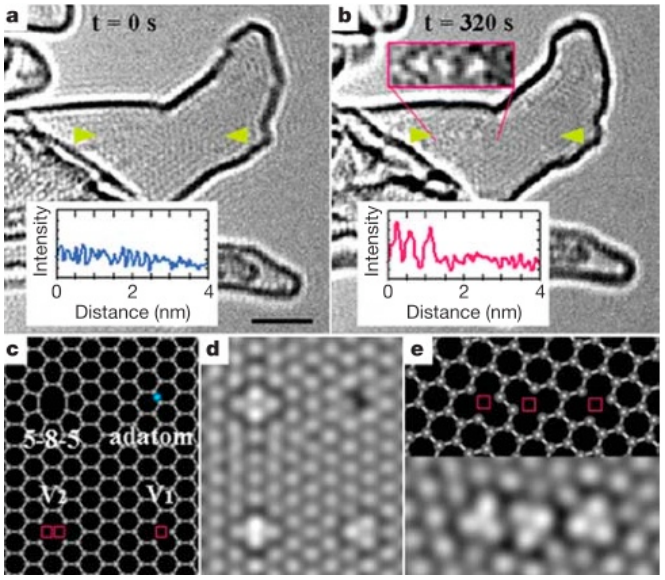


5/7 pairs

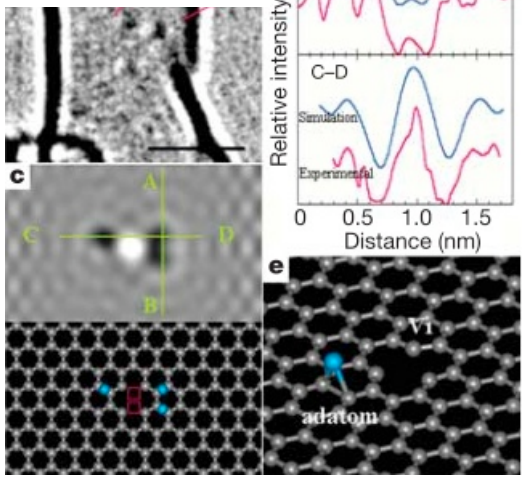


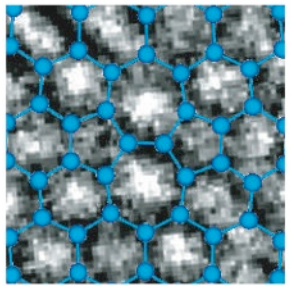
Stone-Wales

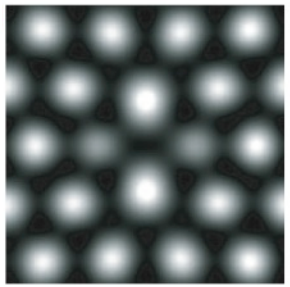




adatom







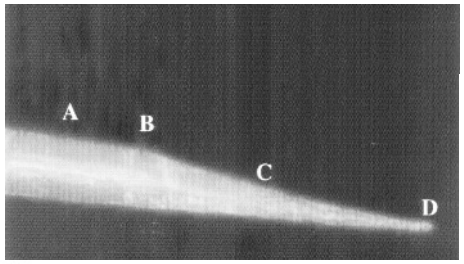
vacancy / di-vacancy

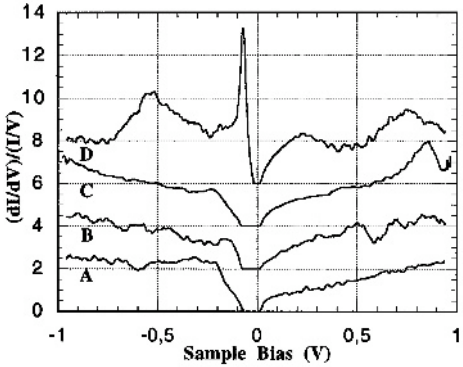
Hashimoto *et al.*, Nature 2004
Suenaga *et al.*, Nature Nanotech. 2007

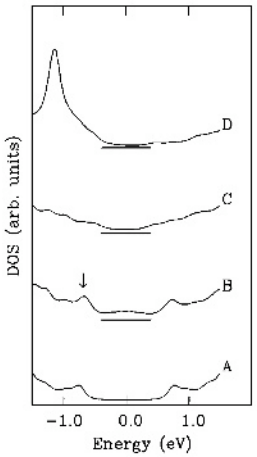
Direct evidences for atomic defects

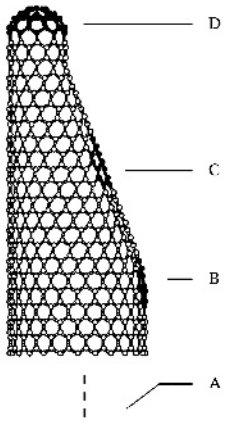
(2) Indirect experimental approach : STS

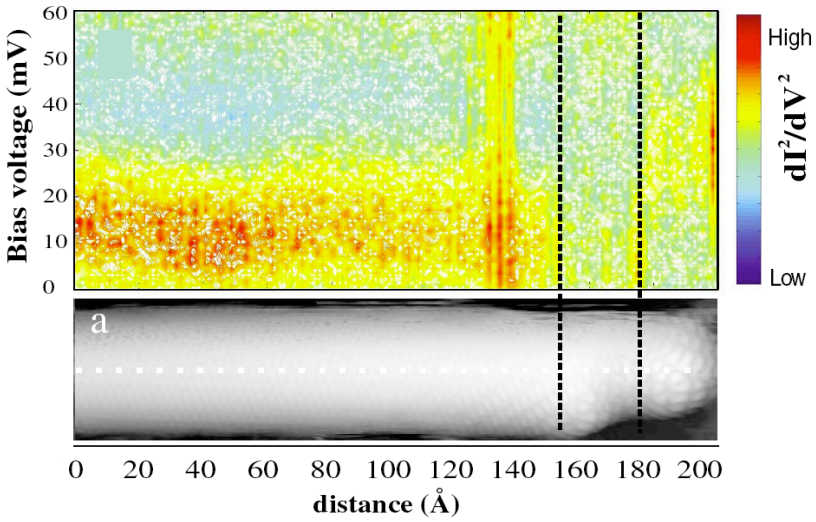
Variation of the local electronic density of states









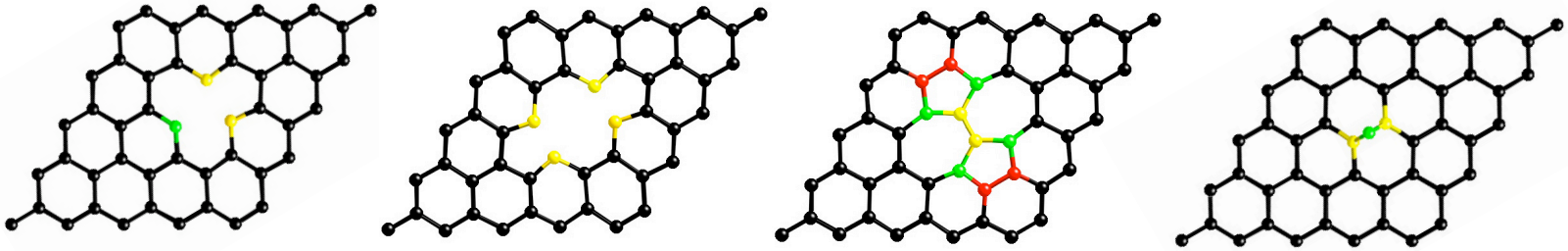


Carroll *et al.*, PRL 1997

Vitali *et al.*, PRL 2004

⇒ Importance to propose a list of defects in sp^2 carbon nanostructures in order to predict their identification.

First-principles calculations : Defects in graphene



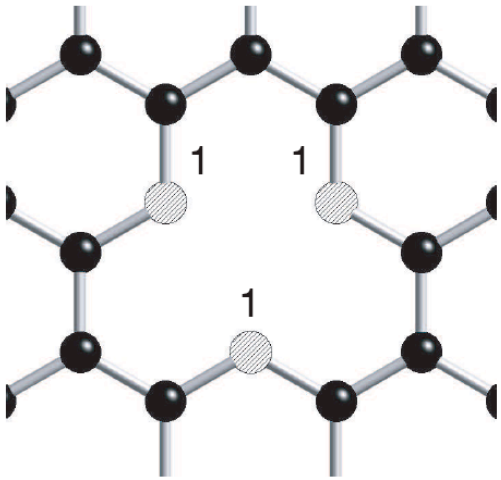
Density Functional Theory (DFT)
Local Density Approximation (LDA)
Norm-conserving pseudopotentials (Carbon atom)
Plane wave expansion (30 Ha) and (3x3) MP k-points 2D grid
Supercell geometry [(5x5) or (6x6) cells of 50 - 72 atoms]
Cold smearing method of Marzari (smearing : 0.002 Ha)
Relaxation of the atomic position until the forces on the atoms are reduced to within 1.0d-6 eV/Å
Code :

http://www.abinit.org

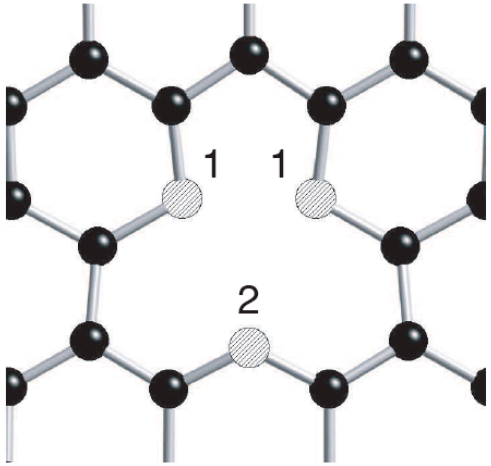
abinit

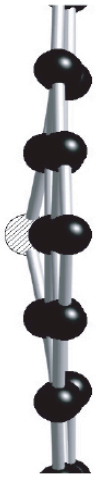
Vacancy in graphene...

D_{3h} vacancy

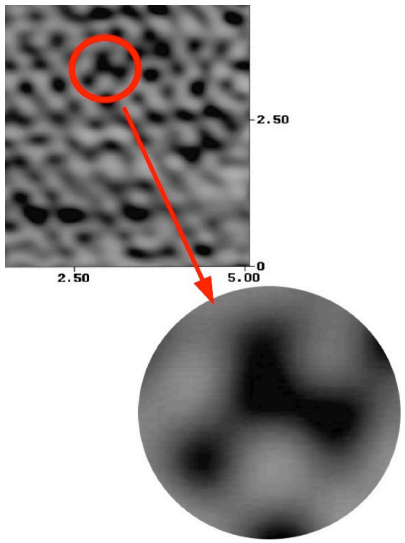


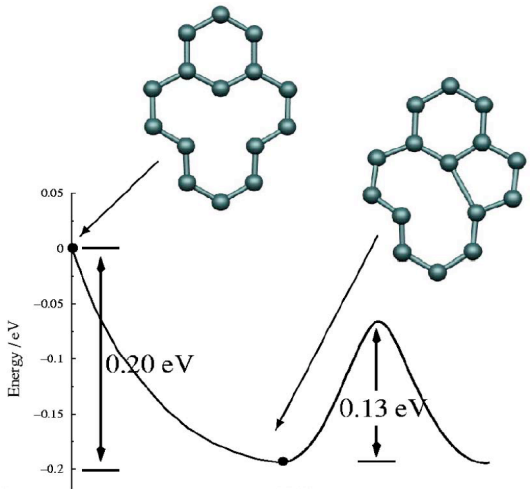
C_s vacancy





Experimentally





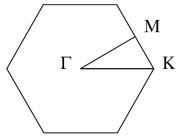
- Vacancy reconstruction
  $D_{3h} \Rightarrow C_s$
- Formation energy (ABINIT)
  $\Delta E \approx 0.23$ eV

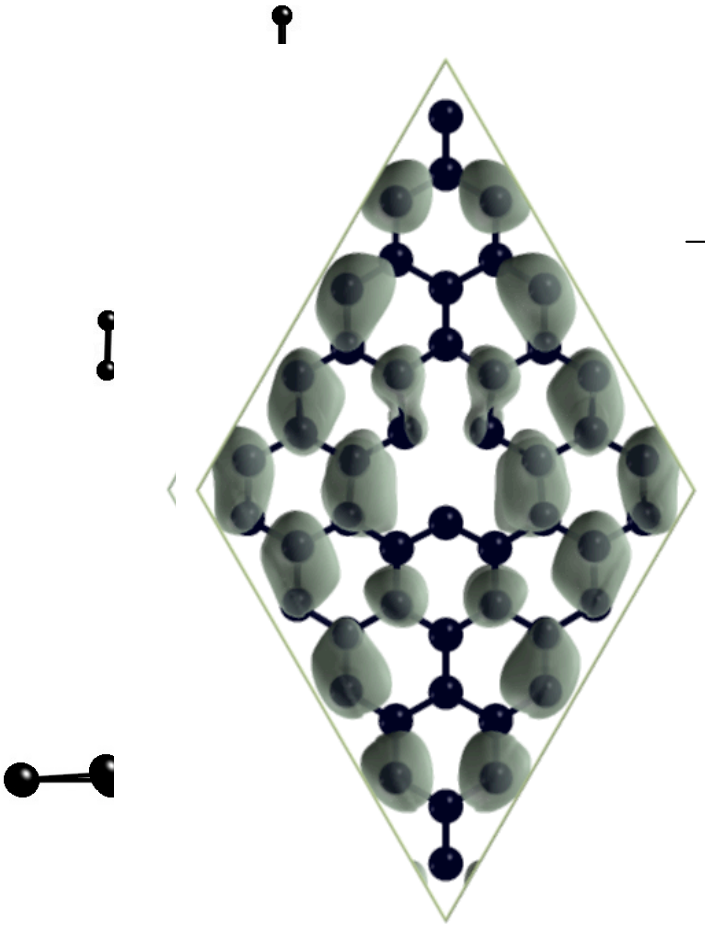
Amara *et al.*, PRB 76, 115423 (2007)

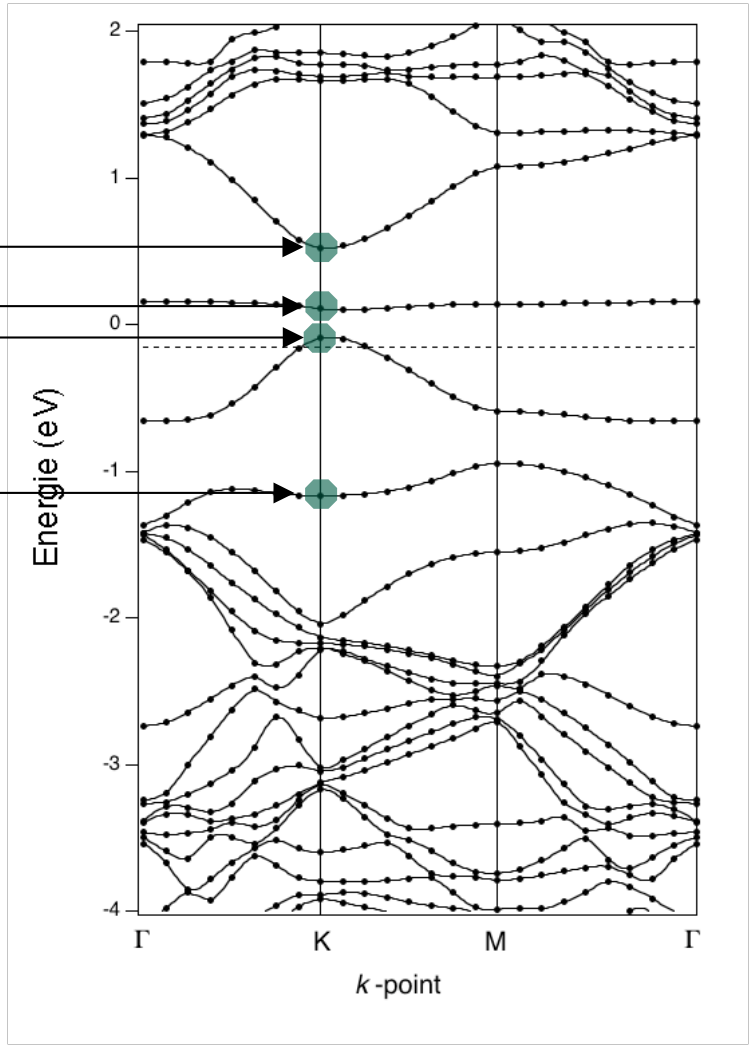
Electronic properties of Defects

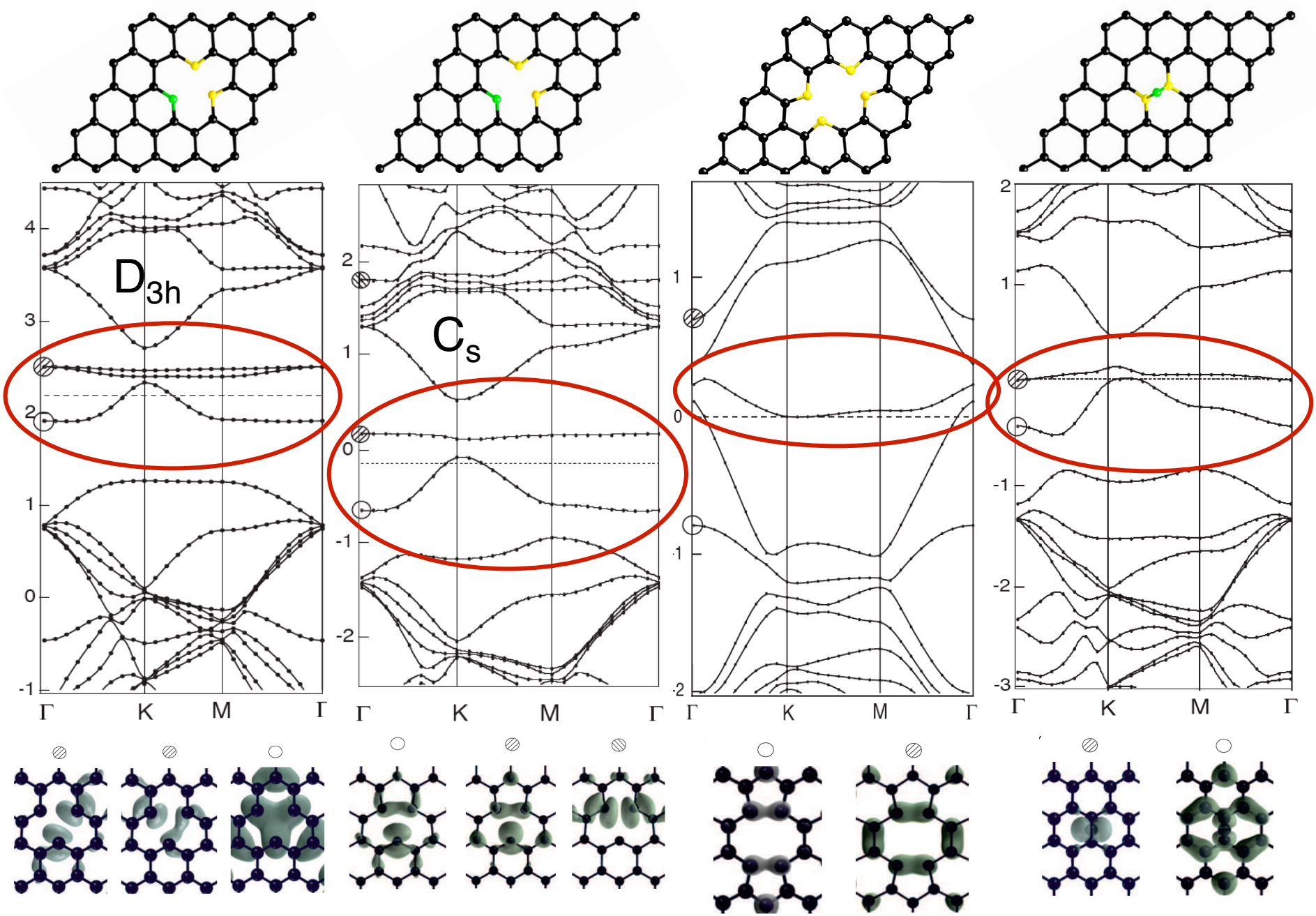
Supercell 5x5 : 49 atoms

C_s - vacancy





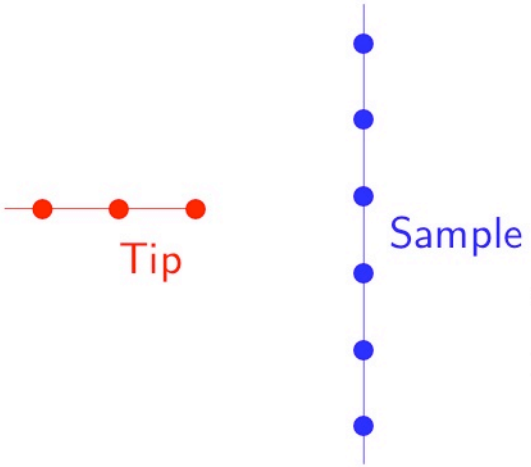




➡ Electronic states are quite localized !

Simulations of STM images

- Useful technique to investigate nanoscopic systems at the nanoscale.
- The electron transfer is allowed from occupied states of the sample to unoccupied states of the tip (or inversely).
- For weak difference of potential between the sample and the metallic tip (0-1eV), tunnelling current is sensible to the electronic states of the sample close to E_F.



First-order time-dependent perturbation theory

$$P_{\alpha\to\beta}(t) \sim \frac{2\pi}{\hbar} t\,|\langle\alpha|v|\beta\rangle|^2 \delta(E_\beta - E_\alpha) \text{ at large } t$$

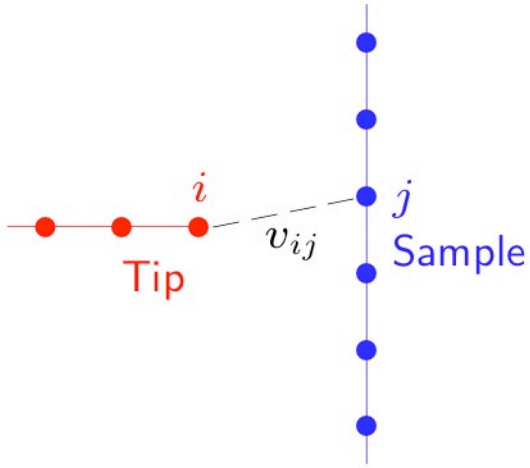
where $|\alpha\rangle$ and $|\beta\rangle$ are electronic states of the tip and sample, respectively, and v is the coupling Hamiltonian.

The total tunnelling current is

$$I = \frac{2\pi e}{\hbar} \int dE\,[f_t(E) - f_s(E)] \sum_{\alpha,\beta} |\langle\alpha|v|\beta\rangle|^2 \delta(E - E_\alpha)\delta(E - E_\beta)$$

Simulations of STM images

STM tight-binding theory



In tight binding, assuming one orbital per atom,

$$|\alpha\rangle = \sum_{i\in t} \chi_i^\alpha |\eta_i\rangle \ , \ |\beta\rangle = \sum_{j\in s} \psi_j^\beta |\theta_j\rangle \ .$$

Let $v_{ij} = \langle \chi_i | v | \theta_j \rangle$ be the tip-sample coupling element between two atomic orbitals. The tunnelling current at 0 K is

$$I = (2\pi)^2 \frac{e}{h} \int_{E_F - eV}^{E_F} dE \sum_{i,i'\in t} \sum_{j,j'\in s} v_{ij} v_{i'j'}^* n_{ii'}^t (E - \delta E_F - eV) n_{jj'}^s (E)$$

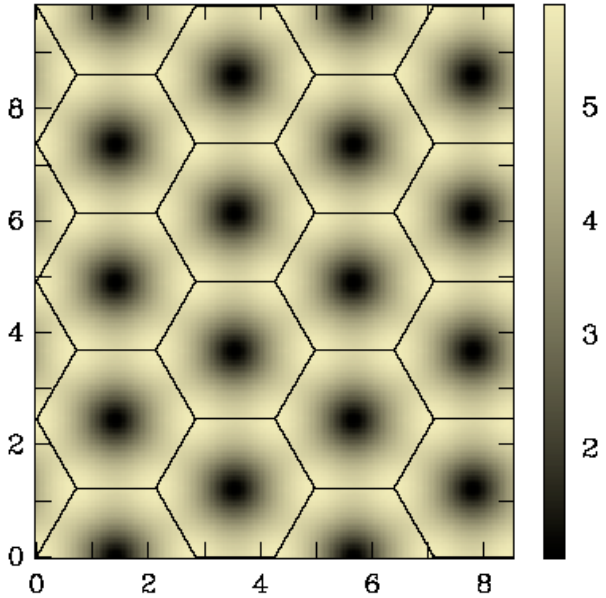
V is the tip–sample bias potential ($e > 0$), $\delta E_F = E_F^t - E_f^s$,

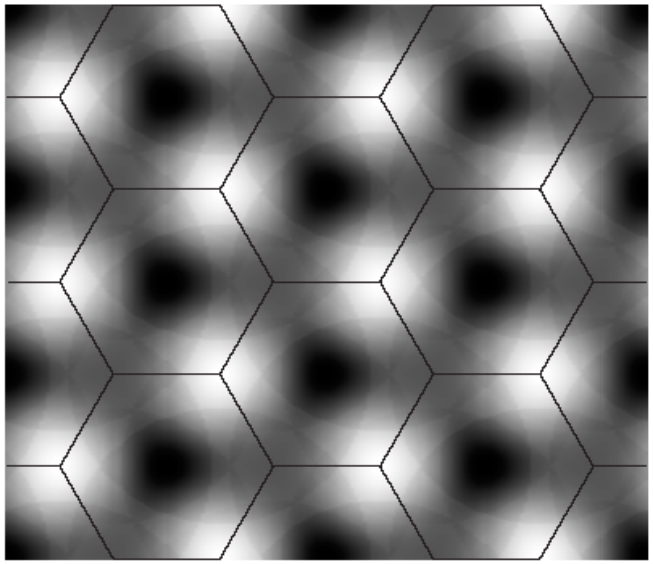
$$n_{jj'}^s (E) = \sum_\beta \psi_j^{\beta *} \delta(E - E_\beta) \psi_{j'}^\beta = (-1/\pi) \ \mathrm{Im} \ G_{jj'}^s (E + i0^+)$$

with $G_{jj'}^s$ a Green function element of the sample.

Meunier *et al.*, PRL 1998

Graphene versus Graphite





Calculated STM curent map at constant height (0.5 nm) above a single graphene layer (V_t = +0.2V).

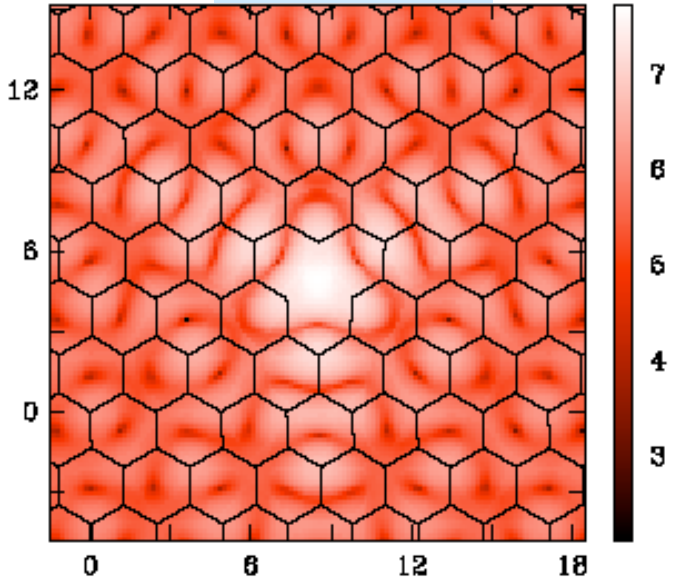
- In graphene, all the C atoms look identical...
- The hexagonal structure is perfecly reproduced...

Calculated STM current map at constant height (0.5 nm) above multilayered graphite (V_t = 0.2V) .

- The B atoms are clearly resolved, while the A atoms are not...

STM images of a vacancy in graphene

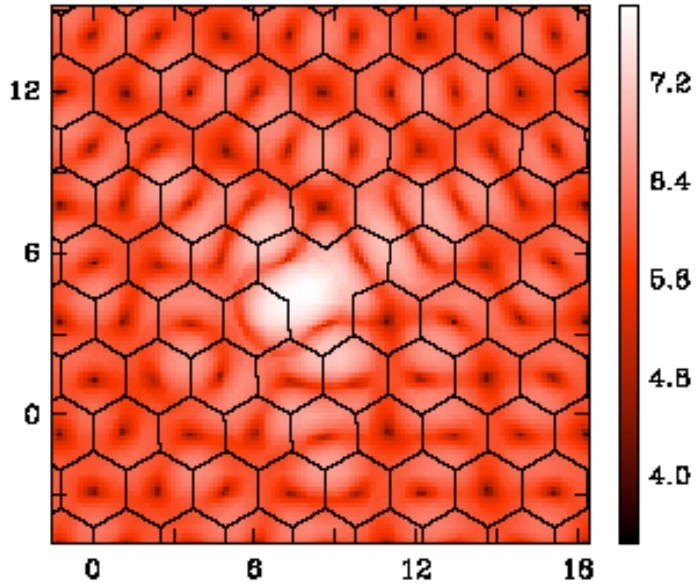
D_{3h} vacancy



Localized electronic states induced by the three dangling bonds => Large protrusion in the form of a hillock with trigonal symmetry at the center of the defect (V_t = +0.2V).

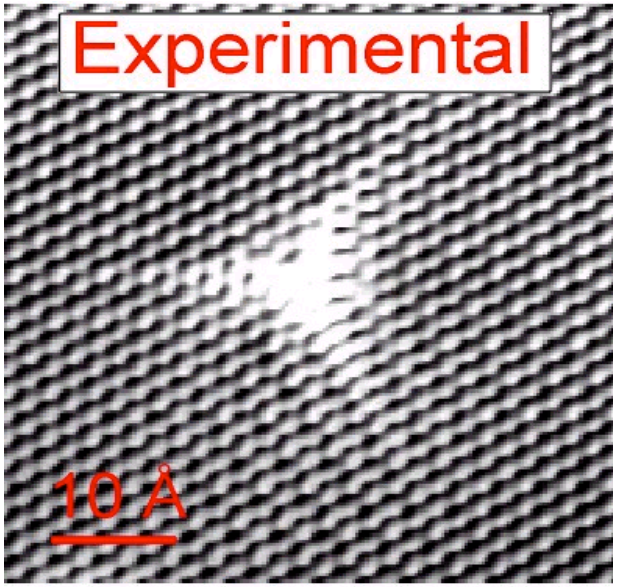
Amara *et al.*, PRB 76, 115423 (2007)

C_s vacancy

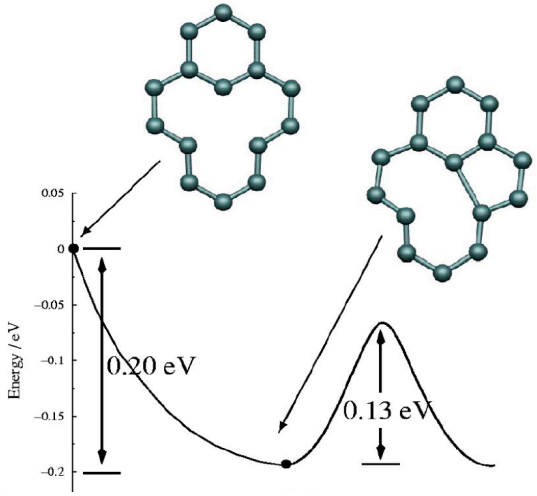


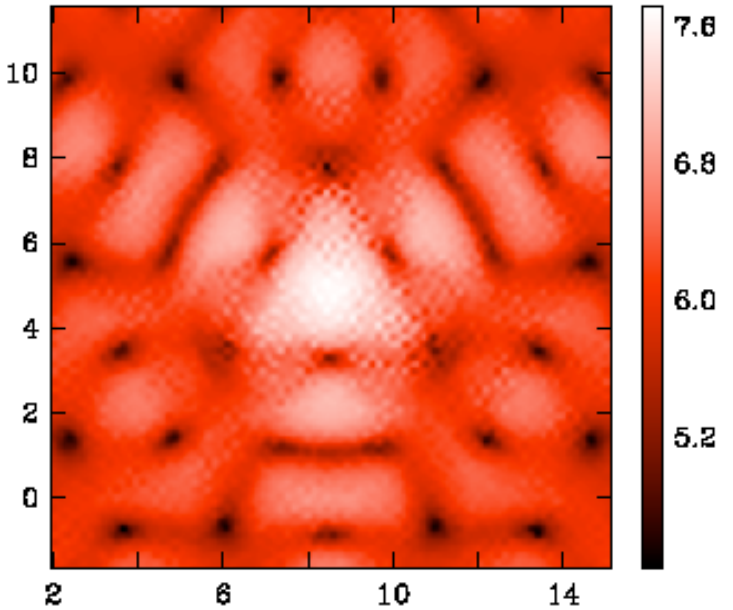
The largest protrusion is located on the two-coordinated atom located in front of the pentagon with a long C-C bond produced by the reconstruction (V_t = +0.2V). The trigonal symmetry of the image can be restored by invoking a dynamical Jahn-Teller effect, where the pentagon rotates by +/-2π/3. The image would then be an average of three structures equivalent to that rotated by +/-2π/3.

Experimental data



Kushmerick *et al.*, JPC 1999



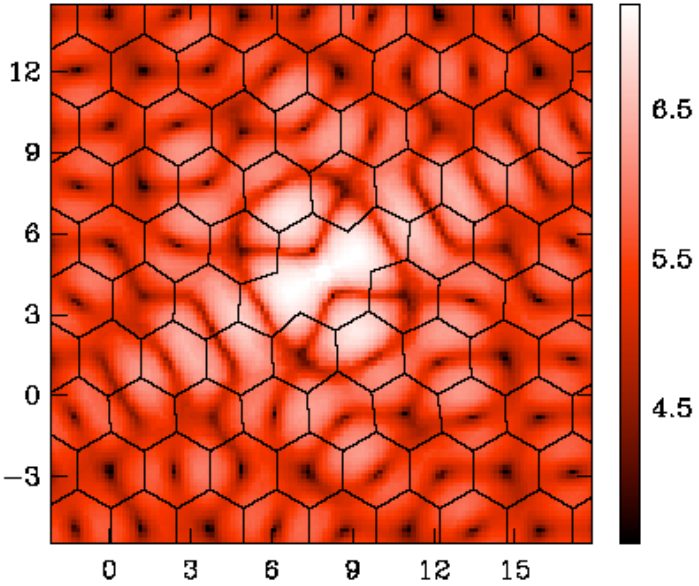


Most often, experimental STM image of irradiated graphite show defects in form of protrusions with three-fold symmetry and $\sqrt{3} \times \sqrt{3}$ superstructure around them.[1] This observation is consistent with the reconstructed C_s vacancy if one invokes a dynamical Jahn-Teller effect,[2] thanks to which the observed image is an average of three equivalent structures rotated by $\pm 2\pi/3$

[1] J. Valenzuela-Benavides *et al.*, Surf. Sci. (1995)
[2] A. A. El-Barbary *et al.*, PRB, (2003)

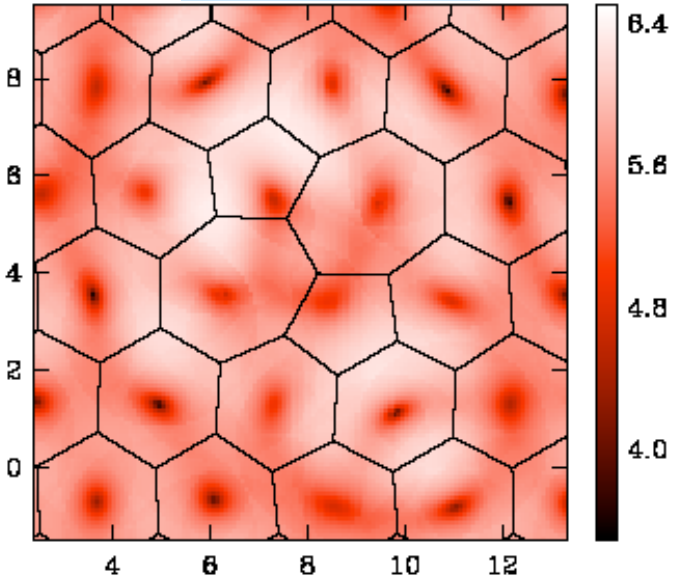
STM images of a di-vacancy and SW in graphene

Di-vacancy



There is no dangling bond in the structure. A dumbell-like feature decorates the two pentagons. Interestingly, the maximum of protrusion is realized right at the center of the defect, where there is no atom. In perfect graphene, the centers of the hexagons corresponds lead to depressions (V_t = +0.2V).

Stone-Wales



Elongated ring of protrusion having its major axis parallel to the Stone Wales bond and extending from 0.3 to 0.5 nm around the center of the defect (V_t = +0.2V).

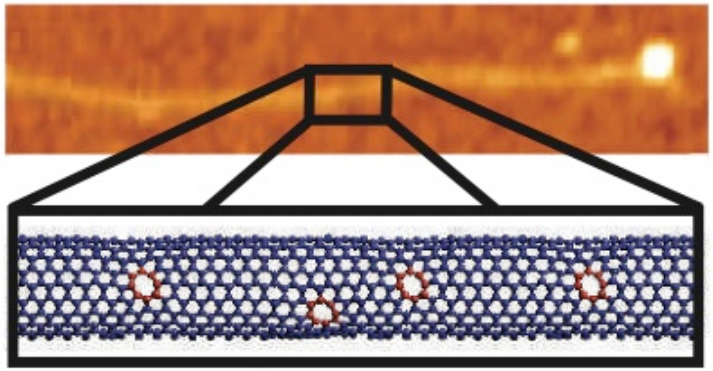
Amara *et al.*, PRB 76, 115423 (2007)

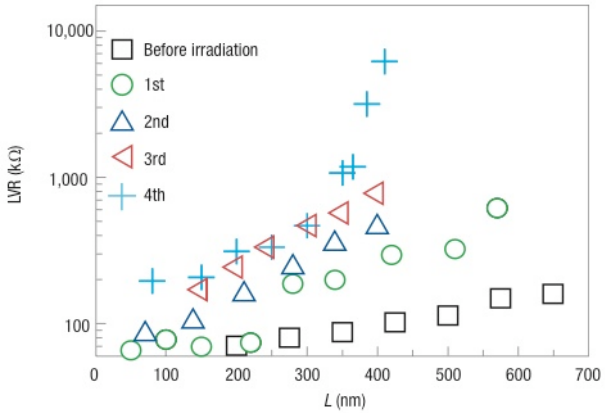
NANOTUBES

Controlling conductance

Gomez-Navarro *et al.*, Nat. Mat. 2005

Most of the outstanding properties of carbon nanotubes rely on them being almost atomically perfect, but the amount of imperfections, and the effect that they have on the tube properties, has, to date, been poorly understood. New work shows that even a very low concentration of missing atom-pairs in the nanotubes has a large effect on their electrical conductance.



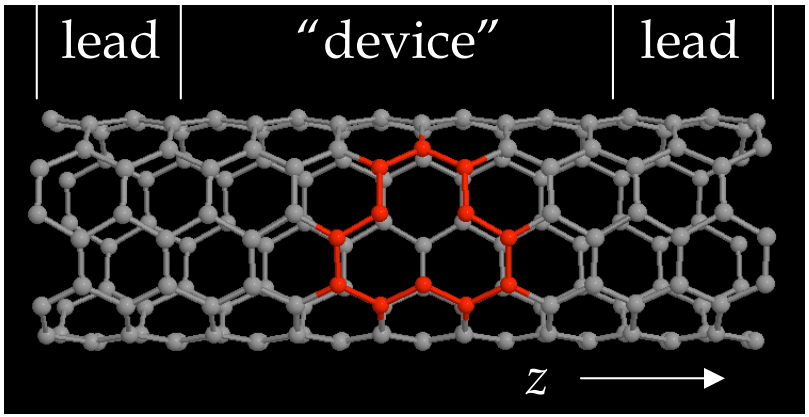


It is crucial to understand the influence of defects on the transport properties in order to conquer their detrimental effects, but also because controlled defect introduction may be used to tune nano-tube properties in a desired direction (i.e. gas sensing property).

First-principles calculations :

Density Functional Theory (DFT)
Local Density Approximation (LDA)
Pseudopotentials
Supercell geometry **(10Å vacuum between tubes)**
(Max. Force < 0.01eV/Å ; Z_{min} calculated for each case !)
Localized Atomic Orbitals (DZP basis)

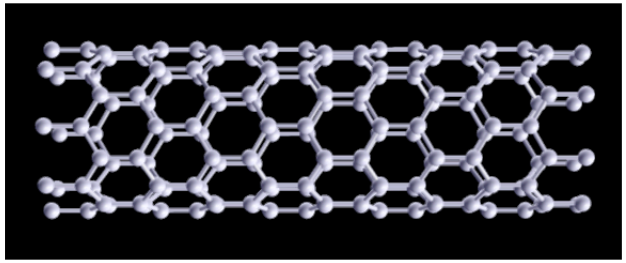
Quantum transport :



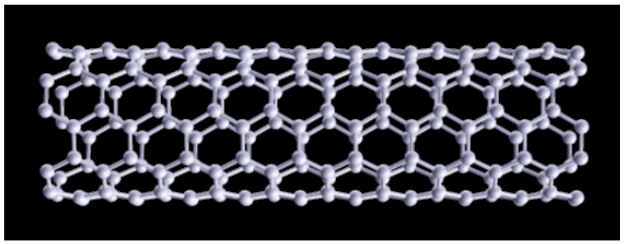
Smeagol **is an *ab initio* electronic transport code based on a combination of DFT and Non-Equilibrium Green's function transport methods (NEGF).**
It has been designed to describe two-terminals nano-scale devices, for which the potential drop must be calculated accurately (+ spintronics).

Quantum conductance : ideal CNTs

Zigzag (8,0)



Armchair (5,5)



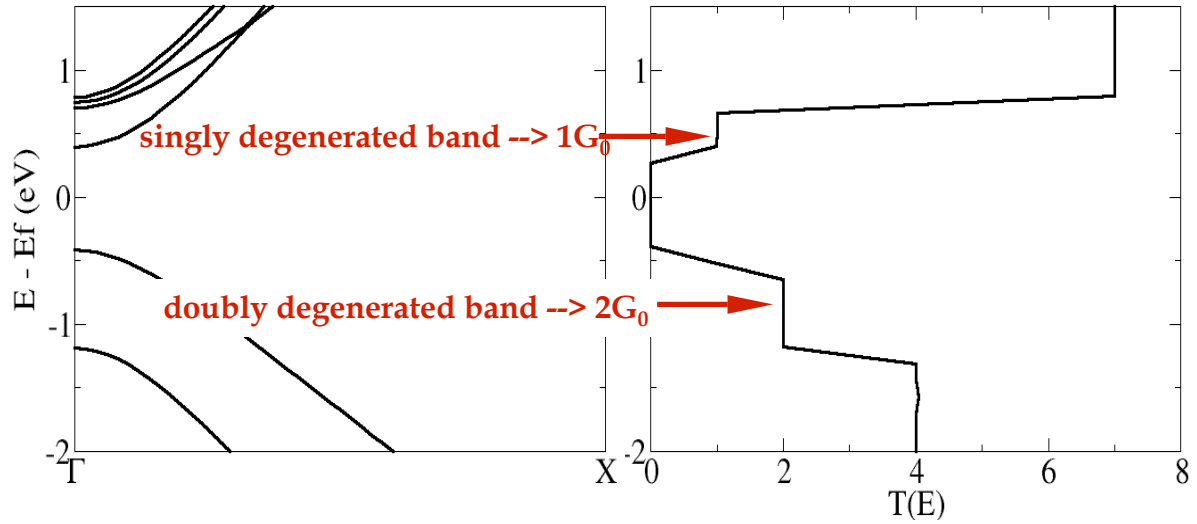
Landauer-Büttiker [PRB **31**, 6207 (1985)] equilibrium transport @ 0K and V=0 : **$G(E) = T(E)G_0$**

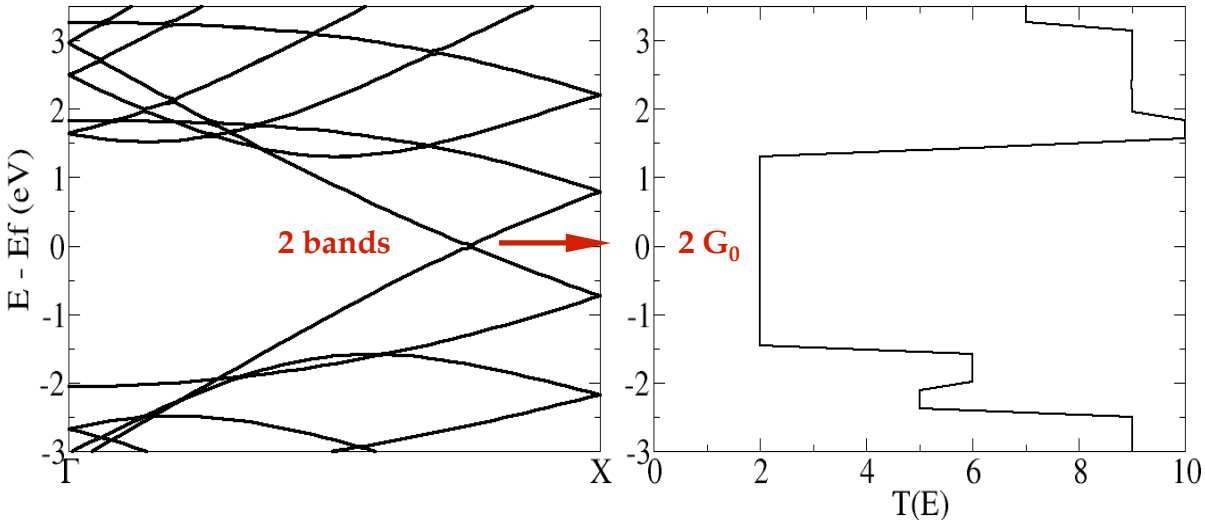
where

$G_0 = 2e^2/h$ = quantum of conduct.

T(E) = q.m. transmission coeff. of scattering theory

T(E) ~ #conduction channels @E
= #bands @E





Two bands cross at the Fermi level

⇒ Conductance ≡ $T(E_F) = 2$ units of $2e^2/h \approx (12.9\ k\Omega)^{-1}$

UCL Université catholique de Louvain

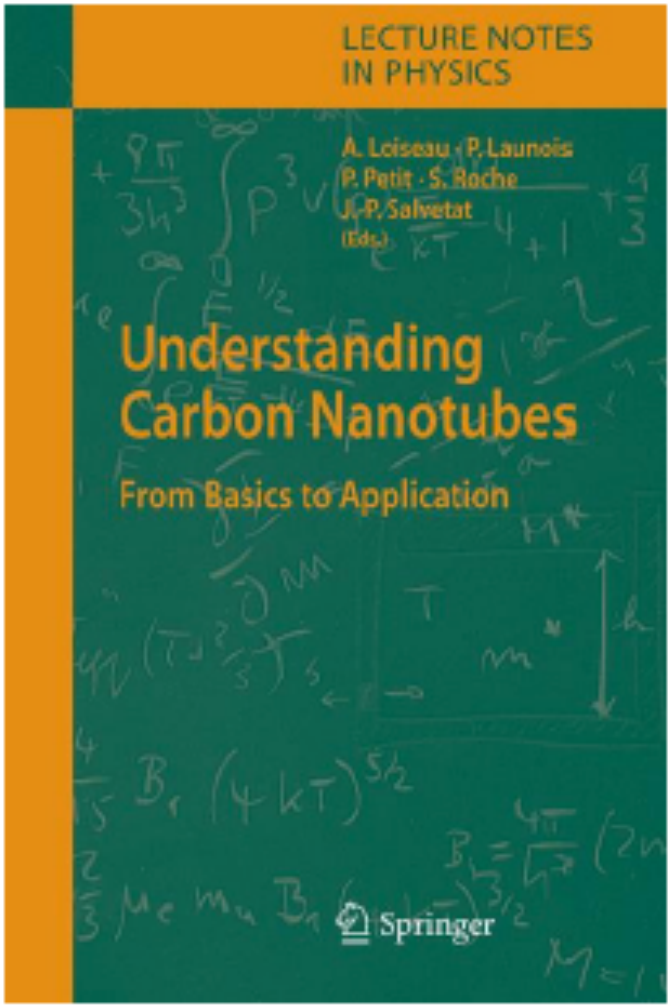
Conclusions

- **Electronic properties of CNTs containing defects, dopants and with random coverage of physisorbed molecules.**
  - **surface modification of CNT = important topic**
- **Transport properties of « modified CNTs » :**
  - **different quantum regimes of conduction**
  - **gas sensing properties...**
  - **magnetic properties => spin-transport !**

Collaborators

Zeila Zanolli	**Univ. of Louvain, Belgium**
Hakim Amara	**CEA - Saclay, France**
Sylvain Latil	
Stephan Roche	**CEA - Grenoble, France**
Xavier Blase	**CNRS - Grenoble, France**
Philippe Lambin	**Univ. of Namur, Belgium**

Textbooks & Review articles



REVIEWS OF MODERN PHYSICS, VOLUME 79, APRIL–JUNE 2007

Electronic and transport properties of nanotubes

Jean-Christophe Charlier*

Unité de Physico-Chimie et de Physique des Matériaux (PCPM), Université Catholique de Louvain, 1 Place Croix du Sud, B-1348 Louvain-la-Neuve, Belgium

Xavier Blase†

Université de Louvain, F-69000, France, Laboratoire de Physique de la Matière Condensée et Nanostructures, Université Lyon I, CNRS, UMR 5586, Domaine scientifique de la Doua, F-69622 Villeurbanne Cedex, France

Stephan Roche‡

Commissariat à l'Energie Atomique, DSM/DRFMC/SPSMS/GT, 17 rue des Martyrs, 38054 Grenoble Cedex 9, France

(Published 16 May 2007)

This article reviews the electronic and transport properties of carbon nanotubes. The focus is mainly theoretical, but when appropriate the relation with experimental results is mentioned. While simple band-folding arguments will be invoked to rationalize how the metallic or semiconducting character of nanotubes is inferred from their topological structure, more sophisticated tight-binding and *ab initio* treatments will be introduced to describe more subtle physical effects, such as those induced by curvature, tube-tube interaction, or topological defects. The same approach will be followed for transport properties. The fundamental aspects of conduction regimes and transport length scales will be presented using simple models of disorder, with the derivation of a few analytic results concerning specific situations of short- and long-range static perturbations. Further, the latest developments in semiempirical or *ab initio* simulations aimed at exploring the effect of realistic static scatterers (chemical impurities, adsorbed molecules, etc.) or inelastic electron-phonon interactions will be emphasized. Finally, specific issues, going beyond the noninteracting electron model, will be addressed, including excitonic effects in optical experiments, the Coulomb-blockade regime, and the Luttinger liquid, charge density waves, or superconducting transition.

Thanks !