Shining Light on Transport in Disordered Graphene

Towards amorphous graphene and Magnetic ordering fingerprints
OUTLINE

1. “Clean versus dirty graphene?”

2. From long range to short range disorder
   Towards amorphous sp2 carbon membrane

3. Local magnetic ordering (hydrogenation) and metal-insulator transition

4. Band gap tunability using a mid-infrared laser field
The “clean 2D world”

Ph. Kim's group [PRL 99, 246803 (2007)]


Suspended graphene

\[ \mu \sim 10^6 \text{cm}^2\text{V}^{-1}\text{s}^{-1} \]

Top gated graphene MOS channels

\[ \mu \sim 23,000 \text{cm}^2\text{V}^{-1}\text{s}^{-1} \]

Large area (catalytic growth) graphene

\[ \mu \sim 3,700 \text{cm}^2\text{V}^{-1}\text{s}^{-1} \]
Pseudospin / e-h symmetry and Berry's phase
Single scatter level

$H_{K+} = u_F \vec{\sigma} \cdot \vec{p}$  
4 Dirac point (2 valley * 2 spin)

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

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

Klein Tunneling
"perfect transmission through a potential barrier of increasing width/depth"

Katsnelson, Novoselov, Geim Nature Physics 2006
Berry’s phase effects and quantum interferences (multiple scattering)

Disorder (static/dynamic) induces multiple scattering events

\[ \sigma(L) = \sigma_{sc} + \delta\sigma(L) \]

\[ \delta\sigma(L) = \frac{2e^2D}{\pi\hbar\Omega} \int_0^\infty dt Z(t)(e^{-t/\tau_\varphi} - e^{-t/\tau_e}) \]

\[ Z(t) = \int d^d r P(r, r, t) \]

B.L. Altshuler and A.G. Aronov (80)

Additional QIE due to Berry’s phase
Weak antilocalization
(Robust metallic state)

Negative magnetoresistance
\[ \Delta G(B)/G(B = 0) \]

\[ B(T) \]
Cooperon (spin/pseudospin driven effect)

Original prediction (cooperon equation)

The spin of electrons rotate (adiabatically) as it moves around the classical path

\[ \sigma = \sigma_{\text{Drude}} + \delta \sigma \]

\[ \delta \sigma = -\frac{2e^2 D}{\pi \hbar \Omega} \int_0^\infty \, dt \, Z(t) \langle Q_{s.o}(t) \rangle \left( e^{-t/\tau_\phi} - e^{-t/\tau_e} \right) \]

\[ |s_{n+1}\rangle = e^{-i \Delta \theta S_z / \hbar} |s_n\rangle \]

\[ \mathcal{R}_t = \mathcal{T} e^{-i \hbar \int_0^t \mathcal{H}_{s.o} \, dt} \]

\[ \mathcal{H}_{s.o} = \frac{\hbar}{4m^2 c^2} \vec{\sigma} \cdot (\vec{\nabla} V(\mathbf{r}) \times \vec{p}) \]

\[ Q_{s.o}(t) = \sum_{\pm} \langle s_0 | \mathcal{R}_{-t}^\dagger | s_f \rangle \langle s_f | \mathcal{R}_t | s_0 \rangle \]
Spin rotates by an angle $-\pi$

Spin rotates by an angle $+\pi$

Because of the complex conjugation these two phases add up to a total rotation of $2\pi$

Total Berry's phase

$$\langle Q_{s.o}(t) \rangle = -\frac{1}{2}$$

Strong so-coupling-antilocalization

Original prediction (cooperon equation)

Magnetococonductance

\[ \frac{\Delta G(B)}{G(B = 0)} \]

G. Bergmann,
*Phys. Rev. Lett. 48, 1046 (1982)*

Thin Mg disordered metallic film (9nm thickness!) –weak so-coupling with Au impurities (strong so coupling)

Experimental observation of
Weak antilocalization
Weak antilocalization in graphene...


No so-coupling... no magnetic impurities

Strictly driven by Berry's phase (pseudospin)
Weak localization in 2D graphene

E. McCann, K. Kchedzhi, V. I. Fal’ko, H. Suzuura, T. Ando, B.L. Altshuler,

Quantum interferences correction (WL/WAL)

\[ \Delta \sigma(B) = \frac{e^2}{\pi \hbar} \left\{ \mathcal{F}\left( \frac{\tau_B^{-1}}{\tau_\varphi} \right) - \mathcal{F}\left( \frac{\tau_B^{-1}}{\tau_\varphi^{-1} + 2\tau_i^{-1}} \right) - 2\mathcal{F}\left( \frac{\tau_B^{-1}}{\tau_\varphi^{-1} + 2\tau_i^{-1} + \tau_\star^{-1}} \right) \right\} \]

- \( \tau_i \) intervalley scattering time
- \( \tau_\varphi \) trigonal warping scattering time
- \( \tau_s \) intravalley scattering time
- \( \tau_B = \hbar / 2 e DB \)

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

Digamma function

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

\[ \tau_i^{-1} = 4\tau_{\perp\perp}^{-1} + 2\tau_{\perp\downarrow}^{-1}, \quad \tau_\varphi^{-1} = 4\tau_{\perp\downarrow}^{-1} + 2\tau_{\downarrow\downarrow}^{-1}. \]

\[ \tau_w^{-1} + \tau_\varphi^{-1} + \tau_i^{-1} = \tau_\star^{-1}. \]

\[ \tau_w^{-1} = 2\tau_0 \left( \frac{e^2 \mu}{\hbar v^2} \right)^2. \]
The real “dirty” graphene?
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”
Graphene Chemical Derivatives

Turning graphene to a true band insulator vs mobility gap material

Hydrogenation of Graphene

Band insulator (towards GRAPHANE)


Anderson insulator (low hydrogen coverage)

Ozone treatment of Graphene

J. Moser et al., PRB 81, 205445 (2010)

Ozone flux \( O_3 \)

Gate-dependent Transport

Low temperature transport
(variable range hopping)

Magnetotransport fingerprints
(weak localization-coherence length-)

\[ \sigma(T) = \exp\left(-\left(T_0/T\right)^{1/3}\right) \]

Localization length

\[ \xi_{VRH} = \sqrt{13.8/k_B \rho T_0} \]
\[ \xi_D = \ell_c \exp\left(\sigma_D/(e^2/h)\right) \]

Disorder Engineering of new functionality...

**Bandgap engineering** (chemical functionalization)

- **Electrochemical switch**
- **Grafting nitrophenyl groups**

**Graphene Nanomesh**
- J. Bai et al., *Nature Nanotech* 2010

**Nitrogen doped graphene**
- J.C. Meyer et al., *Nat. Mat.* 10, 209 (2011)
- L. Zhao et al., *Science* 333, 999 (2011)


L. Zhao et al., *Science* 333, 999 (2011)
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
  
  $1 \mu m^2$ - 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)*
Kubo formula in a nutshell

Electronic system is described by

$$\hat{H}_0 = \frac{\hat{P}^2}{2m} + \hat{V} \quad \text{with spectrum} \quad \varepsilon_k, \left| \Psi_k \right>$$

Perturbation: applying an electric field

$$\tilde{E} = E_0 \cos \omega t \tilde{u}_x$$

Transition between states of the system at equilibrium
(to the first order of time-dependent perturbation theory)

$$\hat{H}_0 = \frac{\hat{P}^2 + eA}{2m} + \hat{V} = \hat{H}_0 + \delta \hat{H}$$

Perturbation

$$\delta \hat{H} = \frac{e}{m} \mathbf{A} \hat{P} = -\frac{eE_0}{2i\omega} (e^{i\omega t} - e^{-i\omega t}) \hat{V}_x$$

(Coulomb gauge)

Transition rate from k to q reads

$$p(t) = \frac{1}{\hbar^2} \left| \int_0^t e^{i(\varepsilon_k - \varepsilon_q) \tau / \hbar} \langle k | \delta \hat{H} | q \rangle \right|^2$$

$$= \frac{2\pi}{\hbar} \left( \frac{eE_0}{2\omega} \right)^2 \left| \langle k | \hat{V}_x | q \rangle \right|^2 \left( \delta(\varepsilon_k - \varepsilon_q + \hbar\omega) + \delta(\varepsilon_k - \varepsilon_q - \hbar\omega) \right)$$

Transition induced energy loss (emission)  Transition induced energy gain (absorption)
Kubo formula in a nutshell

Total absorbed power by the system is computed by evaluating all possible transitions, accounting for state occupancies

\[
\Re \sigma(\omega) = \frac{2\pi e^2 \hbar}{\varepsilon_0^2 \Omega/2} \sum_{kq} \frac{f_q - f_k}{\hbar \omega} \left| \langle k | \hat{V}_x | q \rangle \right|^2 \delta(\varepsilon_k - \varepsilon_q - \hbar \omega)
\]

Kubo-Greenwood formula of quantum conductivity

\[
\Re \sigma(\omega) = \frac{2\pi e^2 \hbar}{\Omega} \int_{-\infty}^{+\infty} dE \frac{f(E) - f(E + \hbar \omega)}{\hbar \omega} \text{Tr}[\hat{V}_x \delta(E \mathcal{H}) \hat{V}_x \delta(E - \mathcal{H})]
\]

\[ \Re \sigma(\omega) = \frac{2\pi e^2 \hbar}{\Omega} \int_{-\infty}^{+\infty} dE \frac{f(E) - f(E + \hbar \omega)}{\hbar \omega} \text{Tr}[\hat{V}_x \delta(E - \hat{H}) \hat{V}_x \delta(E - \hat{H})] \]

\[ \sigma_{dc} = e^2 n(E_F) \lim_{t \to \infty} \frac{d}{dt} \Delta X^2(E_F, t) \]

\[ \Delta X^2(E_F, t) = \langle |\hat{X}(t) - \hat{X}(0)|^2 \rangle_{E_F} \]

\[ \left\langle \tilde{\varphi}_{RP}(t) | \delta(E - \hat{H}) | \tilde{\varphi}_{RP}(t) \right\rangle \]

\[ \left\langle \varphi_{RP} | \delta(E - \hat{H}) | \varphi_{RP} \right\rangle \]

\[ \left\langle \varphi_{RP} | \delta(E - \hat{H}) | \varphi_{RP} \right\rangle = -\frac{1}{\pi} \lim_{\eta \to 0} \Im m \left\langle \varphi_{RP} | \frac{1}{E + i\eta - \hat{H}} | \varphi_{RP} \right\rangle, \]

\[ \frac{1}{E + i\eta - a_1 - \frac{b_1^2}{E + i\eta - a_2 - \frac{b_2^2}{\ldots}}} \]

\[ \text{S.R. et al PRL 79, 2518 (1997); PRL 87, 246803 (2001)} \]
Time-evolution of wavepackets dynamics

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

Conductivity using Kubo approach

\[ \sigma_{dc} = e^2 \rho(E) \lim_{t \to \infty} \frac{d}{dt} \Delta X^2(E, t) \]

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Long range versus short range potential

Long range potential

Intravalley scattering
*(short momentum transfer)*

Short range potential

Intervalley scattering
*(large momentum transfer)*

* Mean free path (el density)
* Quantum interferences & Localization phenomena
* Anomalous vs conventional QHE *(Mirlin)*
Density of states

No disorder
Agrees with analytical result

With Disorder
*) As $W$ is enhanced, DoS increases close to CNP

*) Close to VHs Smoothening (disorder-enhanced Scattering)

N. H. Shon and T. Ando,

Note: no shift of Fermi level
Self Consistent Born Approximation

Conductivity (Kubo)

\[ \sigma_{xx} \sim \text{Tr} \langle v_x \mathcal{S} m G(E + i\eta) v_x \mathcal{S} m G(E + i\eta) \rangle_{\text{conf}}. \]

\[ \langle G(E) G(E') \rangle \sim \langle G(E) \rangle \langle G(E') \rangle \] (semiclassical approximation)

\[ \sigma(E) = \frac{e^2}{\pi \hbar} \left[ 1 + \frac{E - \Delta}{\Gamma} + \frac{\Gamma}{E - \Delta} \right] \text{Atan} \left( \frac{E - \Delta}{\Gamma} \right) \]

\[ \Sigma(E + i\eta) = \Delta(E) - i\Gamma(E) \]

\[ \sigma(E = 0) = \frac{4e^2}{\pi \hbar} \]

(2 spin * 2 valley degeneracy)

Quantum Diffusion

From the maximum of diffusivity

\[ D \sim v_F \ell_e \]

\[ \sigma_{sc} = e^2 \rho(E) v(E) \ell_e \]

\[ \mu(E) = \sigma_{sc}(E) / e n(E) \]
Kubo conductivity (at $D_{\text{max}}$)

Semiclassical part of the conductivity-from Kubo approach-
(short range scattering)

\[ \sigma_{\text{sc}}(E_F = 0) = \frac{4e^2}{(h\pi)} \]

agrees with SCBA

N. H. Shon and T. Ando,
P. M. Ostrovsky, I.V. Gornyi, A. D. Mirlin,
Charge mobilities in 2D graphene

\[ D \sim v_F \ell_e \]

\[ \sigma_{SC} = e^2 \rho(E) v(E) \ell_e \]

\[ \mu(E) = \sigma_{SC}(E) / e n(E) \]

*) Divergence of mfp & mobility as \( E_F \) moves towards CNP

*) Mobility changes agrees with experimental data for poorer quality samples

Experimental data by Ph. Kim (columbia)
Quantum interferences effects

Localization effects - 2D scaling theory of localization -
Lee & Fisher, PRL 47, 882 (81)

$$\sigma(L) = \sigma_{SC} - \Delta \sigma(L)$$
(quantum correction scaling)

$$\Delta \sigma(L) = \left(\frac{G_0}{\pi}\right) \ln\left(\frac{L}{\ell_e}\right)$$

$$\xi$$ (localization length) is defined by

$$\Delta \sigma(L = \xi) = \sigma_{SC}$$

$$\xi = \ell_e \exp\left(\frac{\pi \sigma_{SC}}{G_0}\right)$$

A. Lherbier, B. Biel, YM. Niquet, and SR, PRL 100, 036803 (2008)
Long range and pseudospin effects.

### Charges trapped in the oxide

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

**Long range (Gaussian) potential**

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

- \(\varepsilon_i \in [-W/2, W/2] (\gamma_0\text{-unit})\), \(W = 0.5 - 2\)
- \(\xi = 3a = 0.426\text{nm} \quad \gamma_0 = -2.7\text{eV}\)
- \(n_i = N_i/N = 0.125\%, 0.25\%, 0.5\%\)

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

\(W\) (depth of onsite potential \(\sim\) screening)
Quantum interferences are suppressed by increasing magnetic field

Weak localization phenomenon

\[ \ell_e \in [9, 20] \text{nm} \]

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

\[ \Delta \sigma(B) = \sigma(B) - \sigma(B = 0) \]
Tuning the disorder and valley mixing

At $W=1.5$ a crossover is observed
On the Diffusion coefficient behavior

At $W=1$ the transport regime does not reach the diffusive regime within computational time (~quasiballistic~)
Crossover from WL to WAL

\[ \sigma(E, t = N_t \Delta t) = \frac{e^2 \rho(E) D(E, t)}{2} \]

\[ \Delta \sigma(B) = \sigma(B) - \sigma(B = 0) \]

Not WAL !!
(ballistic regime
Klein tunneling activated)

\[ \Delta \sigma(B) < 0 \]

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

Quantifying the epoxide density?


Ozone flux

O$_3$

![Graph showing Raman shift vs. intensity for pristine and exposed to ozone samples.](image)

![Graph showing conductivity vs. gate voltage for various temperatures.](image)
Epoxide defects

Ab-initio calculations + TB reparametrization

\[ \text{O}_3 \rightarrow \text{O}_2 + \text{C-O-C} \]

Epoxide defect

Van-Hove singularities broadening

Impurity states driven DoS increase

Does Boltzmann conductivity capture Dirac Point Physics?

\[ \sigma^*_{\text{Drude}}(E) = \frac{4e^2}{h} \times k\ell_e(E)/2 \]
\[ \rho(E) = \frac{2|E|}{\pi \times (\hbar v_F)^2} \]

**Fermi Golden Rule Approximations**
- all multiple scattering interferences
- DoS unchanged

\[ \sigma^*_{\text{Drude}} = \frac{2e^2}{h} \left( \sqrt{\pi C_g V_g/e} \right) \ell_e \]
\[ C_g \approx 1.15 \times 10^{-4} \text{Fm}^{-2} \]

\[ e^2/h \sim (6k\Omega)^{-1} \]

Limit of Bloch Boltzmann approach….

\[ \sigma_{\text{Drude}}^*(E) = \left( \frac{4e^2}{\hbar} \right) \times k \ell_e(E)/2 \]

\[ \sigma(E, t) = \left( \frac{e^2}{2} \right) \text{Tr}[\delta(E - \hat{H})]D(E, t) \]

Minimum conductivity
(self-consistent Born approximation)

Scaling behavior of conductivity

\[ \sigma(L) - \sigma \bigg|_{sc} = -\frac{e^2}{\hbar \pi^2} \ln \left( \frac{L}{\sqrt{2} \ell_e} \right) \]

\[ \sigma(L) \sim \exp \left( -\frac{L(t)}{\xi} \right) \]

\[ \xi(E) = \ell_e \exp \left( \pi \sigma_{\text{Drude}} / 2G_0 \right) \]

\[ n_i = 2 - 4\% \]

N. Leconte et al., PRB 84, 235420 (2011)
Towards Amorphous Graphene

J. Kotakoski, A. V. Krasheninnikov, U. Kaiser, J. C. Meyer,
Non Magnetic Structural 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)
Each defect has a specific fingerprint, from an experimental curve, one could unravel the precise nature and density defects

Ugeda et al, PRB 85, 121402(R) (2012)
From dynamics of wavepackets

\[ D_{\text{max}}(E) = v(E)\ell_e(E) \]

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

\[ \mu = \sigma_{sc}(E)/ne \]

Minimum (semiclassical) conductivity

Semiclassical conductivities

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

Upon increasing defect density, Drude conductivity decays until it reaches its minimum value.

\[ \sigma(E) = \frac{4e^2}{\pi \hbar} \]

\[ \sigma_{xx} \sim \text{Tr} \langle v_x \Sigma m G(E + i\eta) v_x \Sigma m G(E + i\eta) \rangle_{\text{conf.}} \]

\[ \langle G(E) G(E') \rangle \sim \langle G(E) \rangle \langle G(E') \rangle \]

( semiclassical approximation )
Quantum interferences & localization

Transport regime tuning from diffusive to Weak / Strong localization

\[ \xi(E) = l_e \exp\left(\pi \sigma_{\text{Drude}} / 2G_0\right) \]

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Room temperature ferromagnetism in partially hydrogenated epitaxial graphene

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(Received 12 March 2011; accepted 18 April 2011; published online 12 May 2011)
Spin-half paramagnetism in graphene induced by point defects

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Here we show that point defects in graphene—(1) fluorine adatoms in concentrations \( x \) gradually increasing to stoichiometric fluorographene \( \text{CF}_{x=1.0} \) (ref. 17) and (2) irradiation defects (vacancies)—carry magnetic moments with spin 1/2. Both types of defect lead to notable paramagnetism but no magnetic ordering could be detected down to liquid helium temperatures.
Observation of hysteresis loops of the magnetoconductance in graphene devices
A. Candini, C. Alvino, W. Wernsdorfer and M. Affronte,

“The hysteresis loops reflect the magnetization reversal of the localized moments, as the conducting graphene layer detects the magnetization behavior through its magnetoconductance.”

Defects? (vacancies....)
Lieb’s Theorem


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

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 \( H \) is unique with spin \( S = \frac{1}{2}(|B| - |A|) = \frac{1}{2}\Delta_{AB} \)

Graphene Nanomesh
J. Bai et al.,
Nature Nanotech 2010

H. Yang et al., PRB 84, 214404 (2011)
Describing Hydrogenated Graphene

**Hubbard Hamiltonian**

Single $\pi$ band with a repulsive Coulomb interaction between electrons with opposite spin occupying the same orbital

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

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

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

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

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

$$
\varepsilon_{i\uparrow} = U \langle \hat{n}_{i\uparrow} \rangle (1 - \langle \hat{n}_{i\downarrow} \rangle) \\
\varepsilon_{i\downarrow} = U \langle \hat{n}_{i\downarrow} \rangle (1 - \langle \hat{n}_{i\uparrow} \rangle) \\
\mathcal{M}_i = \frac{\langle \hat{n}_{i\uparrow} \rangle - \langle \hat{n}_{i\downarrow} \rangle}{2}
$$
Spin texture around Hydrogen defects

Case studies low H- coverage
Absence of any (local) magnetic ordering
Local Antiferromagnetism
Local Ferromagnetism

(1 H per unit cell)
(2 H defects on sites A and B)
(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

$\sigma^{\uparrow,\downarrow}(E, t) = (e^2/2) \text{Tr}[\delta^{\uparrow,\downarrow}(E - \hat{H})] D^{\uparrow,\downarrow}(E, t)$

Spin-resolved DoS  Spin resolved diffusion coefficient

Neglecting quantum interferences

$\sigma^{\text{Drude}}(E) \sim 1/n_x$

For the local ferromagnetic ordering spin splitting and $\sigma^{\uparrow} \neq \sigma^{\downarrow}$

$\sigma^{\text{Drude}}(E) + \sigma^{\text{Drude}}(E) \geq 4e^2/\pi h$

Magnetoresistance signal

$$MR = \frac{\sigma^F - \sigma^{AF}}{\sigma^F + \sigma^{AF}}$$

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

**Ground state**

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

**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.

\[ \xi(E) = \ell_e \exp(\pi \sigma_{\text{Drude}}/2G_0) \]

\[ n_x = 0.25\% \text{ and } 0.8\% \]

\[ \xi(E) \sim 8 - 15 \text{nm} \]

Local Ferromagnetic ordering

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

\[ \sigma_{Kubo} \geq 4e^2/\pi \hbar \]  Suppression of quantum interferences

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

1. **Welcome to the world of “dirty graphene”?**

2. **From structural defects to amorphous \( sp^2 \) membrane (transparent electrodes ?)**

3. **Local magnetic ordering (hydrogenation) and metal-insulator transition**

4. **Band gap tunability using a mid-infrared laser field**
Acknowledgements

**Ph.D students**
Nicolas Leconte  
Dinh Van Tuan

**Postdocs**
Frank Ortmann  
David Soriano

**Collaborations**
Aurelien Lherbier  
Jean-Christophe Charlier  
Pablo Ordejon