Transport Properties in Disordered Graphene :
Effects of Atomic Hydrogen and Structural Defects

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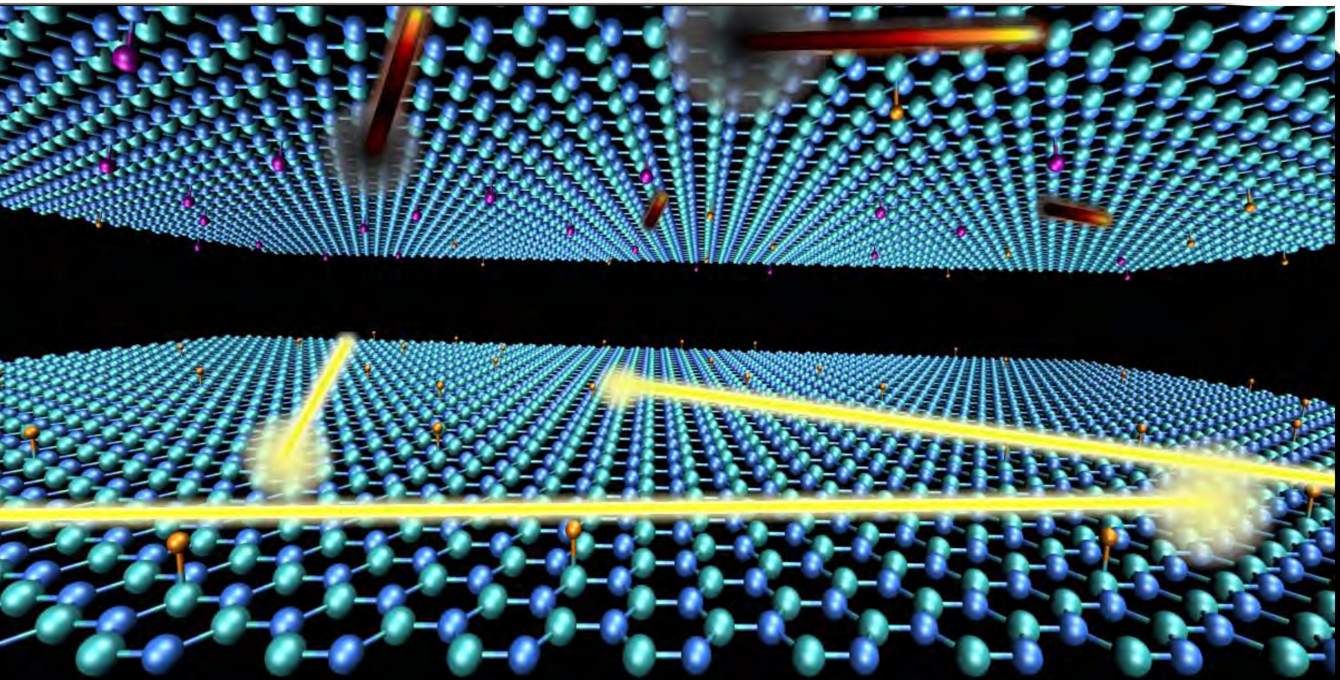
*iCrea
INSTITUCIÓ CATALANA DE RECERCA I ESTUDIS AVANÇATS

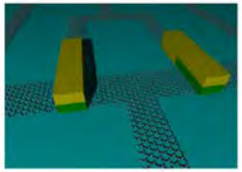
GRAPHENE FLAGSHIP



TNT2011, Tenerife, Monday - November 21, 2011

OUTLINE

1. *Why focusing on "dirty graphene" ?*



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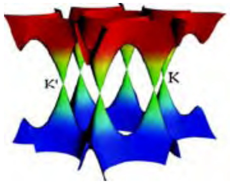

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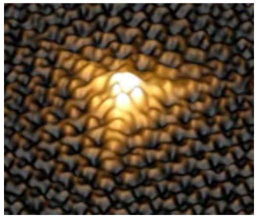

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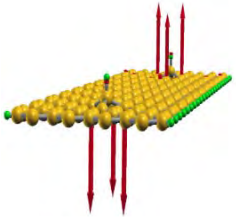
   Local magnetic ordering and metal-insulator transition

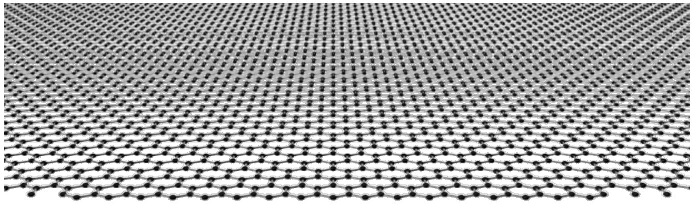


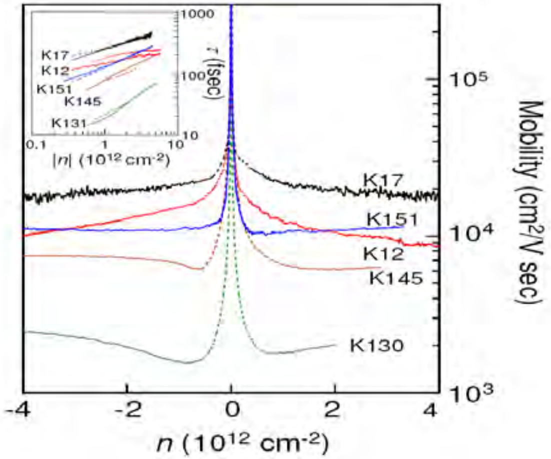
Why focusing on “dirty graphene” ?

ICN Institut Català de Nanotecnologia

A.K. Geim, **Bull. Am. Phys. Soc. 55 (2010)**

Suspended graphene	$\mu \sim 10^6 \mathrm{cm^2V^{-1}s^{-1}}$
Top gated graphene MOS channels	$\mu \sim 23.000 \mathrm{cm^2V^{-1}s^{-1}}$
Large area (catalytic growth) graphene	$\mu \sim 3.700 \mathrm{cm^2V^{-1}s^{-1}}$

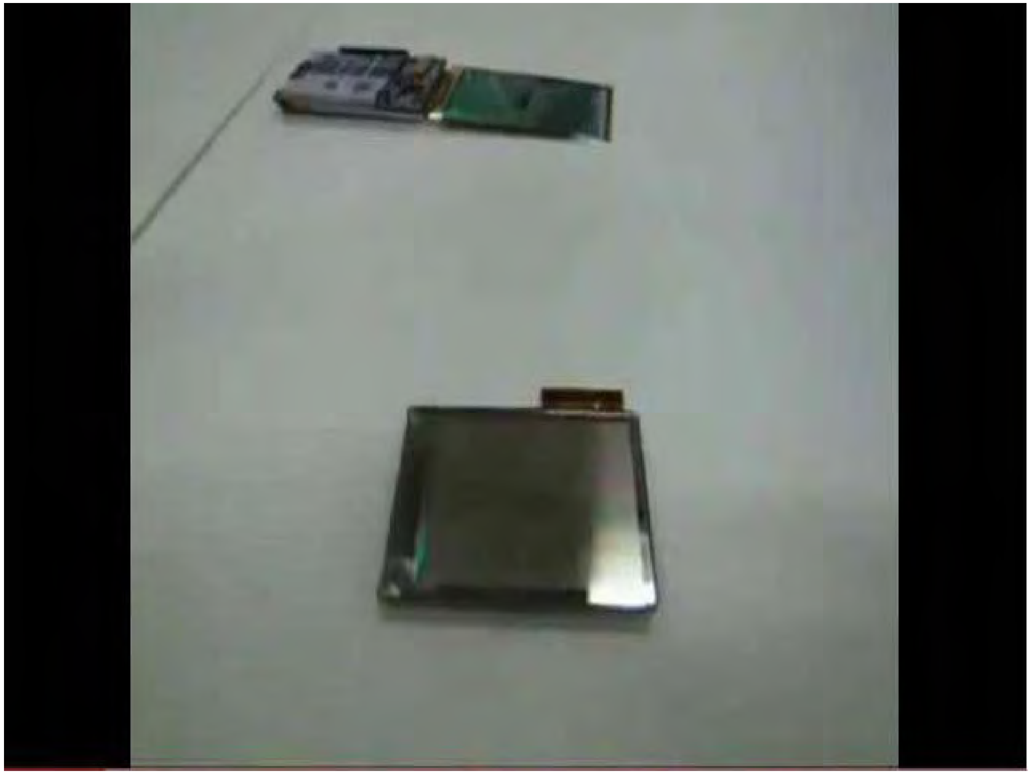




Ph. Kim et al., **PRL 99, 246803 (2007)**

- Understanding mobility reduction in CVD-grown graphene (*transparent electrodes*)
- Band-gap engineering / ON-OFF ratio (*graphene transistors & logic functions*)
- Implementing (bio)chemical sensing capability (*medicine, biotec,….*)
- Diversifying electronic, transport properties of charge, spin, phonons,..
  - *Making graphene magnetic at room-temperature (hydrogenation)*
  - *Making graphene good thermoelectrical converters*
  - *Etc.*

Today s state of the art in graphene-based flexible electronics

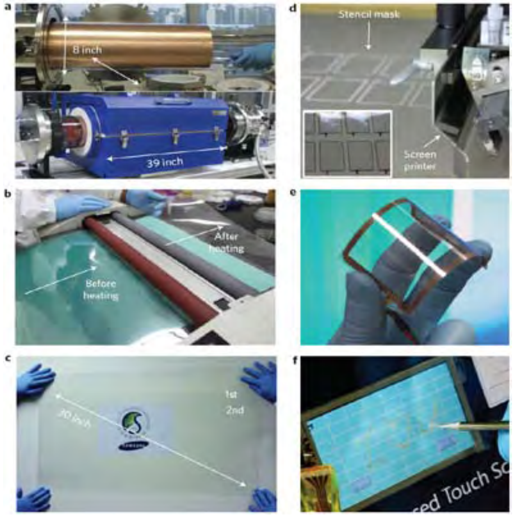


SAMSUNG

NT11,

Graphene Satellite meeting

Cambridge July 2011



CVD grown graphene (roll to roll and material transfer)

used in current prototypes of flexible displays promising but still of relatively poor quality

***Crystalline imperfections** (growth, transfer processes, etc..)*

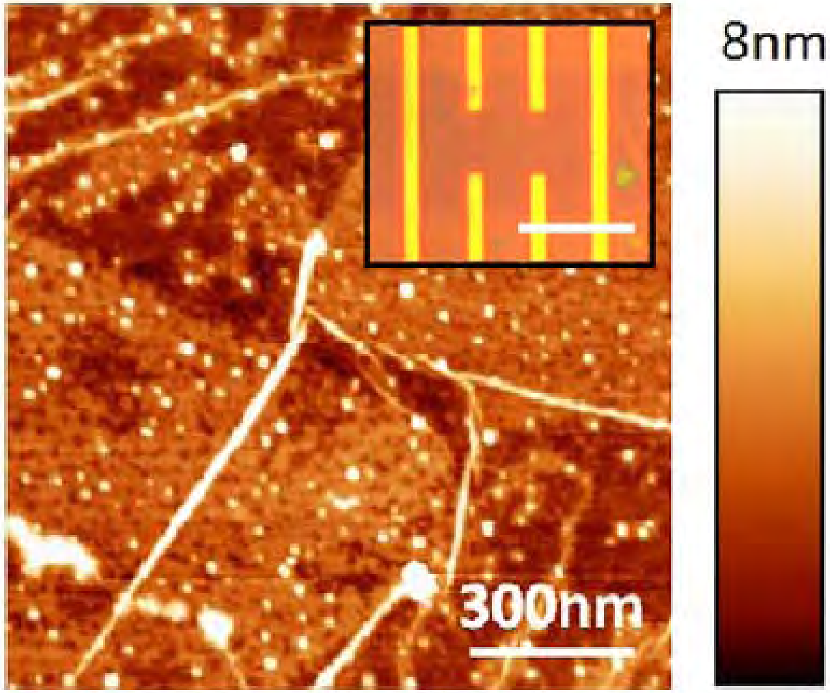
***Work in high dissipation regime**(bias, temperature, heating)*

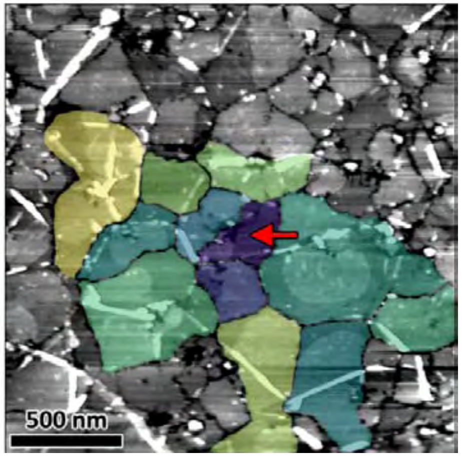
CVD graphene film transferred on SiO$_2$
How does it looks like ?

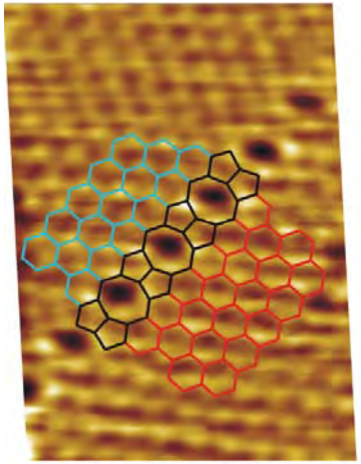
Mesoscopic scale

AFM image

EPL, 94 (2011) 28003





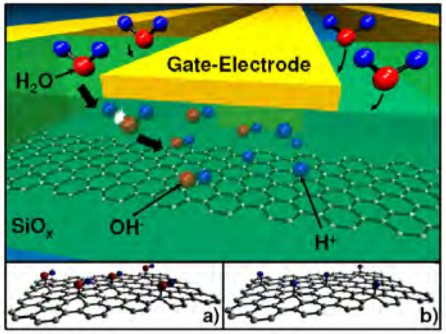


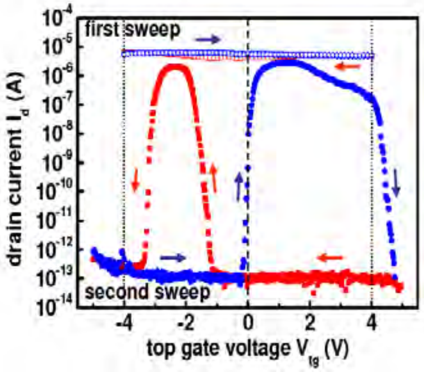
“Different thermal expansion of the Cu foil and the graphene sheet result in the formation of a few nm high ripples. Locally cracks can form during the transfer process and occasionally one is left with PMMA residues”

Disorder Engineering….

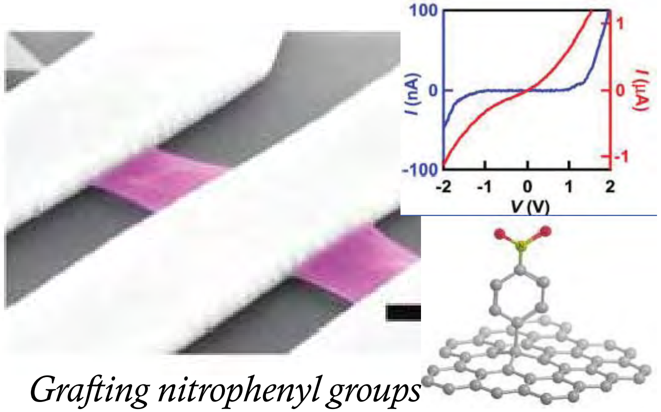
Bandgap engineering (chemical functionalization)

Electrochemical switch





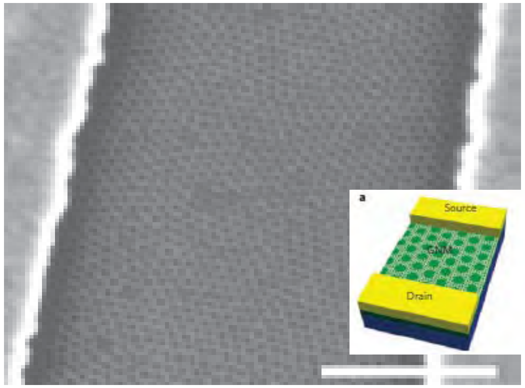
T. Echtermeyer et al, Elec. Dev. Lett. (2008)



Grafting nitrophenyl groups

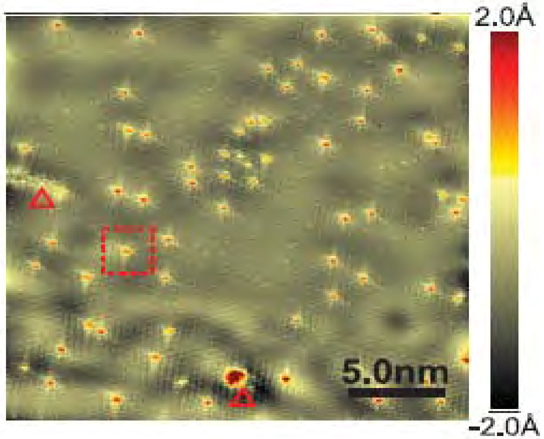
H. Zhang Nano Lett. (in press)

Graphene Nanomesh



J. Bai et al., Nature Nanotech 2010

Nitrogen doped graphene

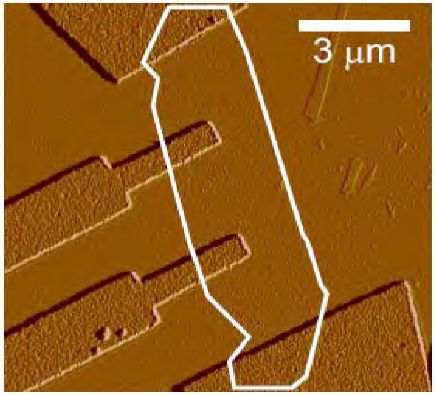


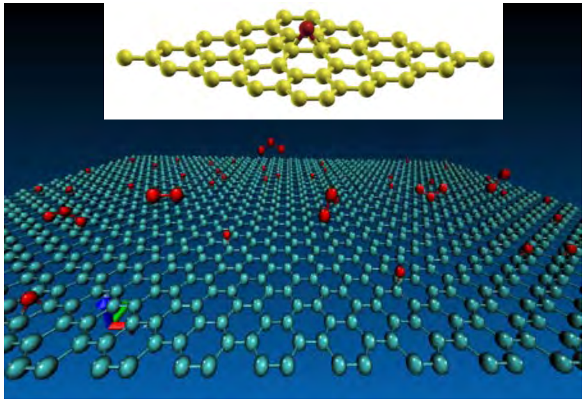
L. Zhao et al., Science 333,999 (2011)

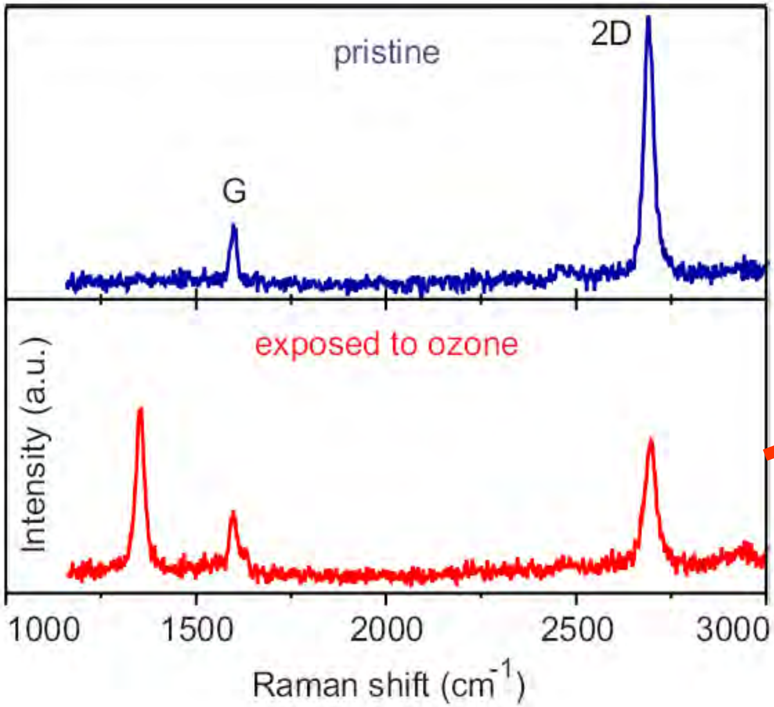
Ozone functionalization of Graphene

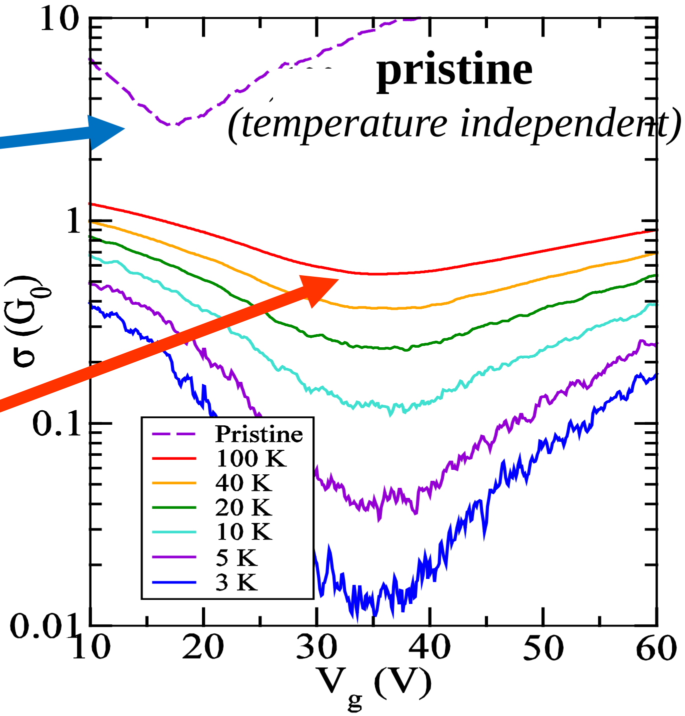
J. Moser et al.,
Phys. Rev. B 81, 205445 (2010)

Ozone flux →









Gate-dependent Damaged Transport

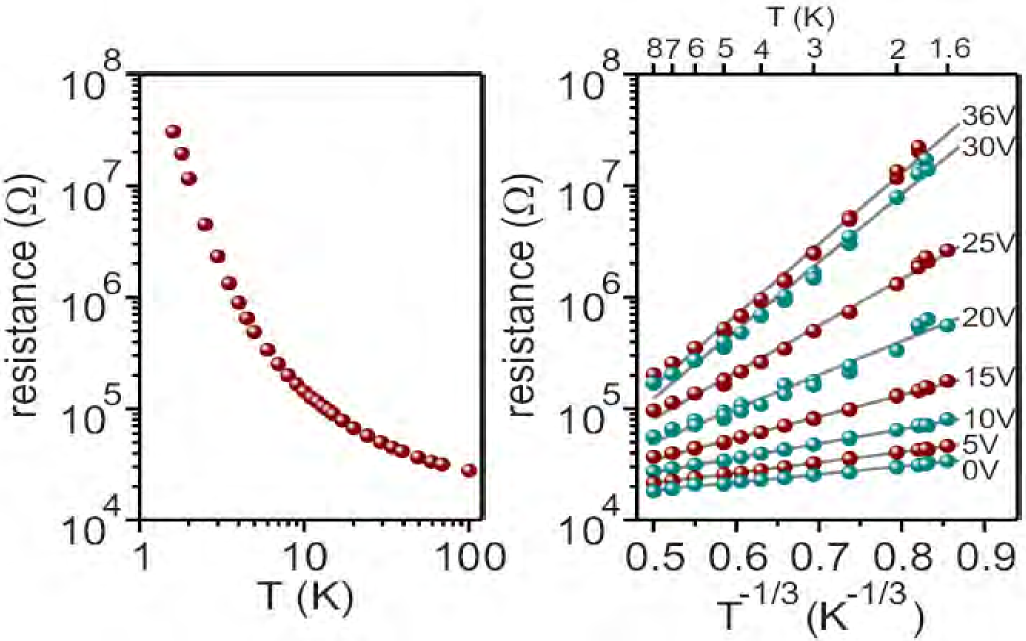
Low temperature transport
(variable range hopping)

$$\sigma(T) = \exp(-(T_0/T)^{1/3})$$

$$\downarrow$$

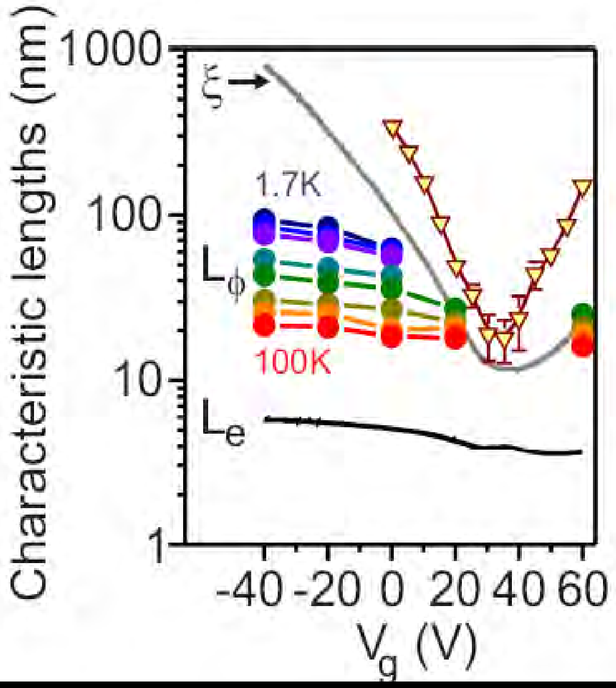
Localization length

$$\xi = \sqrt{13.8/k_B \rho T_0}$$



Analyse of magnetotransport fingerprints
(weak localization-coherence length-)

→ L_ϕ



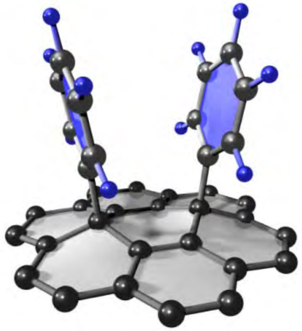
J. Moser, H. Tao, S.R., F. Alsina, C. M. Sotomayor Torres, A. Bachtold, **Phys. Rev B 81, 205445 (2010)**

Complexity & Computational challenges

- Enhanced structural & electronic complexity at the nanoscale
  driven by disorder (defects, deformations,chemical reactivity,...)
- Randomness of defects distribution
- *If quantitative prediction is targeted*

Simulation of **very large system size**

1μm^2 - 10 Millions carbon atoms



Theoretical modelling & simulation

- **First-principles calculations** - *accurate predictions of structures, electronic properties, description of impurity states,…*
- **Reduced Hamiltonian (tight-binding,..)**
- **Order N implementation of transport methodologies** *(Landauer, Kubo)*

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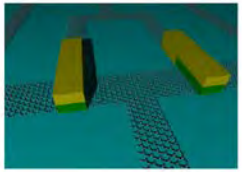

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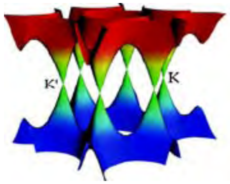

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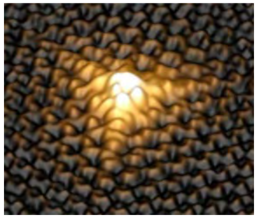
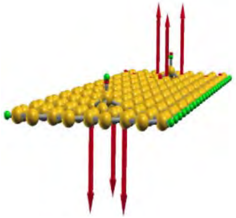
   From Klein Tunneling to weak antilocalization



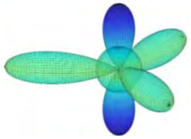
4. *Chemically modified Graphene*

   From electronic insulators to Magnectic materials



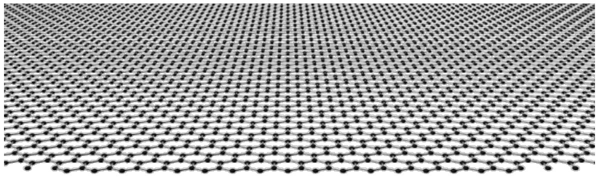
π - Effective Model

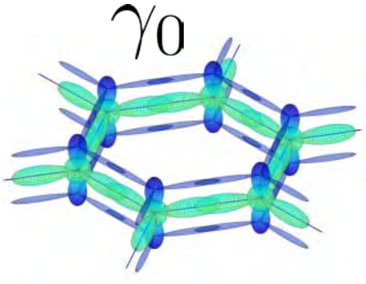
Hybrid Molecular Orbitales



Cohesion $s, p_x, p_y \equiv \sigma$

Electronic Properties in the vicinity of E_F $p_z \equiv \pi$

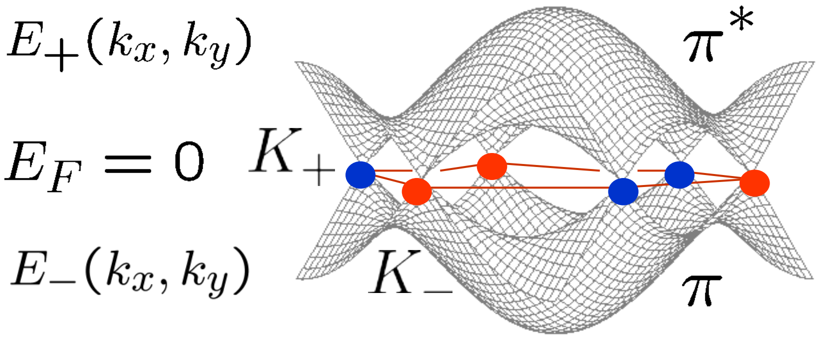


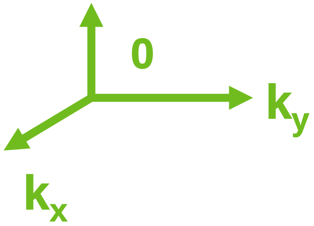


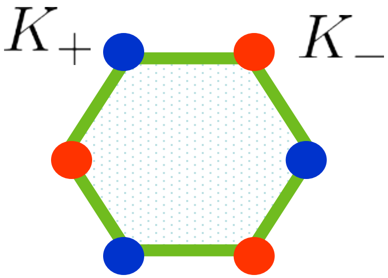
2 atoms/ cell γ_0 nearest neighbor orbital overlap

$$\mathcal{H}_k = \begin{pmatrix} 0 & h(k) \\ h^*(k) & 0 \end{pmatrix} \quad h_k = -\gamma_0 \sum_{m=1}^{3} e^{-i\mathbf{k}.\mathbf{e}_m}$$

$$E_\pm(k_x, k_y) = \pm\gamma_0 \Big(3 + 4\cos(\frac{\sqrt{3}k_x a}{2})\cos(\frac{k_y a}{2}) + 2\cos(k_y a)\Big)^{1/2}$$

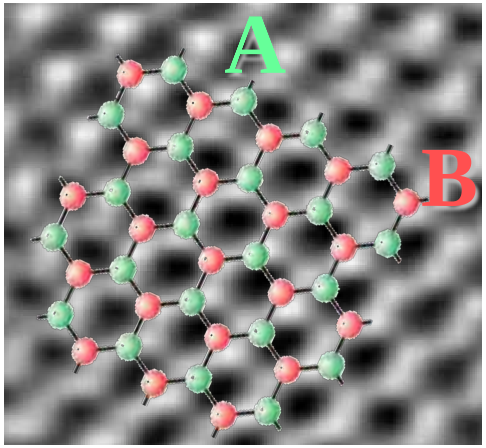


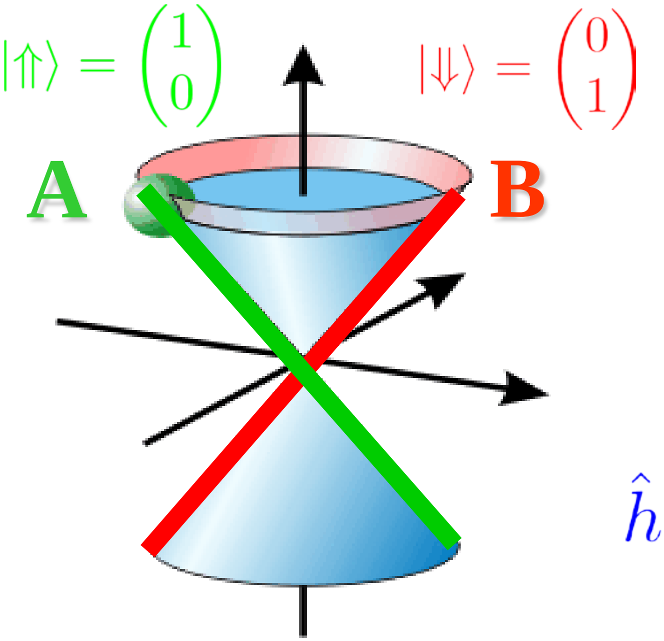




1 Brillouin Zone

Massless Dirac Fermions in 2D





Linearization close to Fermi level

$$\vec{Q} = K_+ + \vec{p}/\hbar$$

$$\boxed{\begin{aligned} \mathcal{H}_{K_+} &= v_F\big(p_x\sigma_x + p_y\sigma_y\big) \\ \mathcal{H}_{K_+} &= -v_F|\vec{p}|_x\sigma_z \end{aligned}}$$

[sublattice basis]

[diagonal basis]

$$E(\vec{p}) = s v_F|\vec{p}|,\, s = \pm 1$$
$$= s\sqrt{v_F^2p^2 + m_*^2v_F^4}$$

Dirac Equation for Massless particles

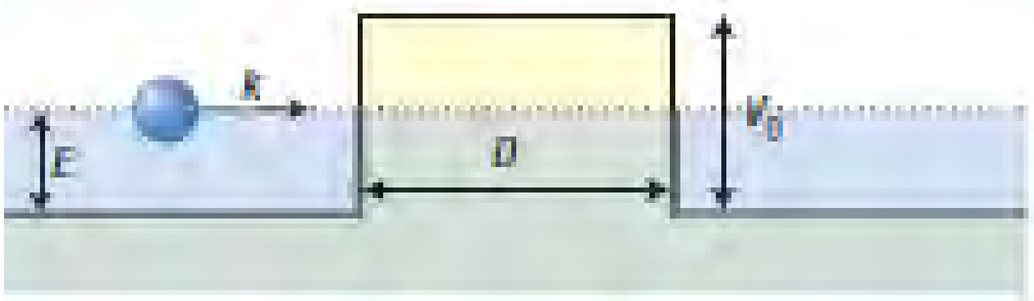
$$\Psi^{\pm}_{\vec{p}} = \frac{1}{\sqrt{2}}\left(\begin{array}{c} \Psi^{\pm}_{p}(A) \\ \Psi^{\pm}_{p}(B) \end{array}\right) = \frac{1}{\sqrt{2}}\left(\begin{array}{c} se^{i\theta/2} \\ e^{-i\theta/2} \end{array}\right)$$

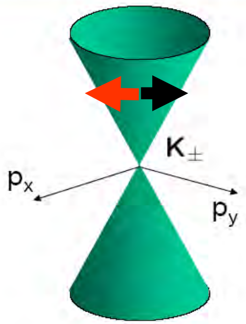
$$\hat{h} = \frac{1}{2}\vec{\sigma}.\frac{\vec{p}}{|\vec{p}|} \qquad \hat{h}|\Psi_{\vec{p}}(s=\pm 1)\rangle = \pm\frac{1}{2}|\Psi_{\vec{p}}(s)\rangle$$

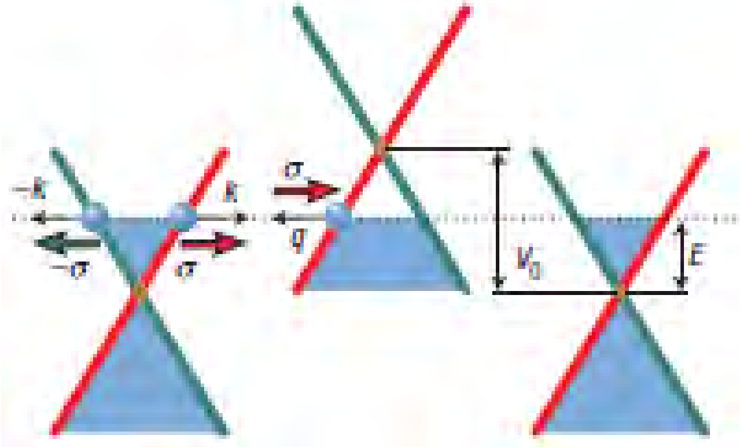
eigenstates have a well defined helicity (good q.n.)

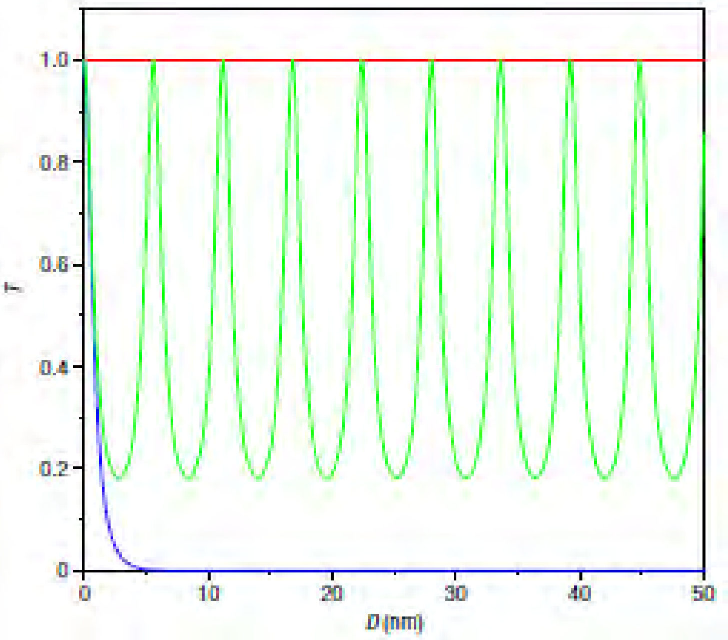
Pseudospin and Klein Tunneling

Katsnelson, Novoselov, Geim Nature Physics 2006









KT-limits : Disorder & valley mixing

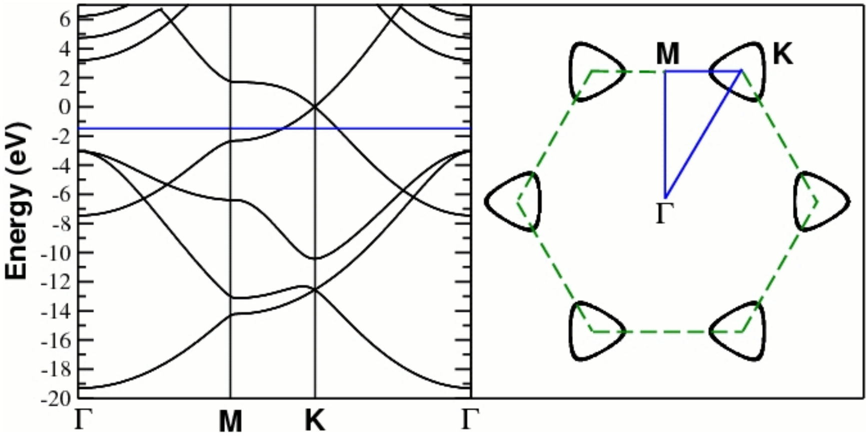
Deviation from linear dispersion

(trigonal warping)

$$E(\vec{p}) = \pm v_F|\vec{p}| + \pm\frac{a_{cc}v_F}{4\sqrt{3}}\sin(3\alpha(\mathbf{p}))|\mathbf{p}|^2 + \mathcal{O}(p^3)$$

Disorder induces (multiple) scattering events

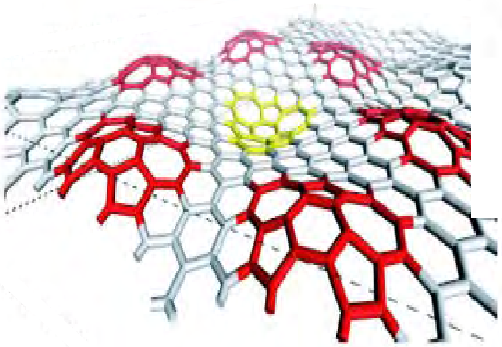
(energy conserved/elastic scattering)

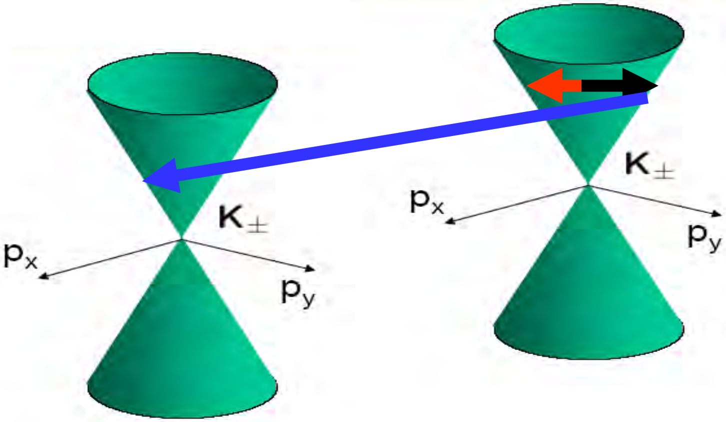


Long range potential

Intravalley scattering

(short momentum transfer)

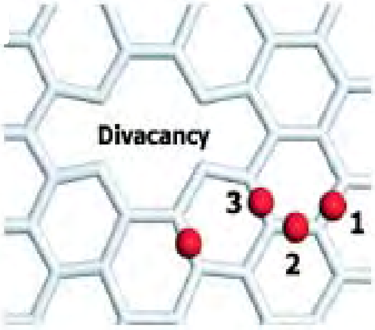




Short range potential

Intervalley scattering

(large momentum transfer)



* **diffusive** (mean free path)

*** Quantum interferences and Localization phenomena**

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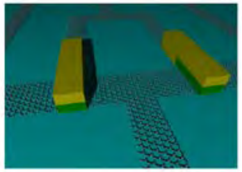

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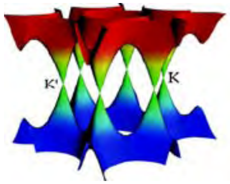

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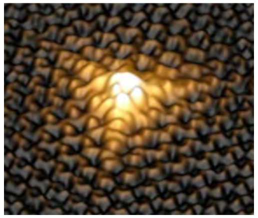

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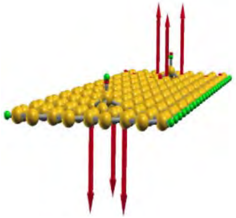
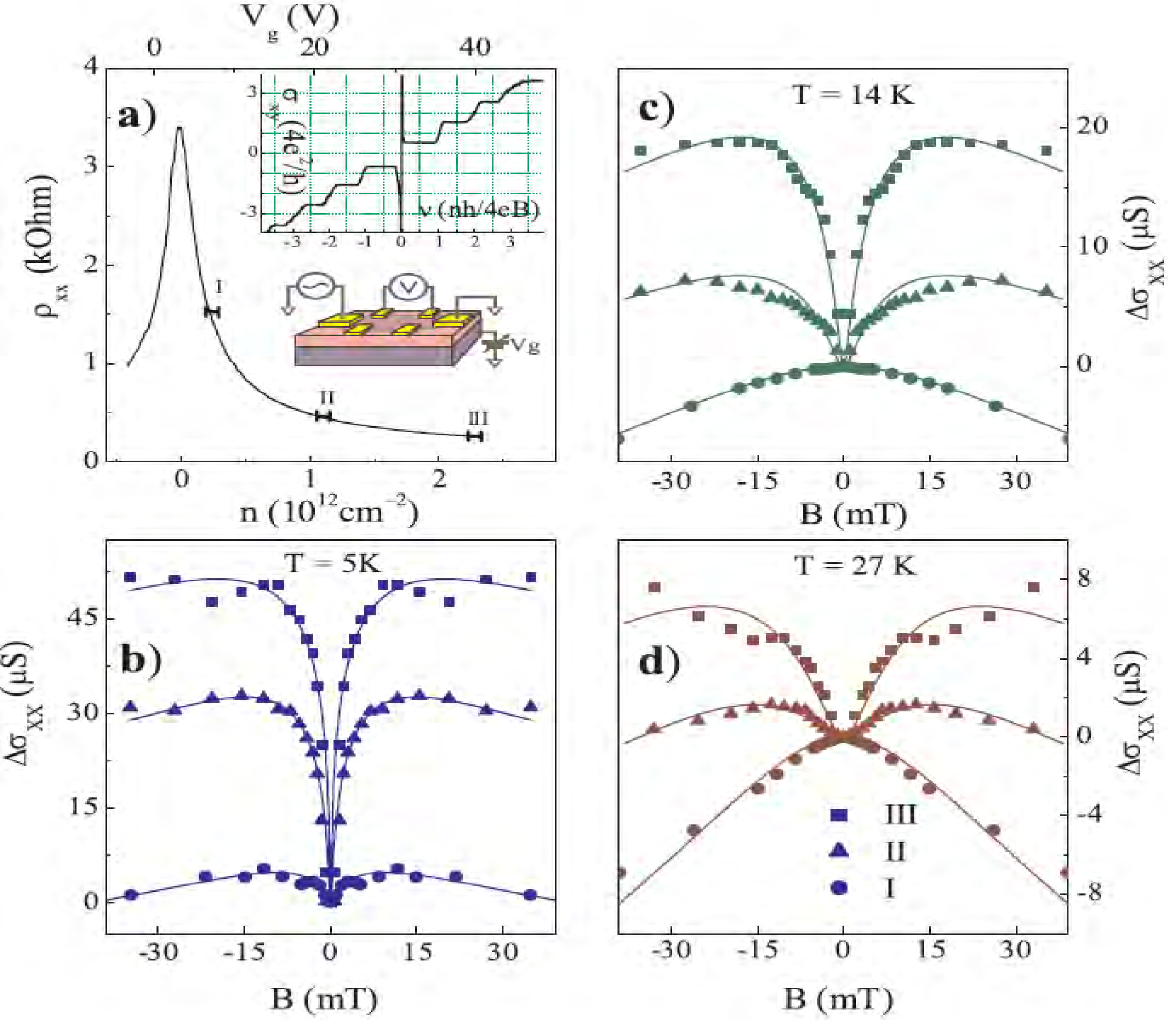


Weak antilocalization in graphene……

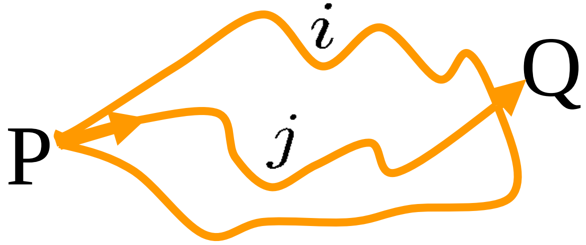
F.V. Tiknonenko et al, **Phys. Rev. Lett 97, 146805 (2007)**



No so-coupling…
no magnetic impurities

Localization Phenomena

Disordered metal



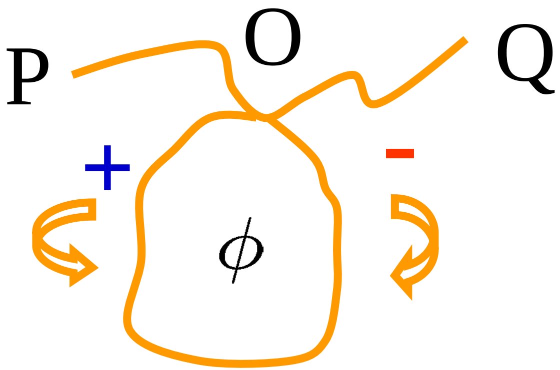
$$G = \frac{2e^2}{h}\mathcal{P}_{P\to Q}$$

Quantum conductance

$$\mathcal{P}_{P\to Q} = \sum_i |\mathcal{A}_i|^2 + \sum_{i\neq j} \mathcal{A}_i\mathcal{A}_j e^{i(\alpha_i-\alpha_j)}$$

Time-reversed trajectories interfere constructively

$$\mathcal{P}_{O\to O} = \left|\mathcal{A}_+ e^{i\alpha_+} + \mathcal{A}_- e^{+i\alpha_-}\right|^2 = 4\left|\mathcal{A}_0\right|^2$$



$$= 2\left|\mathcal{A}_0\right|^2\left(1+\cos\frac{2\pi\phi}{\phi_0/2}\right)$$

Positive magnetoconductance

(weak localization)

Additional phase factor (pseudospin rotation) inducing sign reversal

Disordered Graphene

$$\Psi^{\pm}_{\vec{p}} = \frac{1}{\sqrt{2}}\begin{pmatrix}\Psi^{\pm}_{p}(A)\\ \Psi^{\pm}_{p}(B)\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} s e^{i\theta/2}\\ e^{-i\theta/2}\end{pmatrix}$$

Negative magnetoconductance

(weak antilocalization)

Weak localization in 2D graphene

E. McCann, K. Kechedzhi, V. I. Fal'ko, H.Suzuura, T. Ando, B.L. Altshuler,
Phys. Rev. Lett 97, 146805 (2007)

Quantum interferences correction (WL)

$$\Delta\sigma(B) = e^2/\pi h \left\{ \mathcal{F}\left(\frac{\tau_B^{-1}}{\tau_\varphi^{-1}}\right) - \mathcal{F}\left(\frac{\tau_B^{-1}}{\tau_\varphi^{-1}+2\tau_i^{-1}}\right) - 2\mathcal{F}\left(\frac{\tau_B^{-1}}{\tau_\varphi^{-1}+\tau_i^{-1}+\tau_*^{-1}}\right) \right\}$$

τ_i Intervalley scattering time

τ_ω Trigonal warping scattering time

τ_s Intravalley scattering time

$\tau_B = \hbar/2eDB$

$$F(z) = \ln z + \Psi(1/2 + 1/z)$$

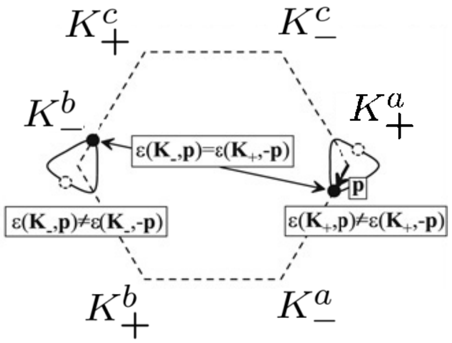
digamma function

Introduction of **several phenomenological parameters** which can not be computed analytically from a given disorder model

$$\tau_w^{-1} + \tau_z^{-1} + \tau_i^{-1} \equiv \tau_*^{-1}.$$

$$\tau_w^{-1} = 2\tau_0(\epsilon^2\mu/\hbar v^2)^2.$$

$$\tau_i^{-1} = 4\tau_{\perp\perp}^{-1} + 2\tau_{z\perp}^{-1}, \qquad \tau_z^{-1} = 4\tau_{\perp z}^{-1} + 2\tau_{zz}^{-1}.$$



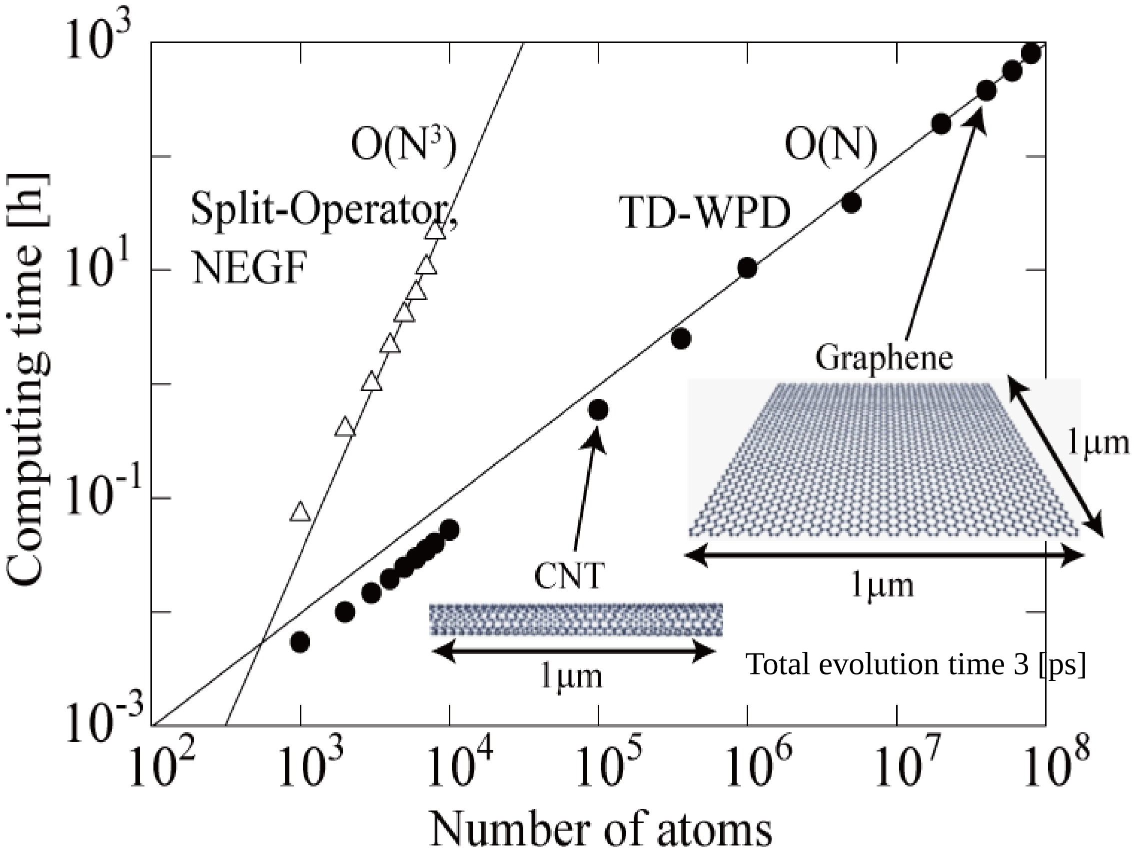
Quantum Transport Methodology

Time-evolution operator

~10

Bessel Chebyshev

$$e^{i\frac{\hat{H}(t)}{\hbar}\Delta t} = \sum_{n=0}^{\boxed{+\infty}} e^{-i\frac{a}{\hbar}\Delta t} h_n i^n J_n\left(-\frac{b\,\Delta t}{\hbar}\right) T_n\left(\frac{\hat{H}(t)-a}{b}\right)$$



Calculation time of conductance using Kubo approach

Quantum Transport

Order-N

Disorder systems

Combined Molecular Dynamics

10-100 million atoms


Copyright 2005. Barcelona Supercomputing Center - BSC

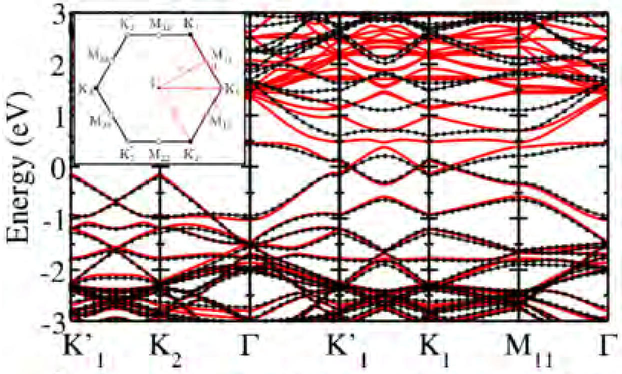
S.R. et al **PRL 79, 2518 (1997)**

C.R. Physique 10, 283-296 (2009)

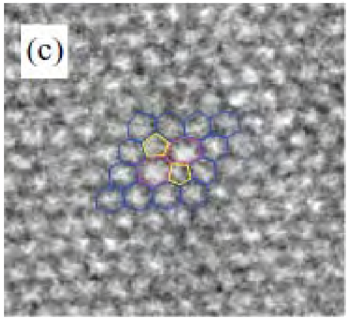
Non Magnetic Defects

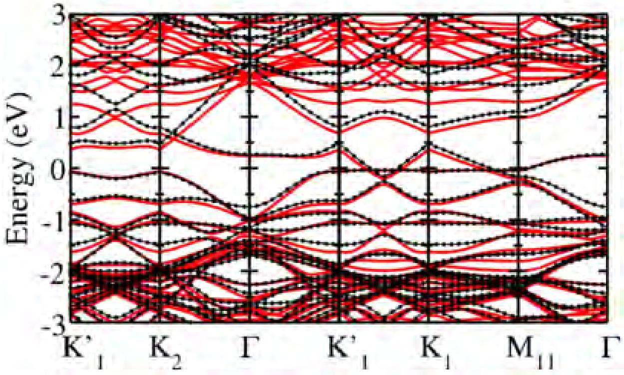
SIESTA ab initio calculations (red)

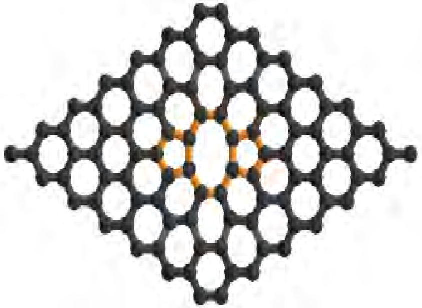
TB-third nearest neighbors (black)



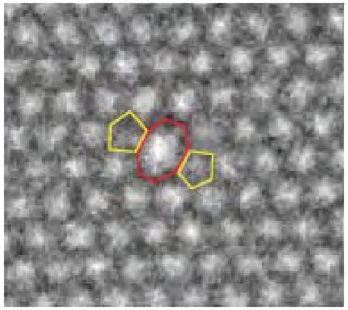
Stone-Wales

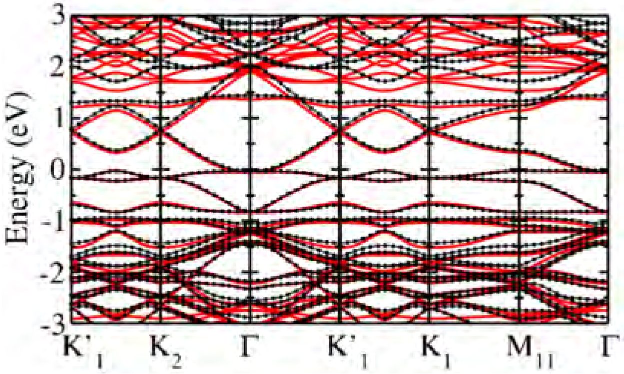






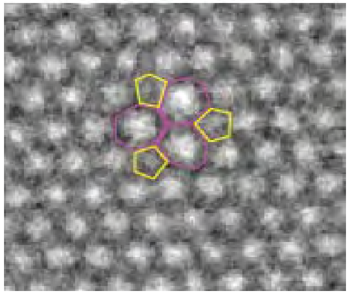
Divacancy 585





Divacancy 555777

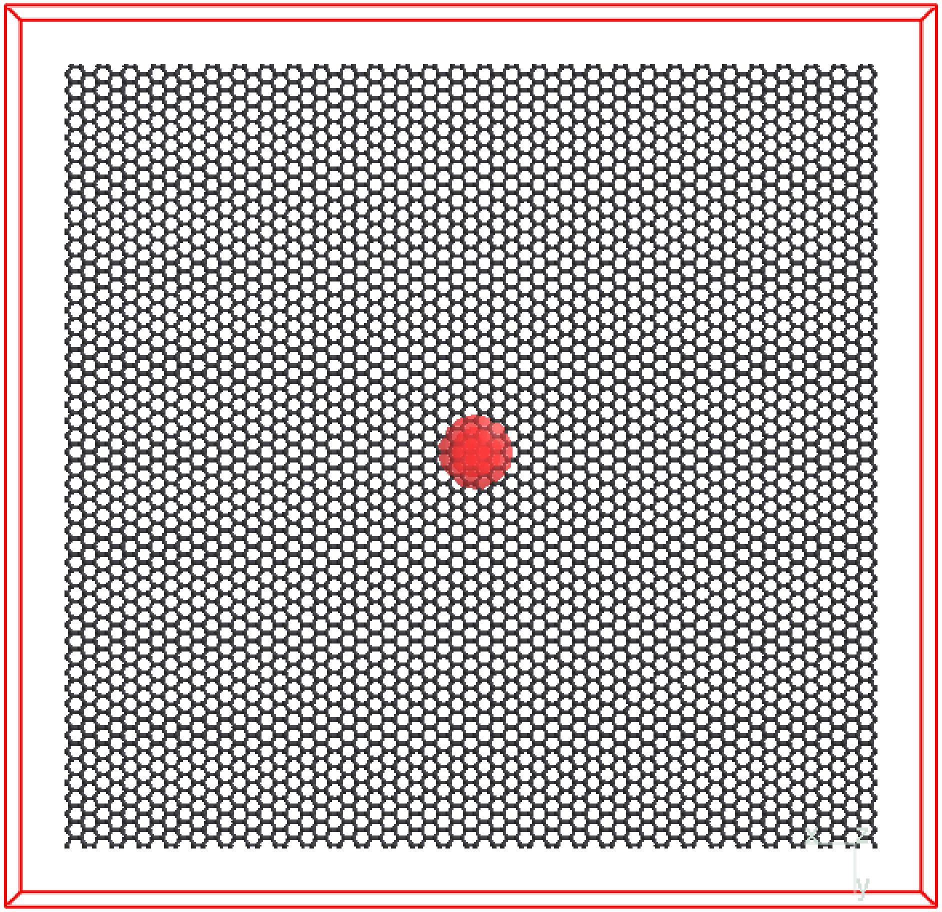
3-fold symmetry axis



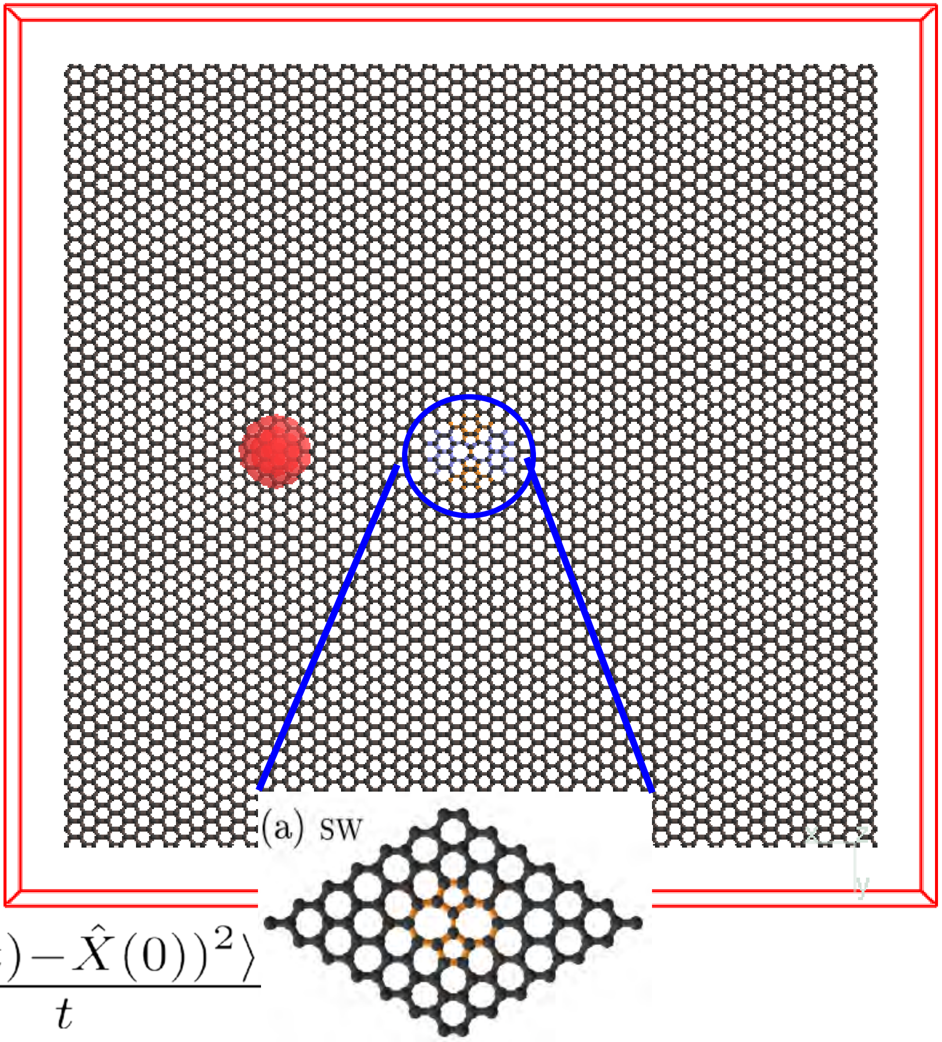
J. Kotakoski et al **PRB 83, 245420 (2011)**

Wavepacket Propagation

Clean Graphene $D(E,t) \sim v^2 t$



Graphene with a single structural defect



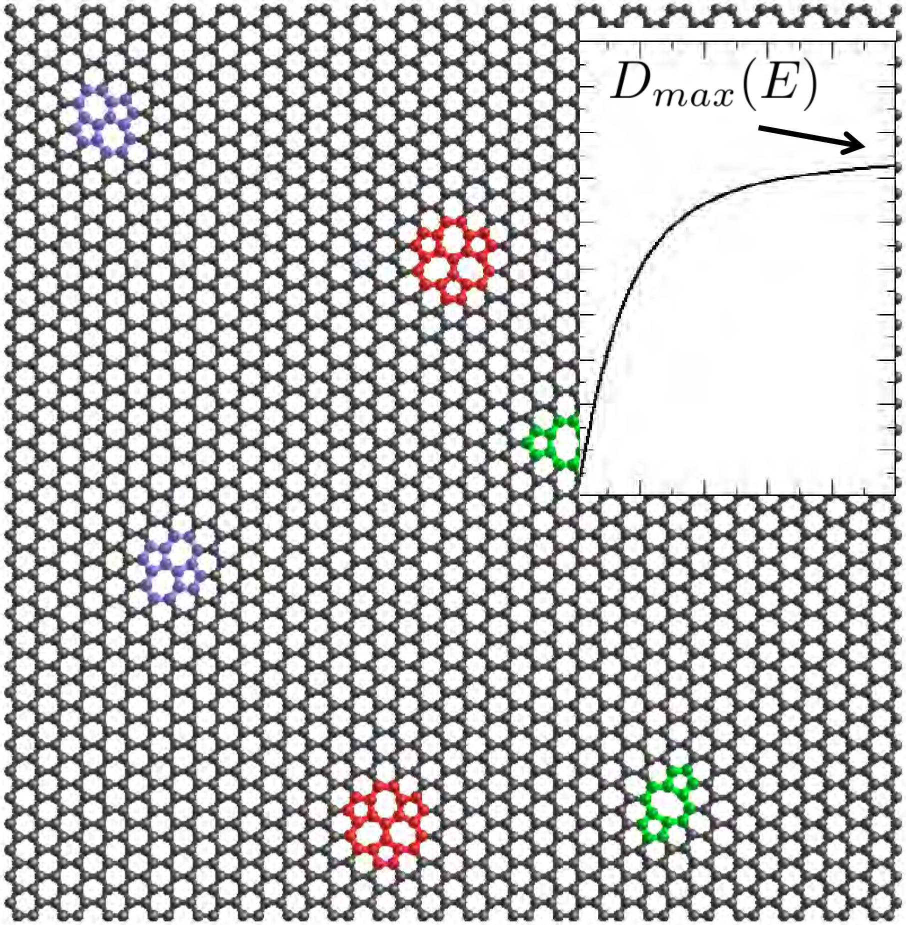
Diffusion coefficient $D(E,t) = \frac{\langle (\hat{X}(t) - \hat{X}(0))^2 \rangle}{t}$

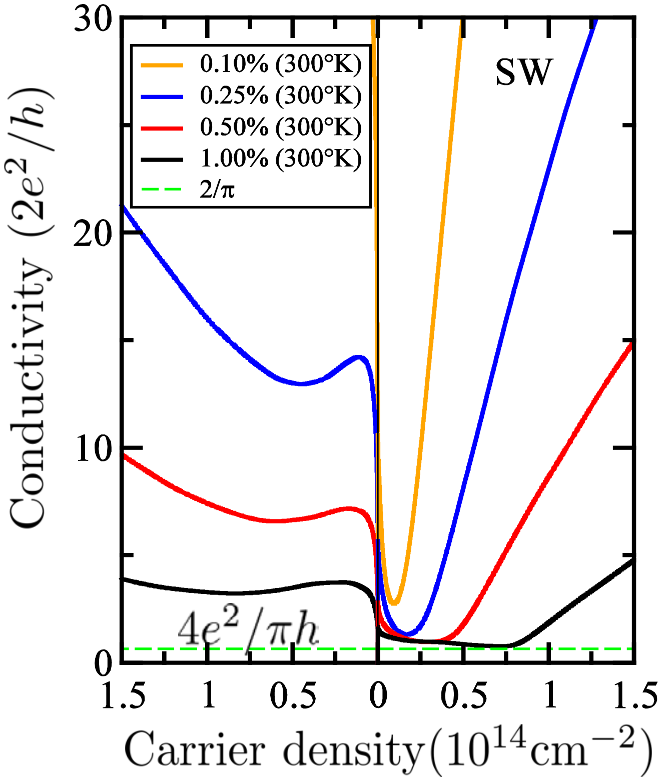
DoS, MFP and SC-Conductivities

From dynamics of wavepackets

$$D_{max}(E) = v(E)\ell_e(E)$$

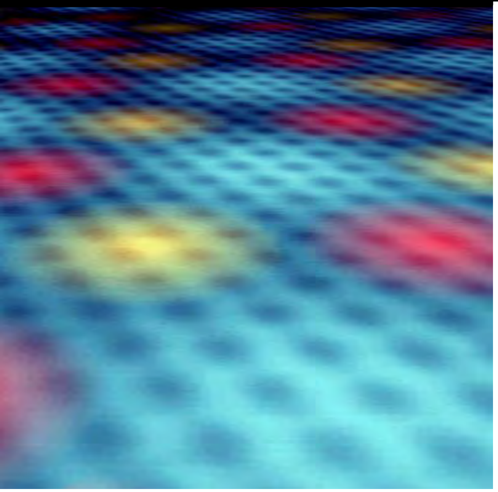
$$\sigma_{sc}(E) = e^2\rho(E)D_{max}(E)/2$$





A. Lherbier et al., **Phys. Rev. Lett 106, 046803 (2011)**

Long range disorder potential



Charges trapped in the oxide

$$\mathcal{H} = \sum_{\alpha} V_\alpha |\alpha\rangle\langle\alpha| + \gamma_0 \sum_{\langle\alpha,\beta\rangle} e^{-i\varphi_{\alpha\beta}} |\alpha\rangle\langle\beta|$$

Long range (Gaussian) potential

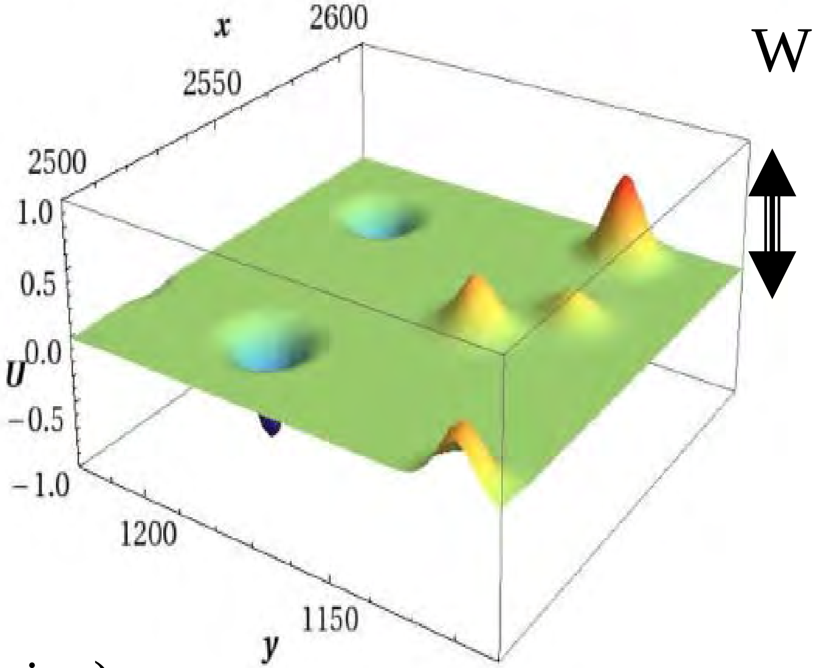
$$V_\alpha = \sum_{i=1}^{N_I} \varepsilon_i \exp(-|\mathbf{r}_\alpha - \mathbf{r}_i|^2/(2\xi^2))$$

$$\varepsilon_i \in [-W/2, W/2](\gamma_0\text{-unit}),\ W = 0.5 - 2$$

$$\xi = 3a = 0.426\text{nm} \quad \gamma_0 = -2.7\text{eV}$$

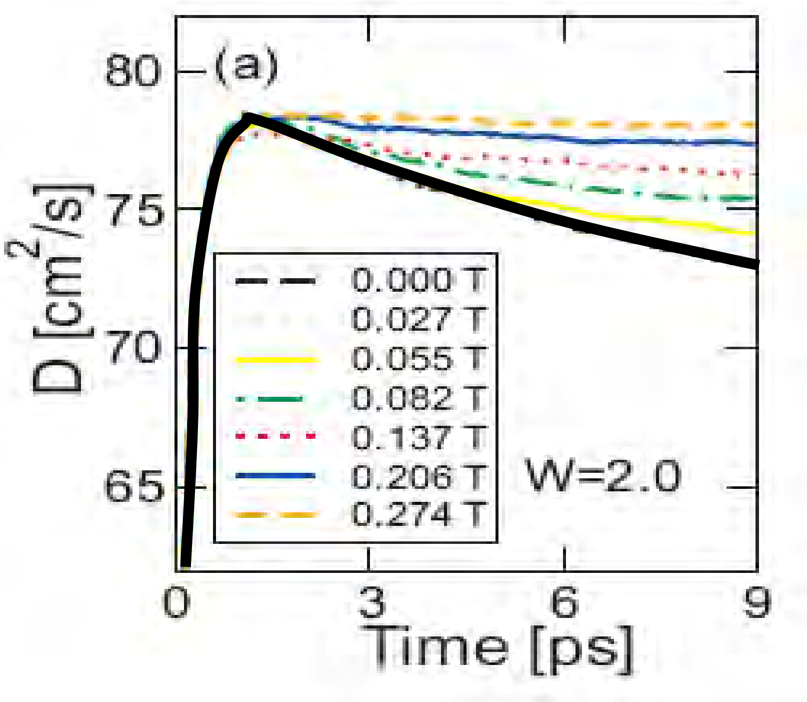
$$n_i = N_i/N = 0.125\%, 0.25\%, 0.5\%$$

Sample size $S \sim 0.3\mu\text{m}^2$

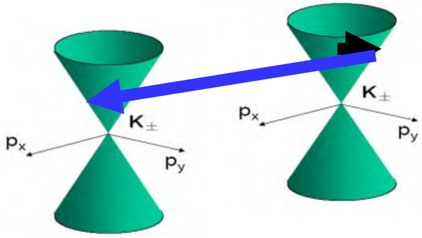


W (depth of onsite potential ~screening)

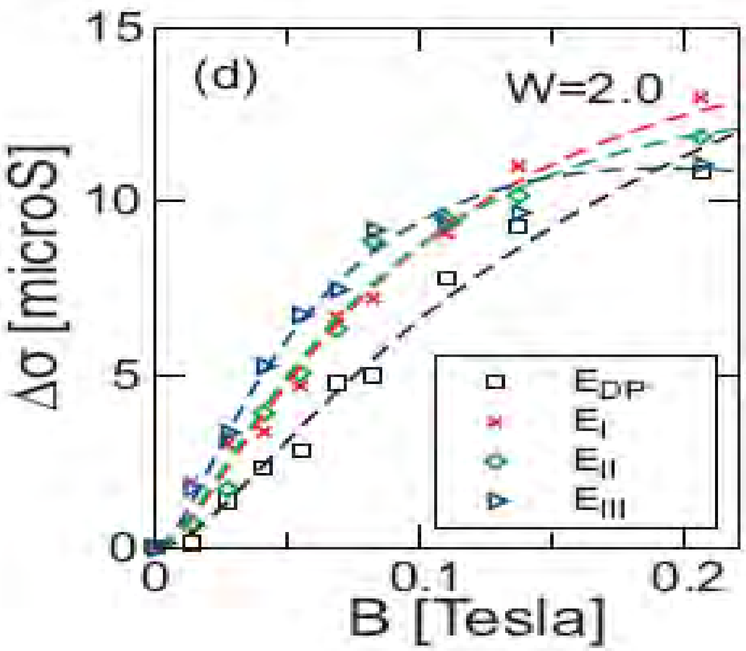
B-suppression of quantum interferences



At B=0 the Diffusion shows onset of localization (time-dependent decay)



$$\Delta\sigma(B) = \sigma(B) - \sigma(B=0)$$



Quantum interferences
are suppressed by increasing magnetic field
Weak localization phenomenon

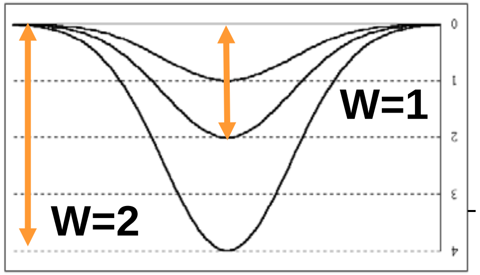
$$\ell_e \in [9, 20]\mathrm{nm}$$

Crossover from WL to WAL

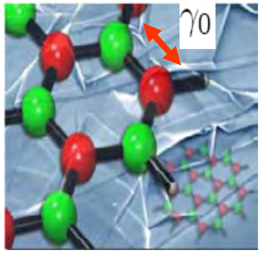
$$\sigma(E, t = N_t\Delta t) = e^2\rho(E)D(E,t)/2$$

$$\Downarrow$$

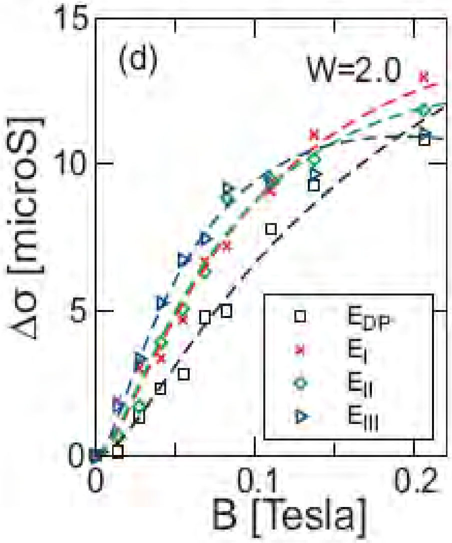
$$\Delta\sigma(B) = \sigma(B) - \sigma(B=0)$$



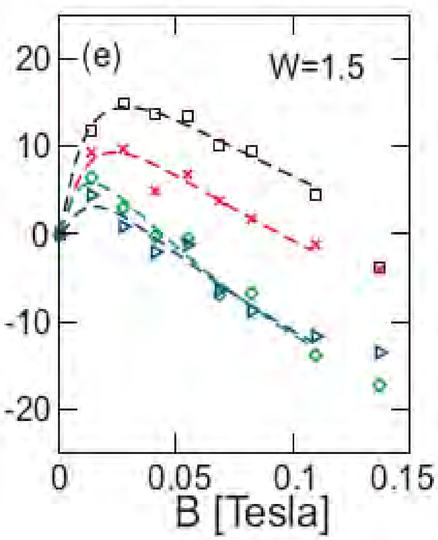
Not WAL !!
(ballistic regime)



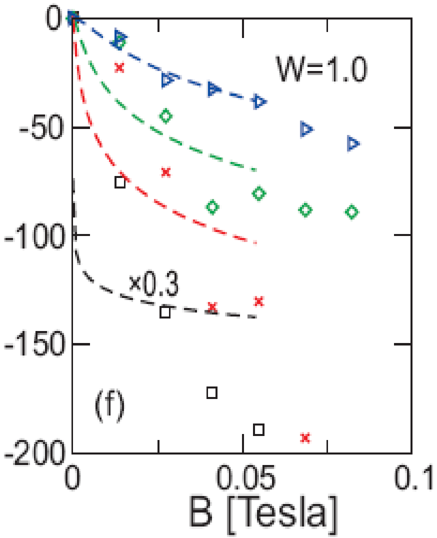
Weak localization



Crossover
Weak Antilocalization



$$\Delta\sigma(B) < 0$$

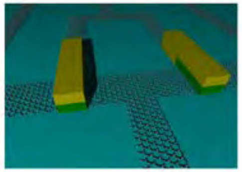


$E_{DP}=0$
$E_I=0.049$eV
$E_{II}=0.097$eV
$E_{III}=0.146$eV

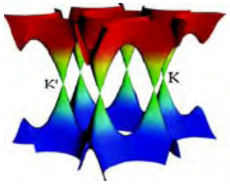
F. Ortmann, A. Cresti, G. Montambaux, SR. **Euro. Phys. Lett. 94, 47006 (2011)**

OUTLINE

1. *Why focusing on "dirty graphene" ?*

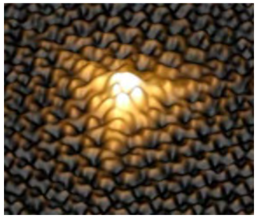


2. *Reminder Electronic Properties*



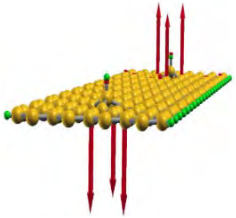
3. *Defects and Transport in Graphene*

   Manifestation of Pseudospin & weak antilocalization

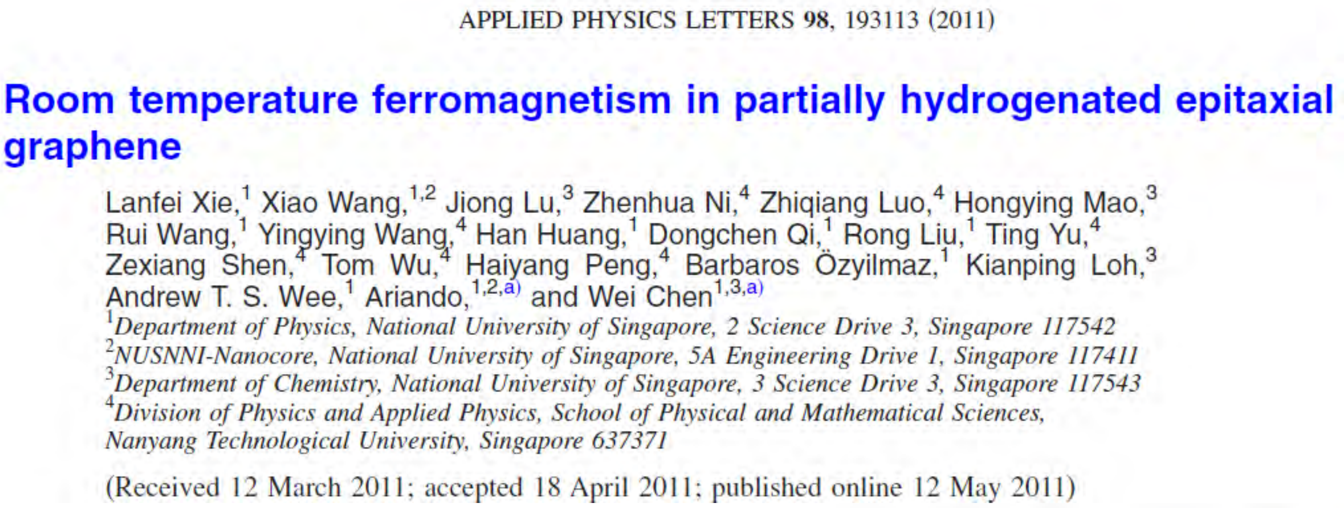


4. *Chemically modified Graphene*

   Local magnetic ordering and metal-insulator transition



Room temperature ferromagnetism



APPLIED PHYSICS LETTERS **98**, 193113 (2011)

Room temperature ferromagnetism in partially hydrogenated epitaxial graphene

Lanfei Xie,[1] Xiao Wang,[1,2] Jiong Lu,[3] Zhenhua Ni,[4] Zhiqiang Luo,[4] Hongying Mao,[3] Rui Wang,[1] Yingying Wang,[4] Han Huang,[1] Dongchen Qi,[1] Rong Liu,[1] Ting Yu,[4] Zexiang Shen,[4] Tom Wu,[4] Haiyang Peng,[4] Barbaros Özyilmaz,[1] Kianping Loh,[3] Andrew T. S. Wee,[1] Ariando,[1,2,a)] and Wei Chen[1,3,a)]

[1] *Department of Physics, National University of Singapore, 2 Science Drive 3, Singapore 117542*
[2] *NUSNNI-Nanocore, National University of Singapore, 5A Engineering Drive 1, Singapore 117411*
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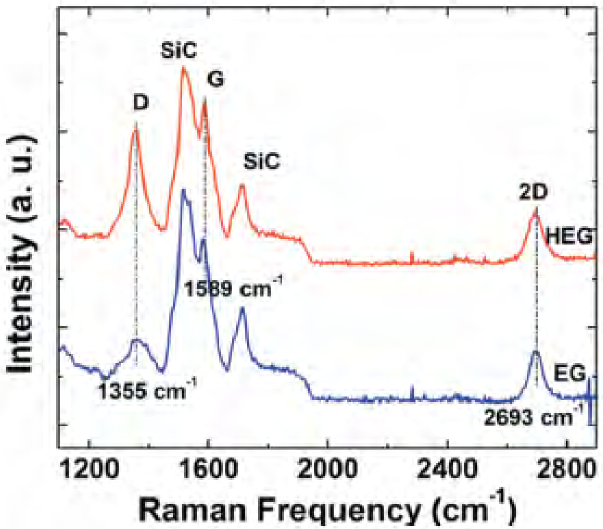
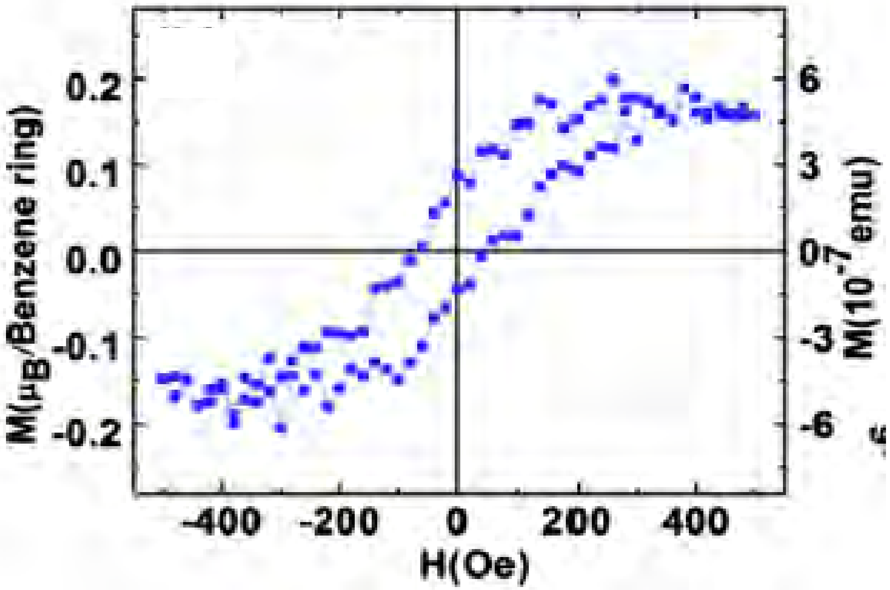
(Received 12 March 2011; accepted 18 April 2011; published online 12 May 2011)

Magnetic hysterisis
at room temperature

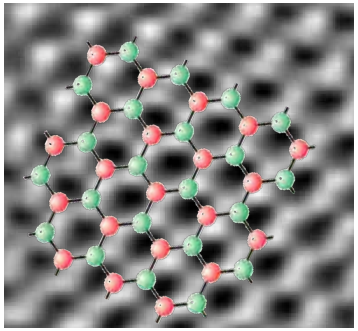




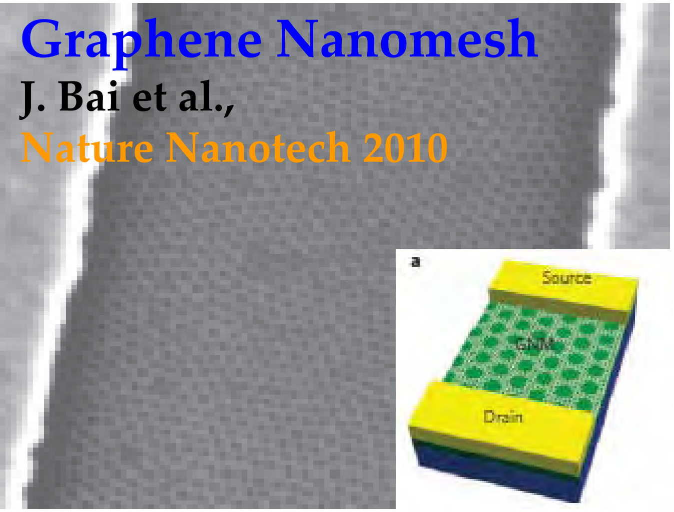
Lieb's Theorem

E.H. Lieb, Phys. Rev. Lett 62, 1201 (1989)

$$\mathcal{H} = \sum_{ij\sigma} t c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} (\hat{n}_{i\uparrow}\langle \hat{n}_{i\downarrow}\rangle + \hat{n}_{i\downarrow}\langle \hat{n}_{i\uparrow}\rangle - \langle \hat{n}_{i\uparrow}\rangle\langle \hat{n}_{i\downarrow}\rangle)$$



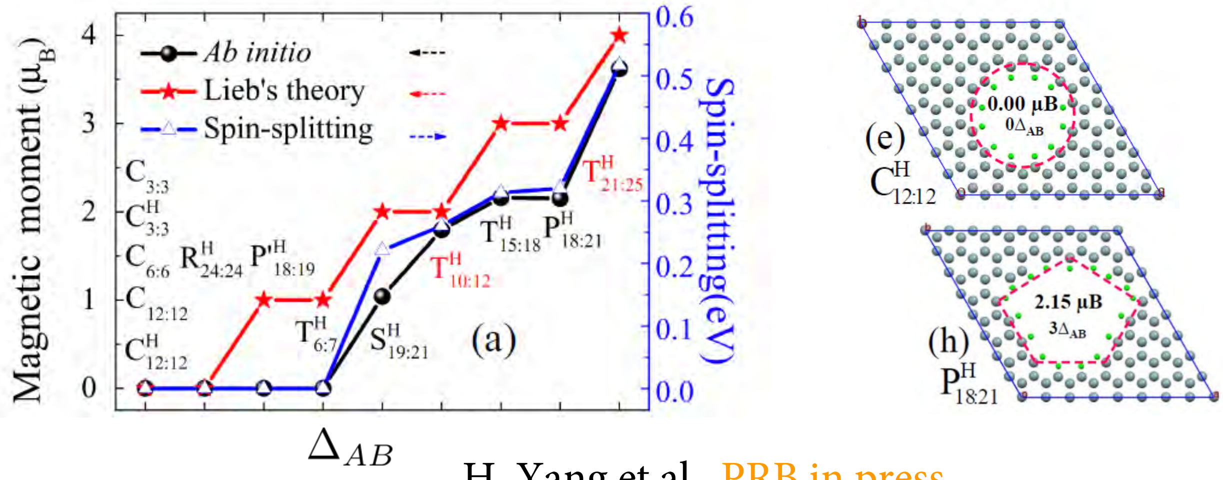
Theorem (repulsive case) : If the lattice is **bipartite** (t couple only A sites with B sites), Assuming number of B larger or equal to number of A sites (and number of electron =total number of sites (half-filled band), then the ground state of $\mathcal{H}$ is unique with spin $S = \frac{1}{2}(\mid B \mid - \mid A \mid) = \frac{1}{2}\Delta_{AB}$



Graphene Nanomesh

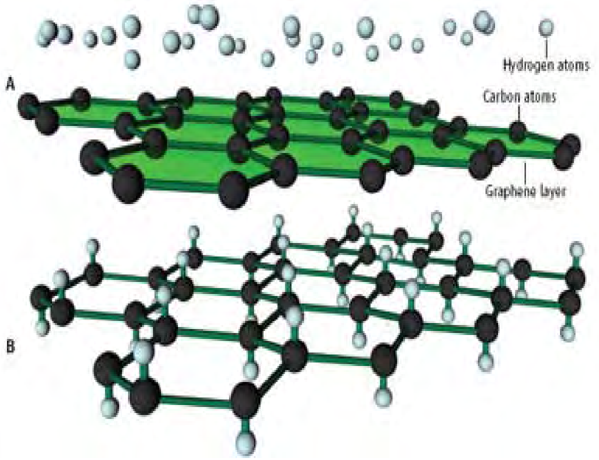
J. Bai et al.,

Nature Nanotech 2010



H. Yang et al., PRB in press

Describing Hydrogenated Graphene



Hubbard Hamiltonian

*Single π band with a **repulsive Coulomb interaction** between electrons with opposite spin occupying the same orbital*

$$\sum_{ij\sigma} t c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} (\hat{n}_{i\uparrow}\langle \hat{n}_{i\downarrow}\rangle + \hat{n}_{i\downarrow}\langle \hat{n}_{i\uparrow}\rangle - \langle \hat{n}_{i\uparrow}\rangle\langle \hat{n}_{i\downarrow}\rangle)$$

$U > 0$ *constant one-site coulomb repulsion raising energy by U when 2 electrons occupy the same orbital*

$$\langle \hat{n}_{i\uparrow}\rangle = \int dE f(E_F - E)\rho_{i\uparrow}(E) \qquad \hat{n}_{i,\uparrow} = c^{\dagger}_{i,\uparrow} c_{i,\uparrow}$$

$$\boxed{\langle \hat{n}_{i\sigma}\rangle_0 \Rightarrow \mathcal{H} \Rightarrow \rho_{i\sigma} \Rightarrow \langle \hat{n}_{i\sigma}\rangle}$$

self-consistent occupation numbers
for spin-down and spin-up electrons

$$\begin{aligned} \varepsilon_{i\uparrow} &= U\langle \hat{n}_{i\uparrow}\rangle(1 - \langle \hat{n}_{i\downarrow}\rangle) \\ \varepsilon_{i\downarrow} &= U\langle \hat{n}_{i\downarrow}\rangle(1 - \langle \hat{n}_{i\uparrow}\rangle) \\ \mathcal{M}_i &= \frac{\langle \hat{n}_{i\uparrow}\rangle - \langle \hat{n}_{i\downarrow}\rangle}{2} \end{aligned}$$

Spin texture around Hydrogen defects

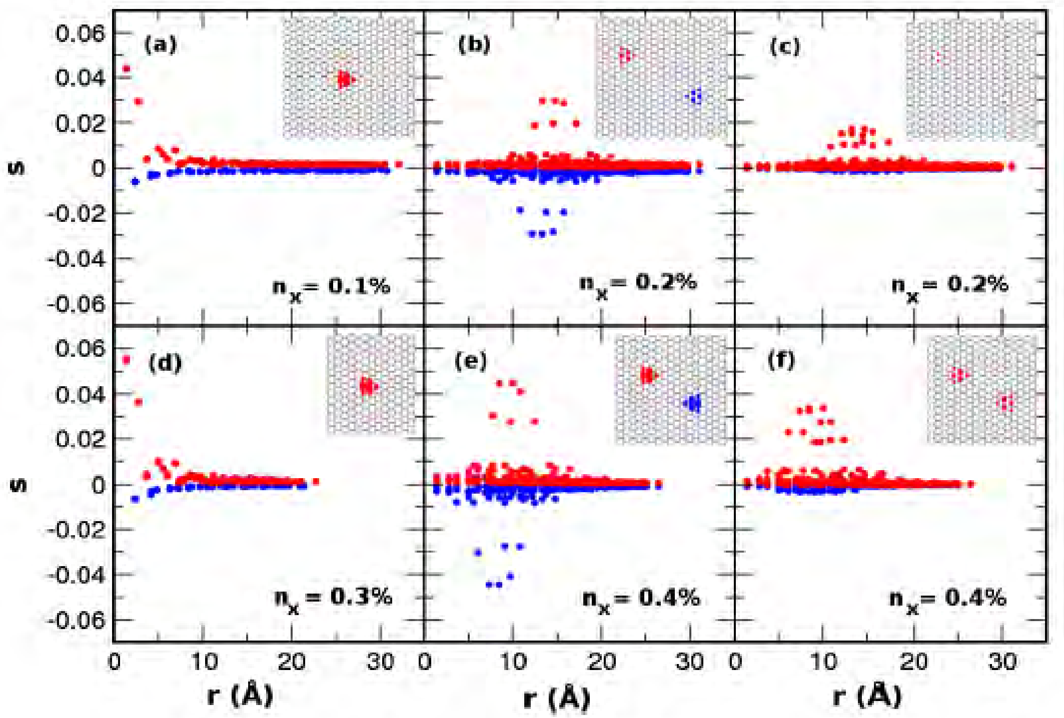
Case studies *low H- coverage*

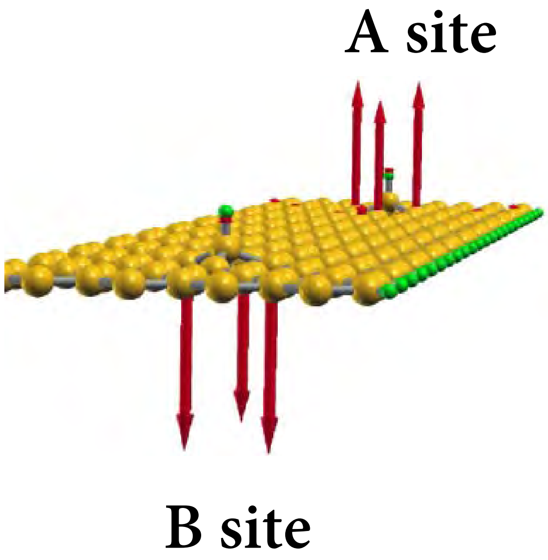
Absence of any (local) magnetic ordering (1 H per unit cell)

Local Antiferromagnetism (2 H defects on sites A and B)

Local Ferromagnetism (2H grafted on the same sublattice A)

or applying magnetic field



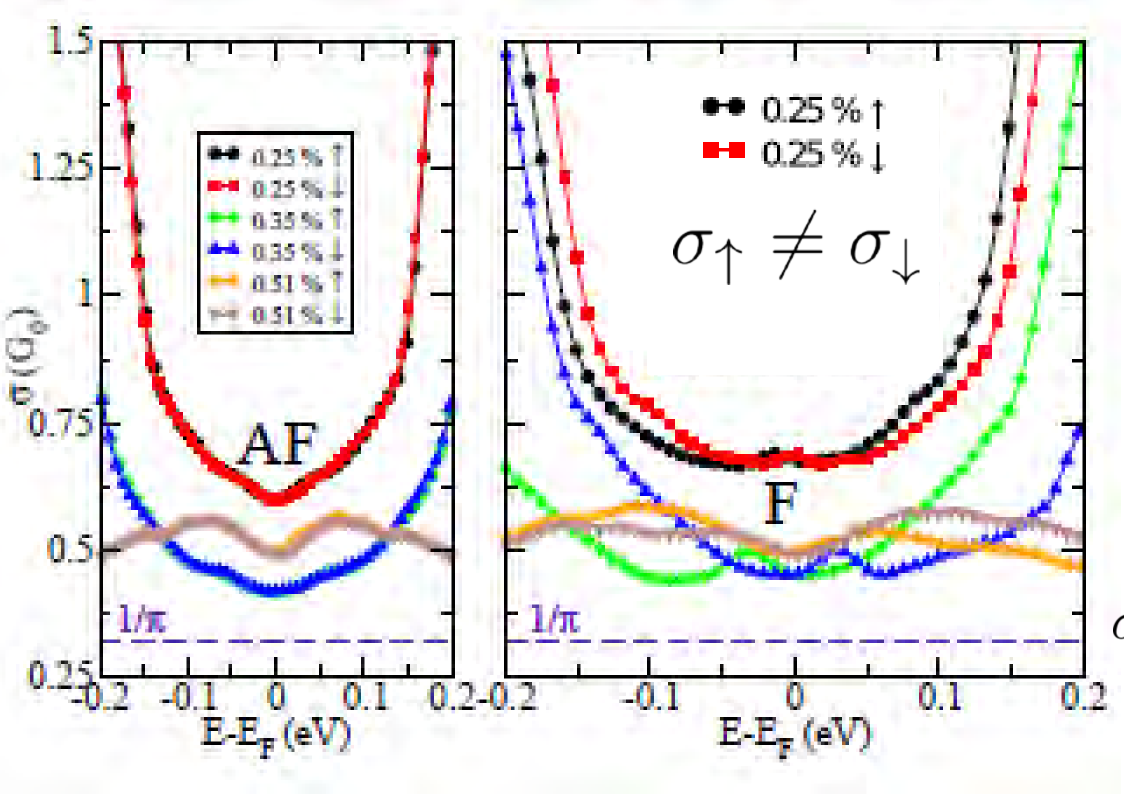


Local (site) spin (s) versus r (*the distance to the center of the supercell*)

Drude Conductivity – magnetic state

$$\boxed{\sigma_{\uparrow,\downarrow}(E,t) = (e^2/2)\mathrm{Tr}[\delta_{\uparrow,\downarrow}(E-\hat{H})]D_{\uparrow,\downarrow}(E,t)}$$

Spin-resolved DoS *Spin-resolved diffusion coefficient*



Neglecting quantum interferences

$$\sigma^{\mathrm{Drude}}_{\uparrow,\downarrow}(E) \sim 1/n_x$$

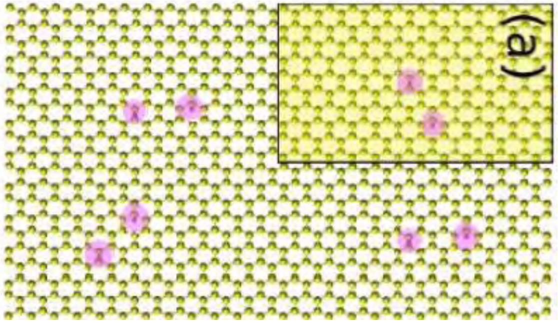
For the local ferromagnetic ordering spin splitting and $\sigma_\uparrow \neq \sigma_\downarrow$

$$\sigma^{\mathrm{Drude}}_{\uparrow}(E) + \sigma^{\mathrm{Drude}}_{\downarrow}(E) \geq 4e^2/\pi h$$

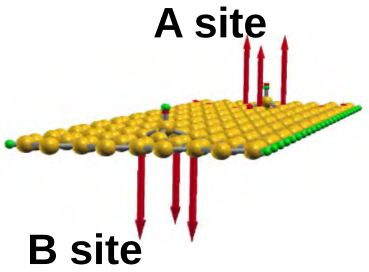
D. Soriano et al., **Phys. Rev. Lett. 107, 016602 (2011)**

Magnetoresistance signal

$$\mathrm{MR} = (\sigma^F - \sigma^{AF})/(\sigma^F + \sigma^{AF})$$

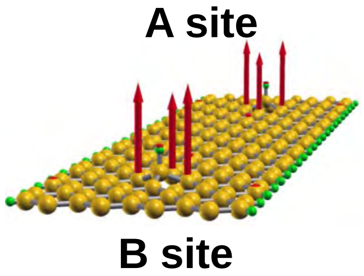


$$\sigma^{AF} = \sigma^{AF}_{\uparrow} + \sigma^{AF}_{\downarrow}$$

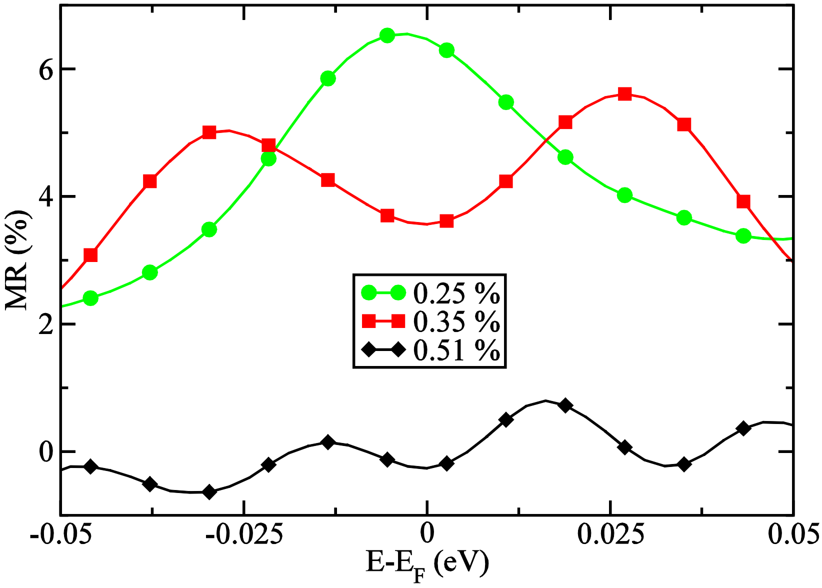


Ground state

$$\sigma^{F} = \sigma^{F}_{\uparrow} + \sigma^{F}_{\downarrow}$$



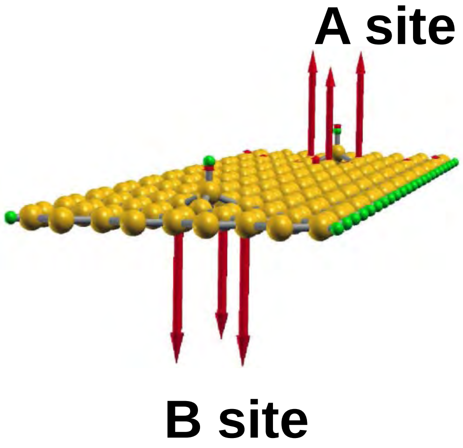
Excited state (applying B)

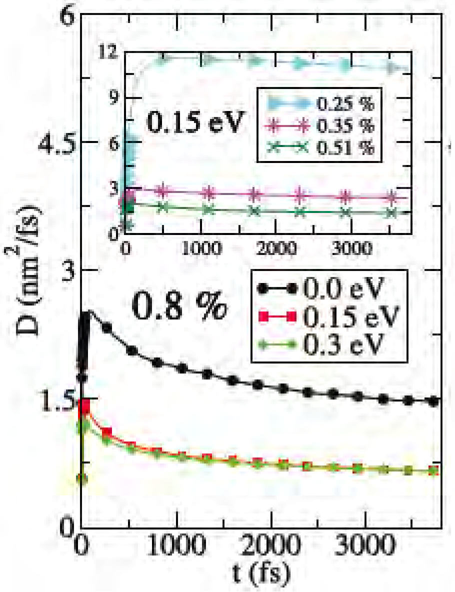


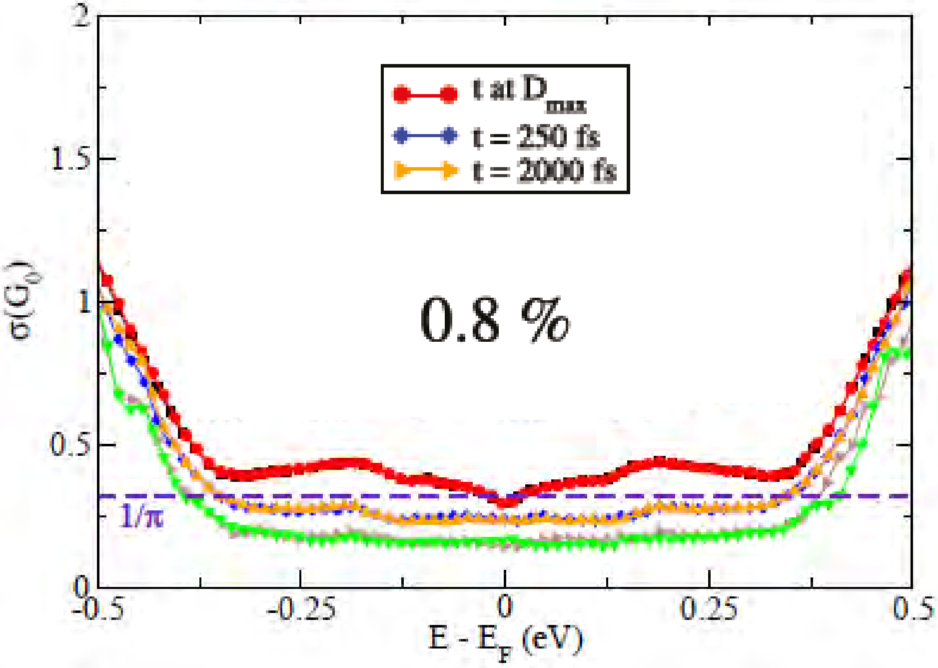
D. Soriano, N. leconte, P. Ordejon, J.C. Charlier, J. Palacios, S.R.

Phys. Rev. Lett. 107, 016602 (2011)

Local Antiferromagnetism / quantum regime







The disordered graphene turns to an insulator

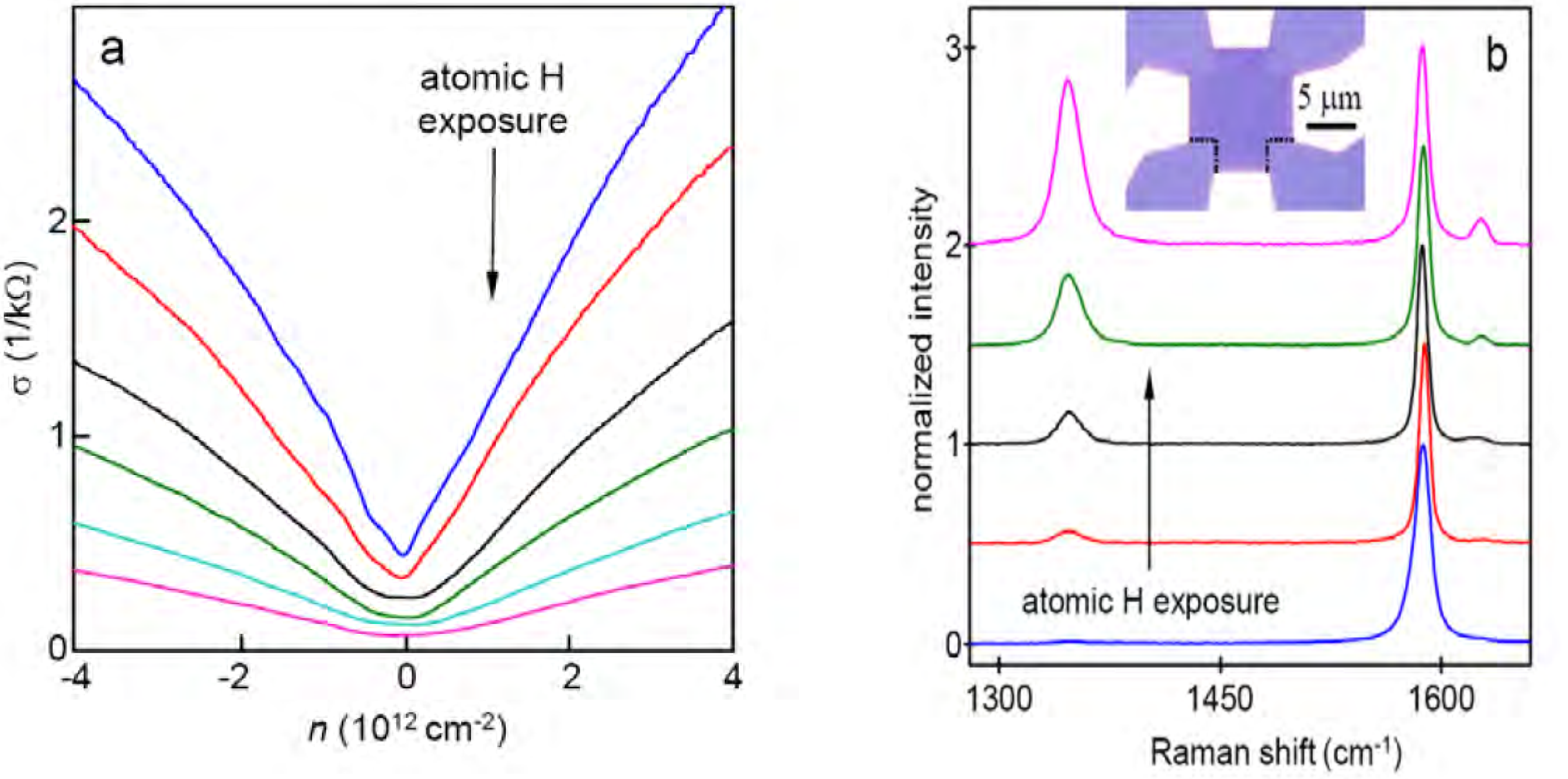
Conductivity strongly decay at low temperatures

$$\xi(E) = \ell_e \exp(\pi\sigma_{\mathrm{Drude}}/2G_0)$$

$$n_x = 0.25\% \text{ and } 0.8\%$$
$$\xi(E) \sim 8 - 15\mathrm{nm}$$

N. Leconte, D. Soriano, S. R. et al. **ACS Nano 5, 3987 (2011)**

Controlled Hydrogenation of Graphene

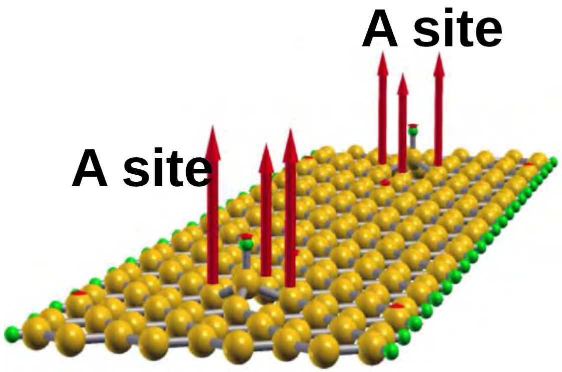


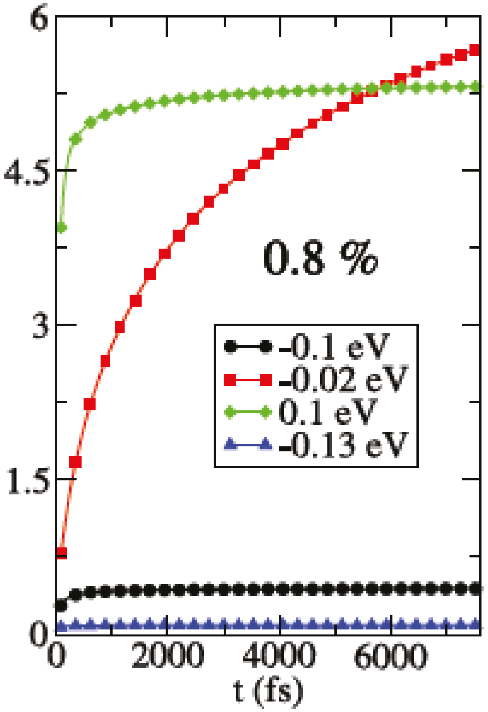
Z. H. Ni, L. A. Ponomarenko, R. R. Nair, R. Yang, S. Anissimova, I. V. Grigorieva, F. Schedin, Z. X. Shen, E. H. Hill, K. S. Novoselov, A. K. Geim

On resonant scatterers as a factor limiting carrier mobility in graphene

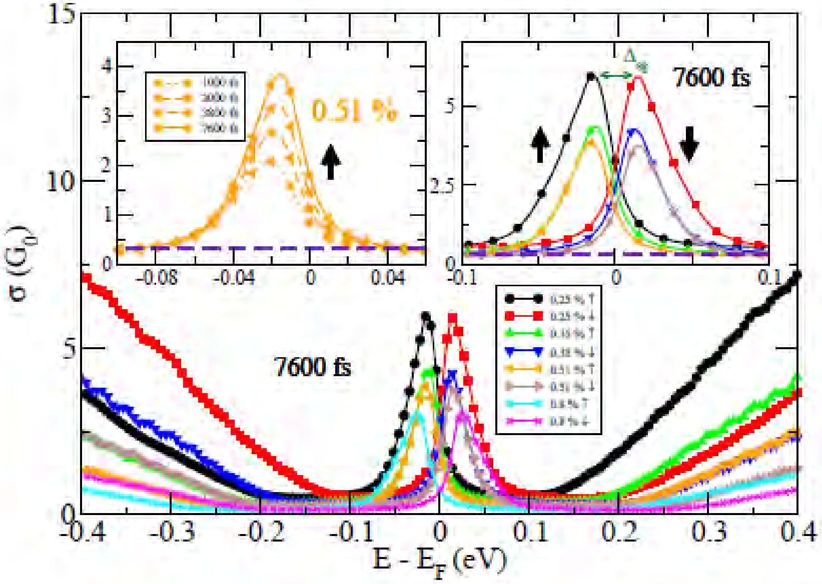
Nano Letters 10, 3868 (2010)

Local Ferromagnetic ordering





$$\Delta_{sg} = |\varepsilon^r_\uparrow - \varepsilon^r_\downarrow| \in [25, 30]\mathrm{meV}$$



Spin Splitting

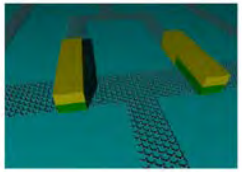
$\sigma_{Kubo} \geq 4e^2/\pi h$ Suppression of quantum interferences

The disordered graphene remains metallic
conductivity insensitive to localization
Effects at low temperatures

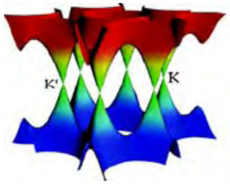
N. Leconte, D. Soriano, S. R. et al. **ACS Nano 5, 3987 (2011)**

OUTLINE

1. *Why focusing on "dirty graphene" ?*

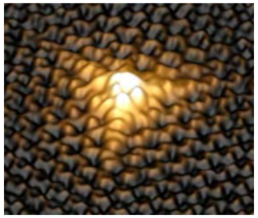


2. *Reminder Electronic Properties*



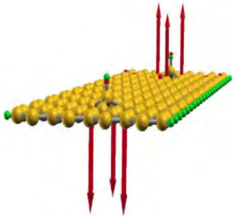
3. *Defects and Transport in Graphene*

   Manifestation of Pseudospin & weak antilocalization



4. *Chemically modified Graphene*

   Local magnetic ordering and metal-insulator transition



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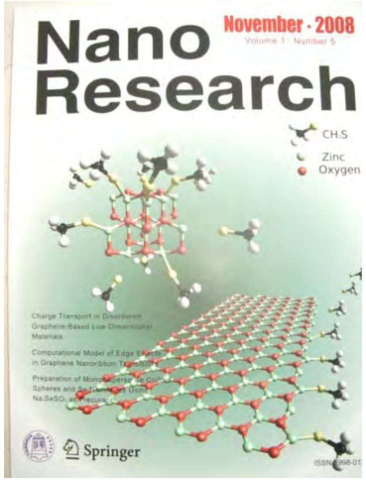
GRAPHENE FLAGSHIP

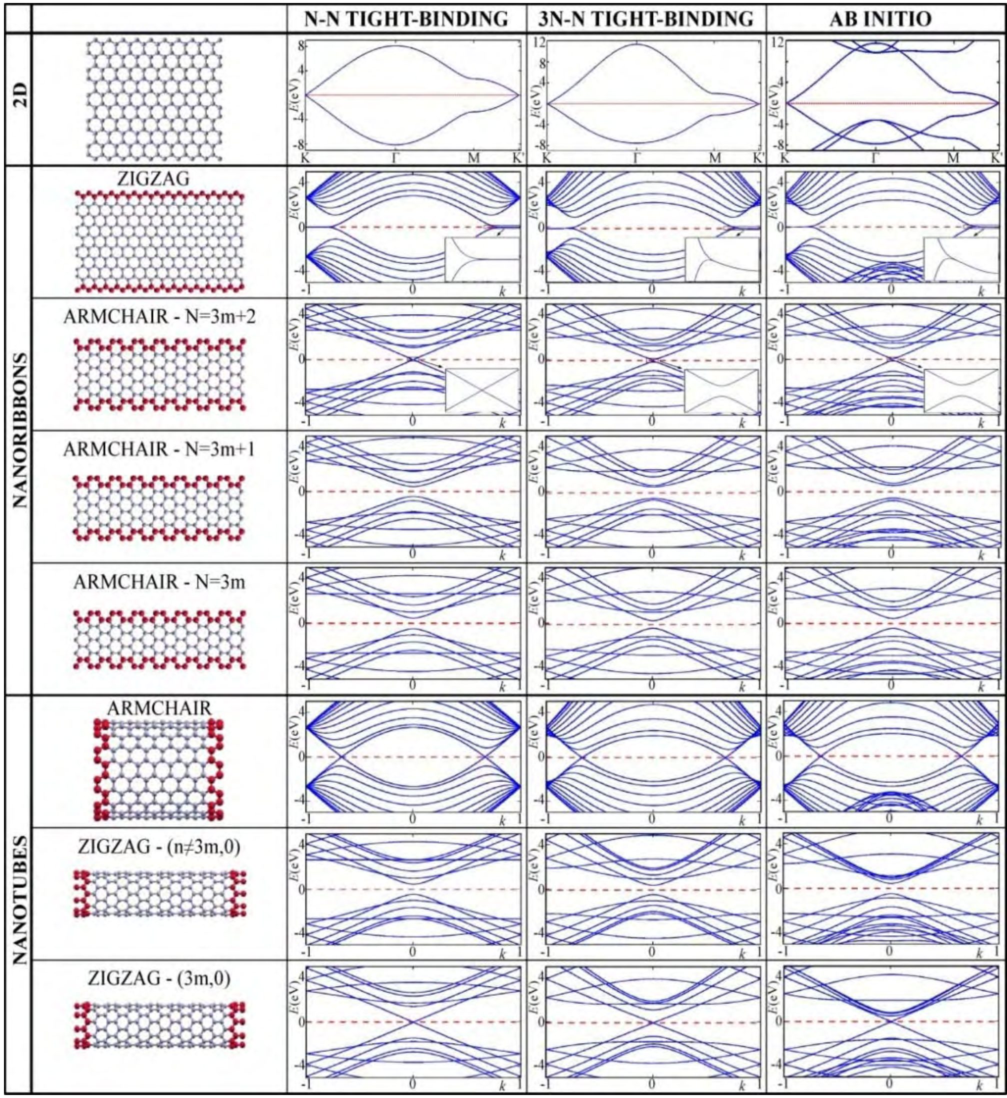
First-principles and TB-modelling

A. Cresti, et al..
Charge Transport in Disordered
Graphene-Based Low Dimensional Materials
Nano Research 1, 361-394 (2008)

Tight-binding vs ab-initio (the clean case)



siesta A linear-scaling density-functional method



Limits of oversimplified description of the electronic structure and « disordered » graphene based materials!!