# Graphene: massless electrons in flatland.




**Enrico Rossi**

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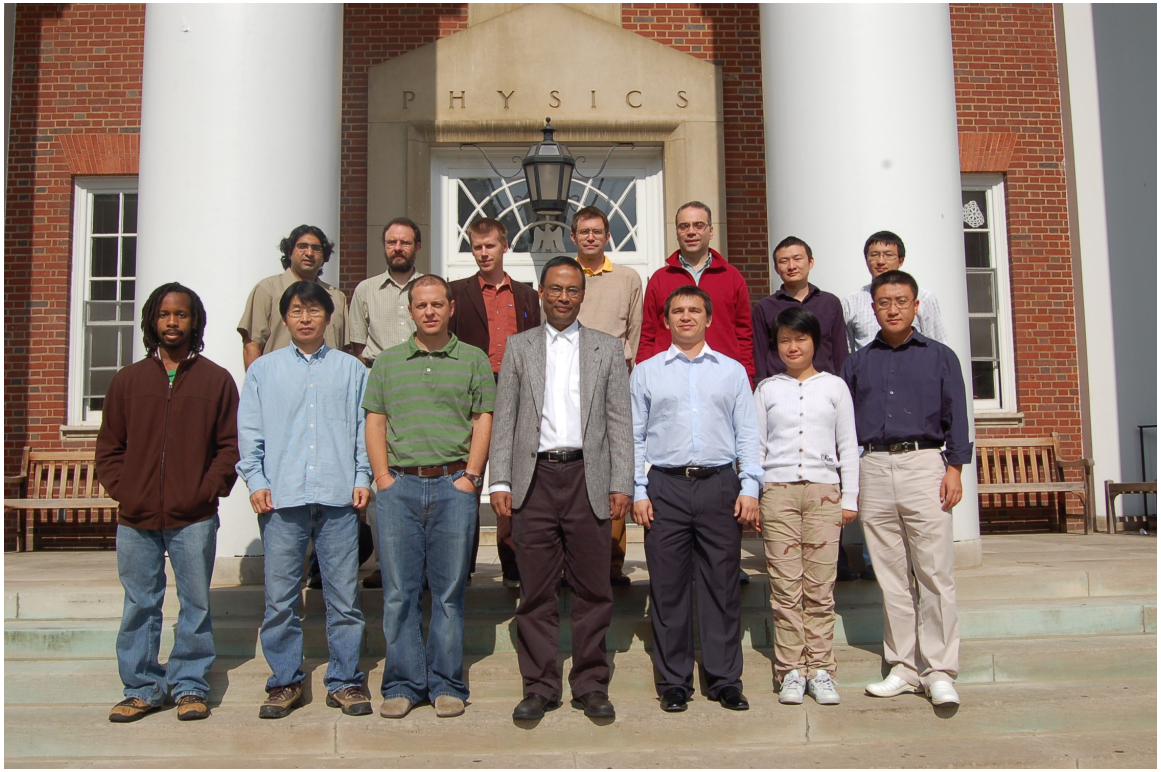
# Collaorators

## CMTC, University of Maryland




**Sankar Das Sarma**

Shaffique Adam

Euyuong Hwang

Roman Lutchin

## Close collaboration with experimental groups of:

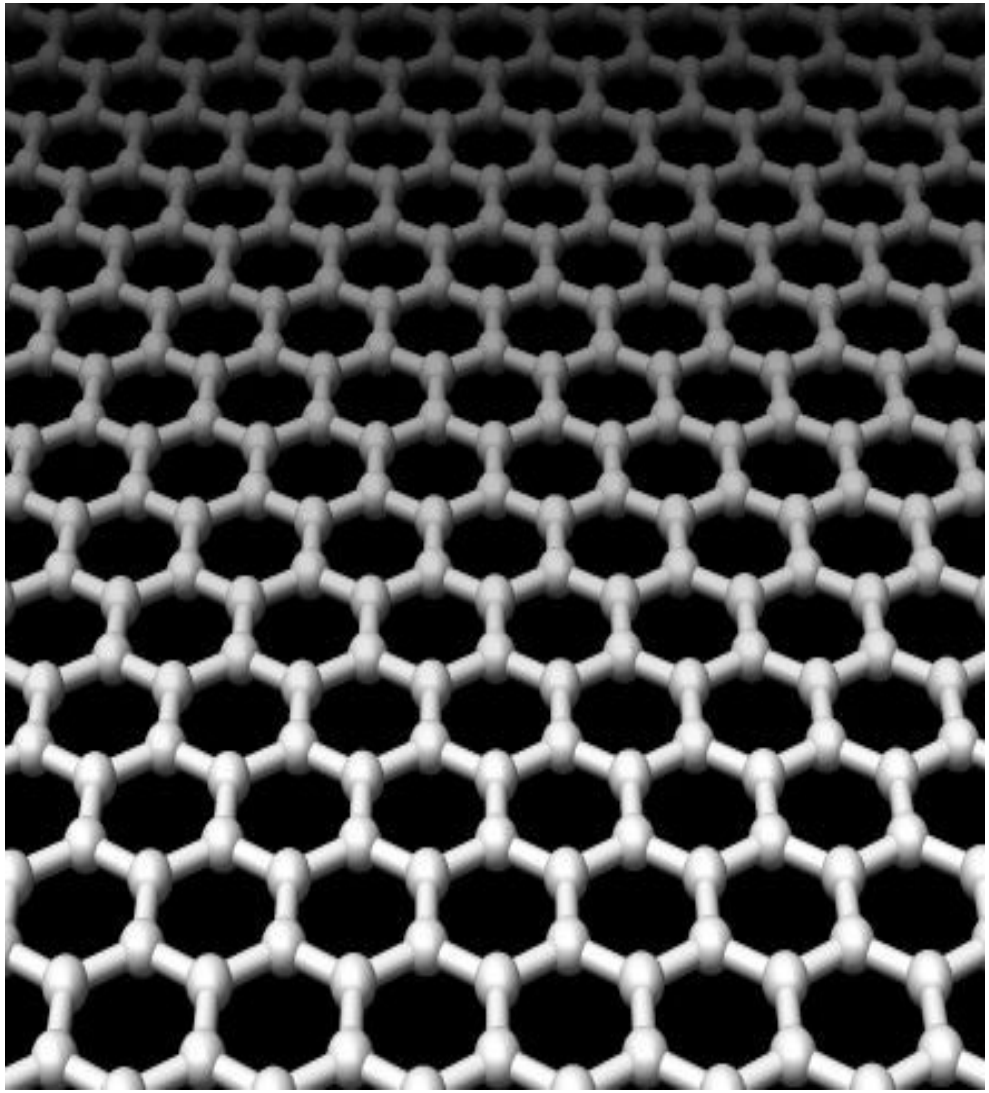
**Michael Fuhrer**,
University of Maryland

**and**

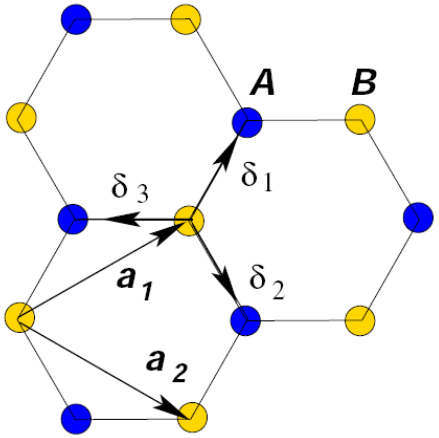
**Ellen Williams**,
University of Maryland

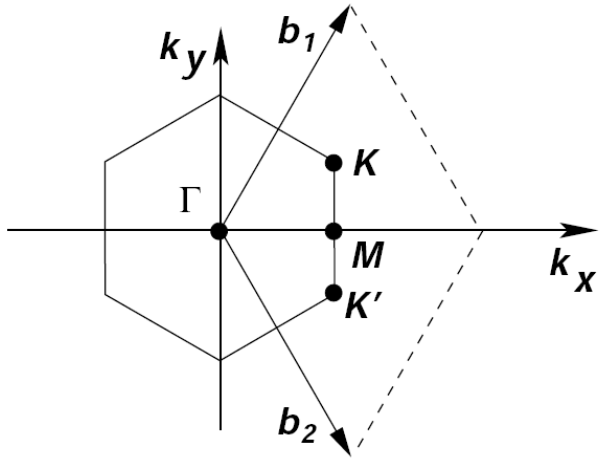
Jianhao Chen
Chau Jang

# What is graphene



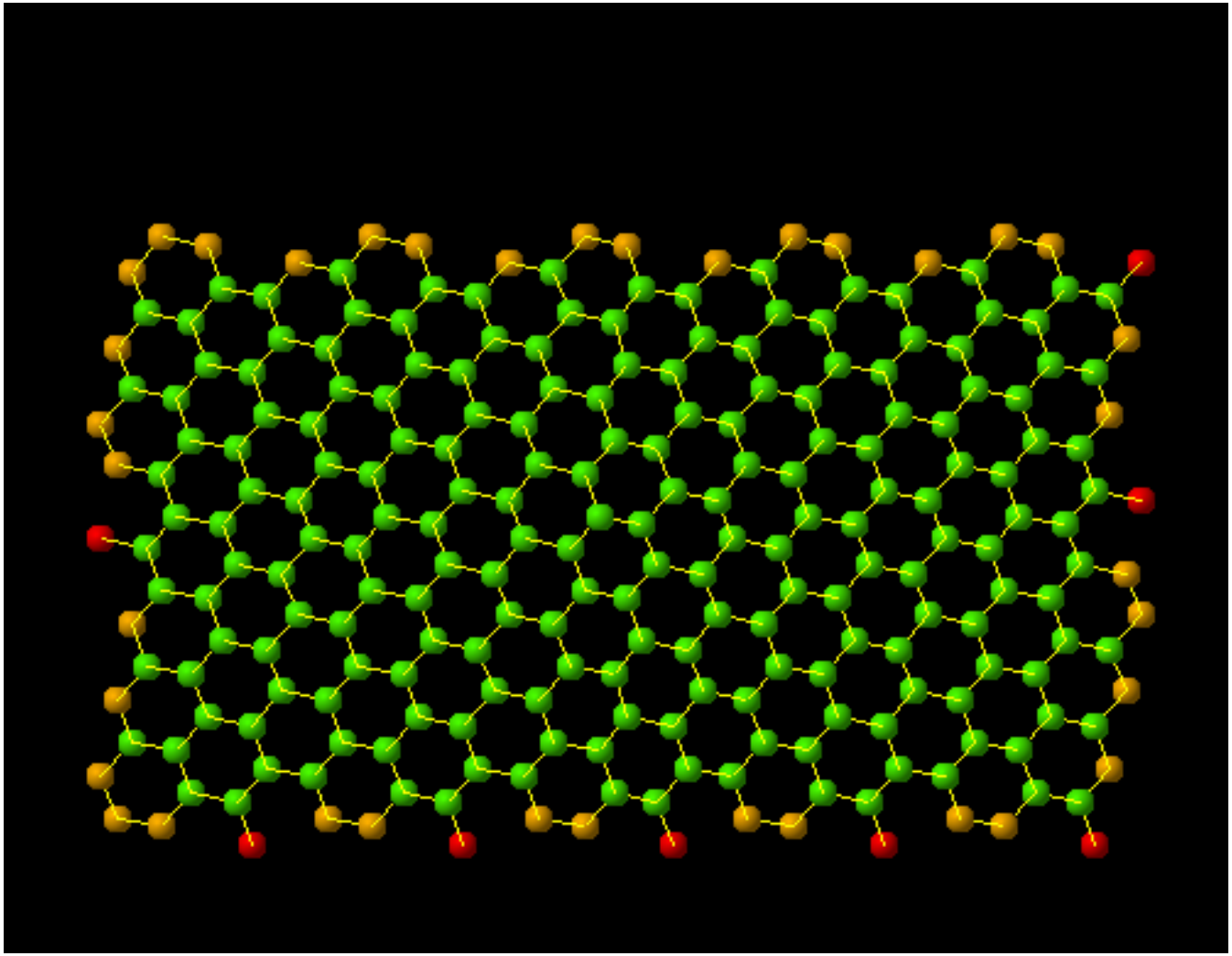
One atom thick layer of carbon atoms arranged in a hexagonal/honeycomb structure. More precisely it can be seen as a triangular Bravais lattice with a basis.



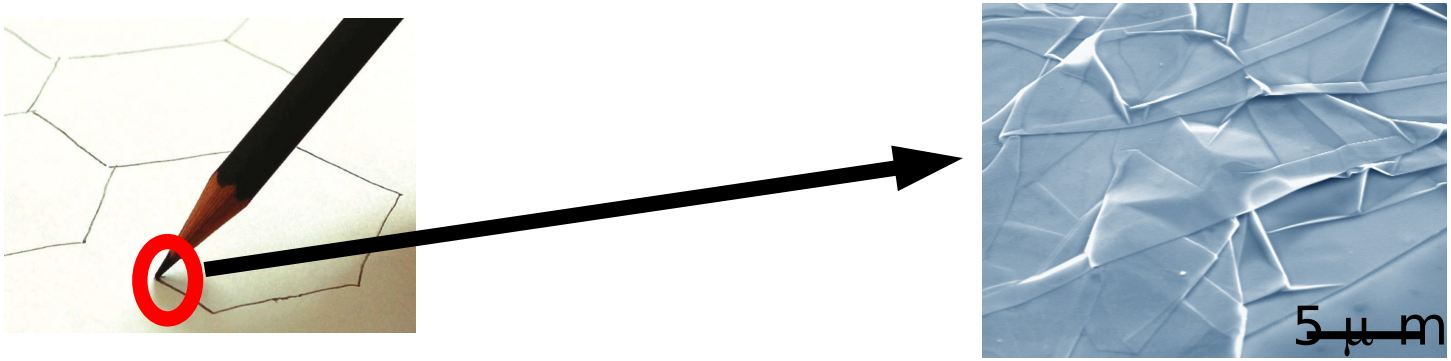

The fact that the Bravais lattice has a basis is a key element to explain many of the properties of graphene.

# Graphene as an unrolled nanotube



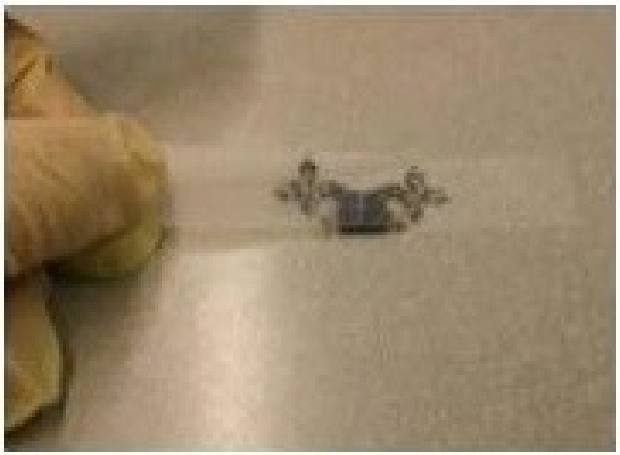
# A brief history

- 1564: “Lead pencil” based on graphite was invented



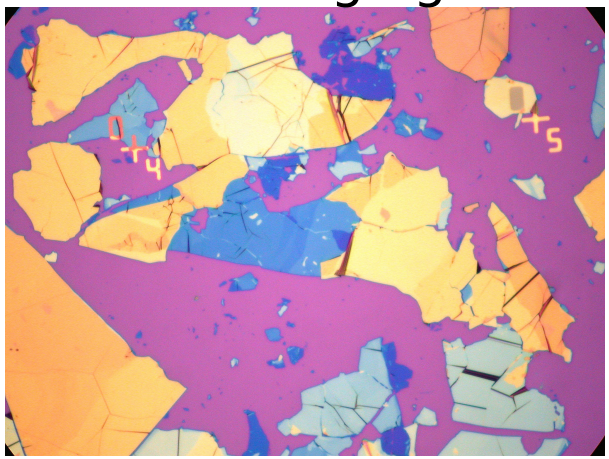

- 1946 P. R Wallace writes paper on band structure of graphene
- 2004 K.S. Novoselov et al. realize and identify graphene experimentally

scotch



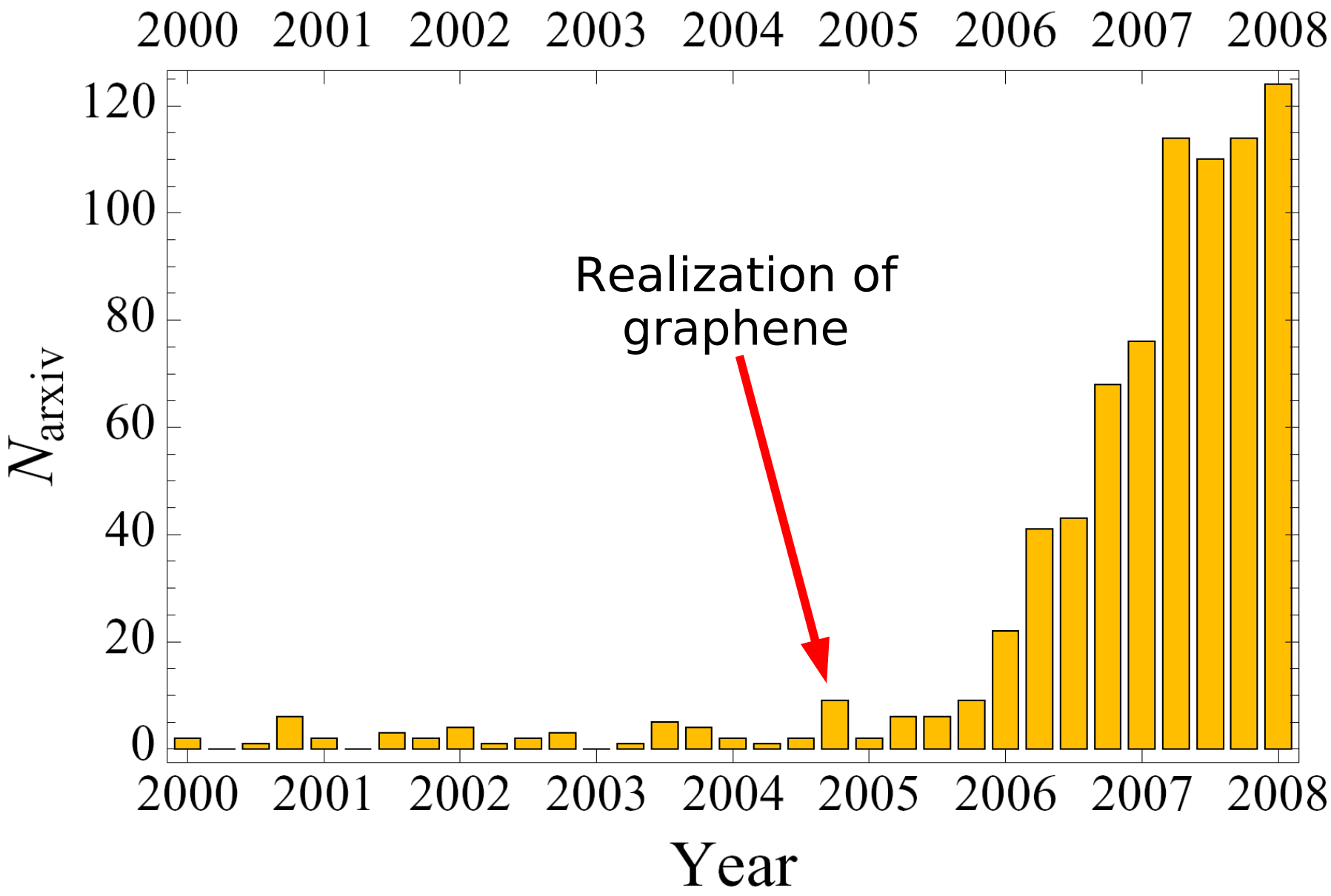
+

Imaging

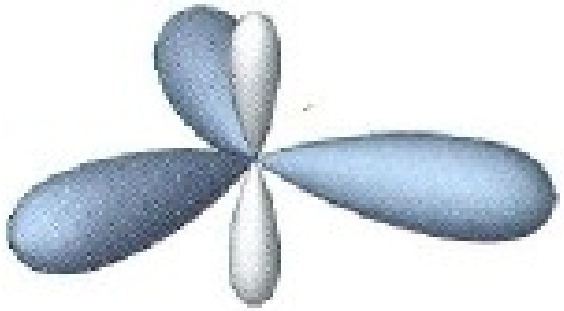


- 2005 Y.B. Zhang et al observe quantum Hall effect and Berry's phase in graphene

# Is it interesting?



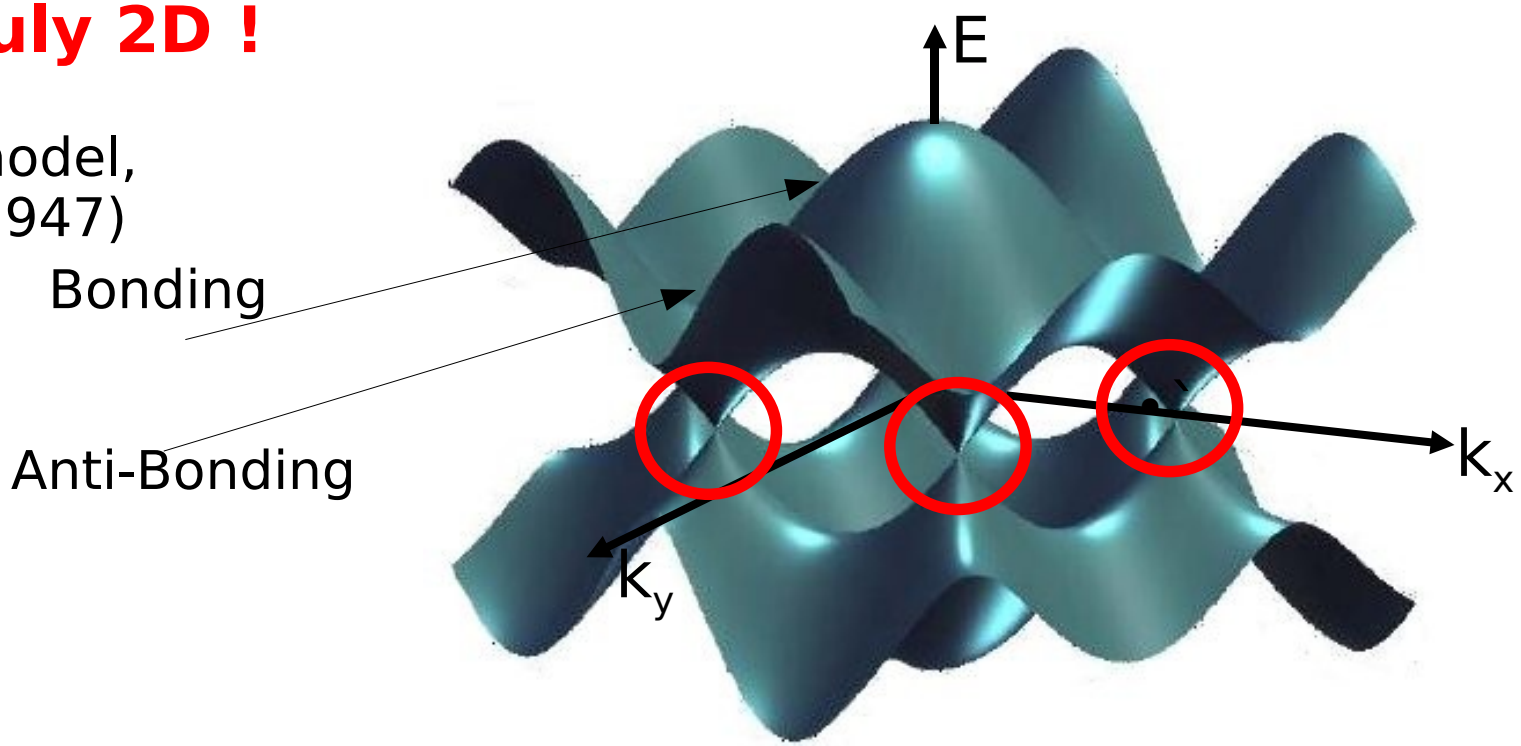
# Why is graphene interesting: band structure



Each carbon atom as 4 bonds, 1 pz and 3 sp2 orbitals. The sp2 (s hybridized with p) leads to trigonal planar structure with formation of  of a σ-bond between carbon atoms. The pz orbitals bind covalently with neighbors forming a half filled π-band

- **Graphene is truly 2D !**

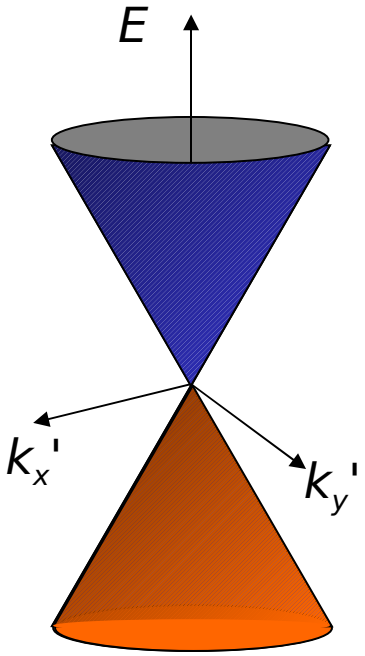
Tight binding model,
P. R. Wallace (1947)




- **Graphene has 2D Dirac cones**

# Dirac cones in graphene

From tight binding model we have that at the corners of the BZ the low energy Hamiltonian is:




$$H = \hbar v_F \sigma \cdot \mathbf{p}$$

**Chiral Massless Dirac Fermions**

**Electrons obey laws of 2D QED!**

The Fermi velocity $v_F$ is ~ 1/300 the speed of light c. We have *slow* ultrarelativistic electrons.

**QED with a pencil and some scotch!**

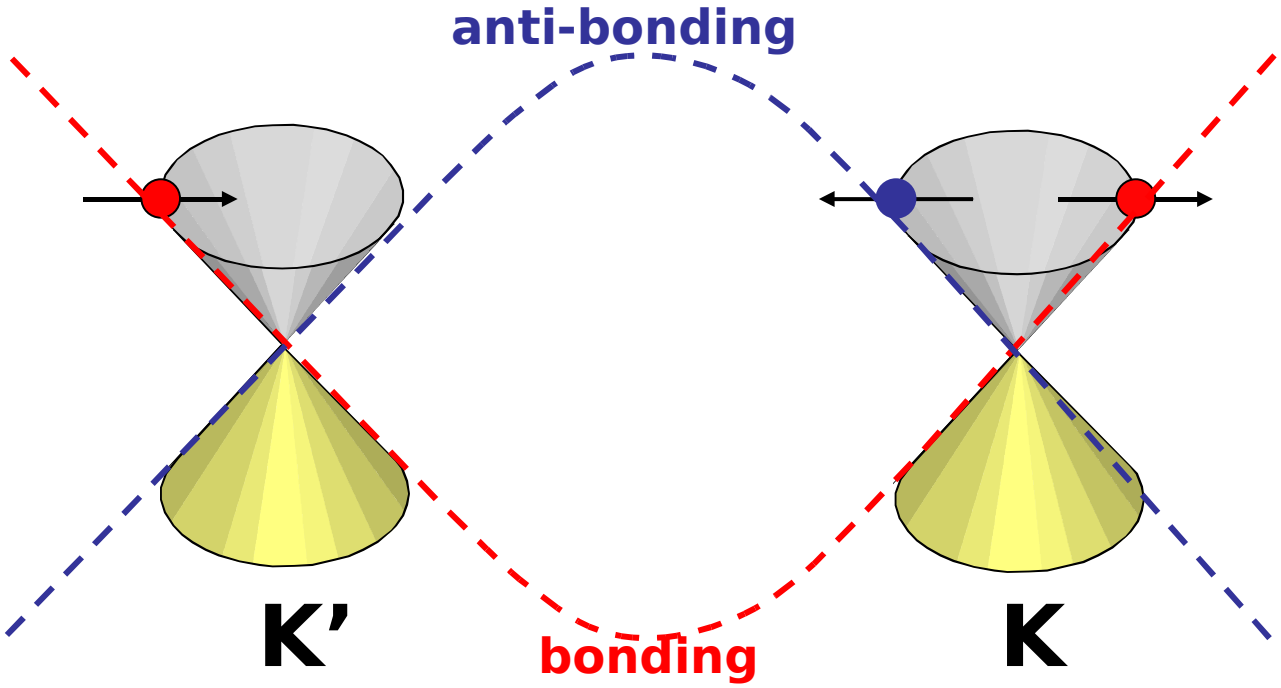
# Chirality

The sublattice symmetry implies that we have a conserved quantity:

**chirality**

defined by the operator:

$$\hat{h} \equiv \frac{1}{2}\sigma \cdot \frac{\mathbf{p}}{|\mathbf{p}|}$$




*Courtesy of M. Fuhrer, University of Maryland*

The Dirac point is protected by the conservation of chirality.

Transport implication:

Back-scattering is suppressed.

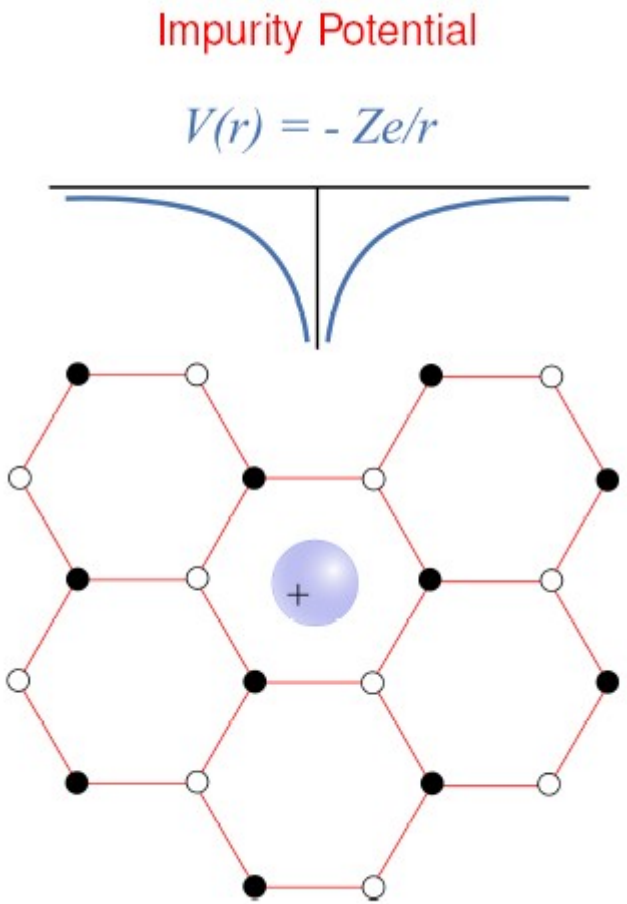
# Klein paradox

If we solve the Dirac equation in presence of a potential barrier :

**We find that for particular directions the transmission probability, T, is equal to 1,
in particular T=1 for forward scattering:**


**The never before observed Klein paradox has been observed for the first time in graphene**

# Screening of charge impurities in graphene




$$\frac{H}{\hbar v_f} = \sigma \cdot \mathbf{p} + Z\alpha \frac{1}{r}$$

1971 г. Ноябрь Том 105, вып. 3

УСПЕХИ ФИЗИЧЕСКИХ НАУК

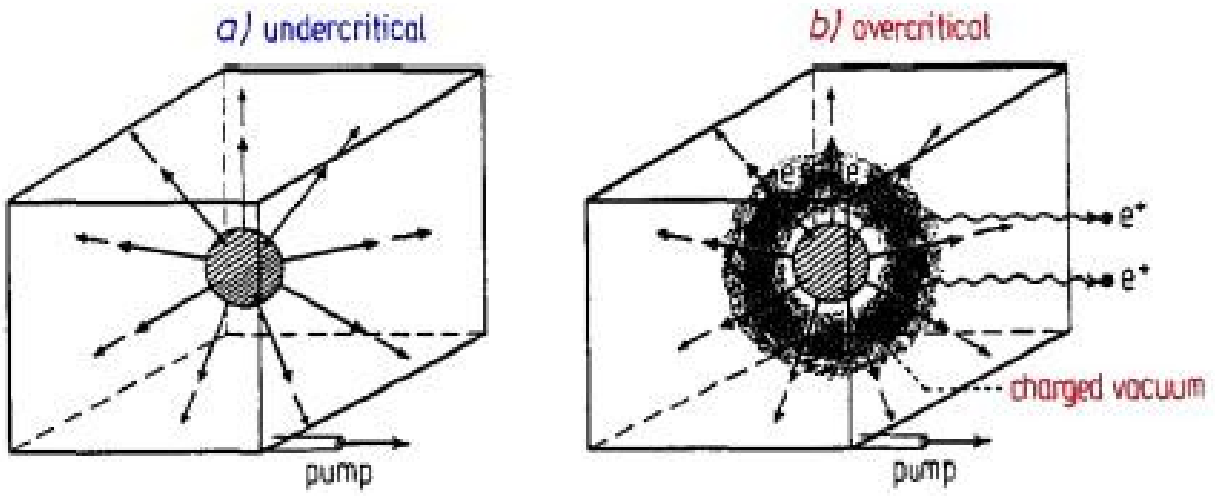
ЭЛЕКТРОННАЯ СТРУКТУРА СВЕРХТЯЖЕЛЫХ АТОМОВ

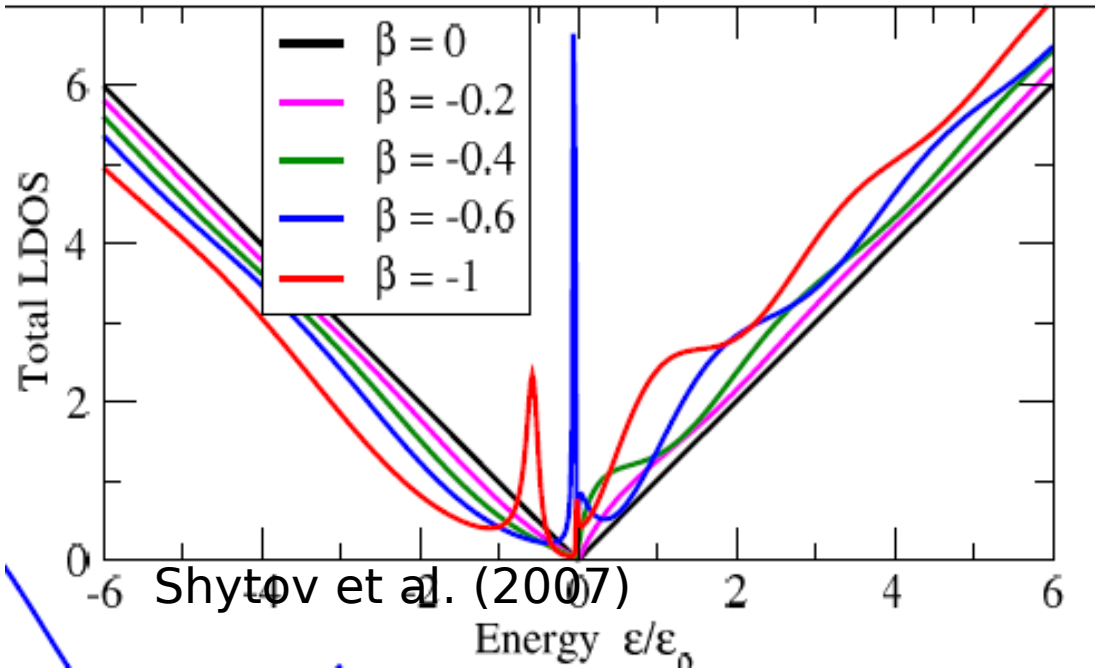
Я. Б. Зельдович, В. С. Попов

Gershtein, Popov, Zeldovich, Perolomov, Greiner, *et al.*
*Electronic Structure Of Superheavy Atoms*
Ya. B. Zeldovich *et al.*, Sov. Phys. Usp. 14 673 (1972)

Shytov et al. PRL (2007);Pereira et al PRL (2007); Novikov PRB (2008);...

# Undercritical and supercritical screening



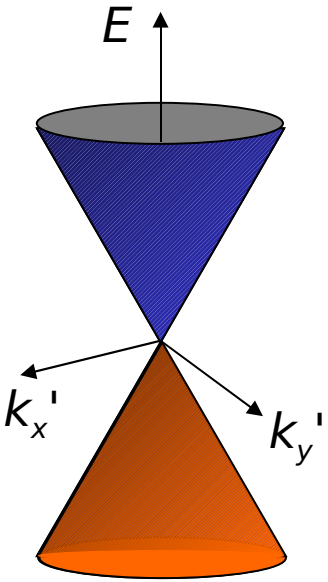



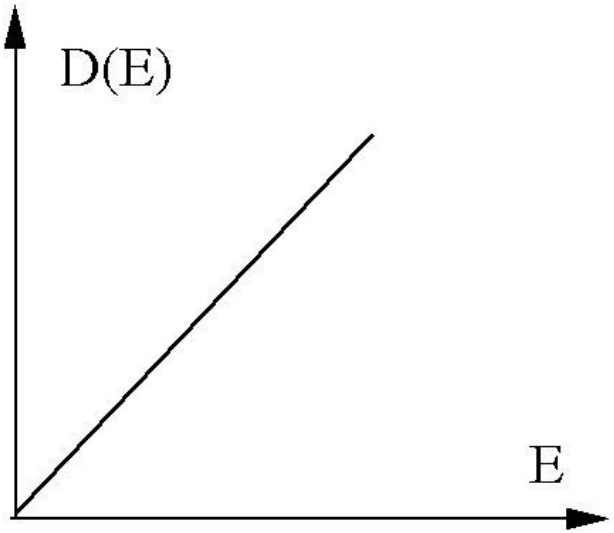

Shytov et al. (2007)

**Difficult to test in QED, we need Z > 137.**

**But in graphene α ~ 1; we only need Z ~ 1**

# Problem: transport at the Dirac point



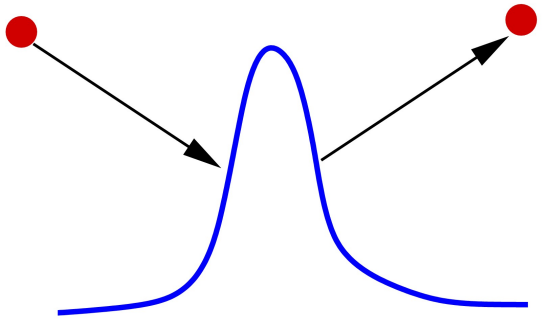




$$\sigma \propto D(E)\tau$$

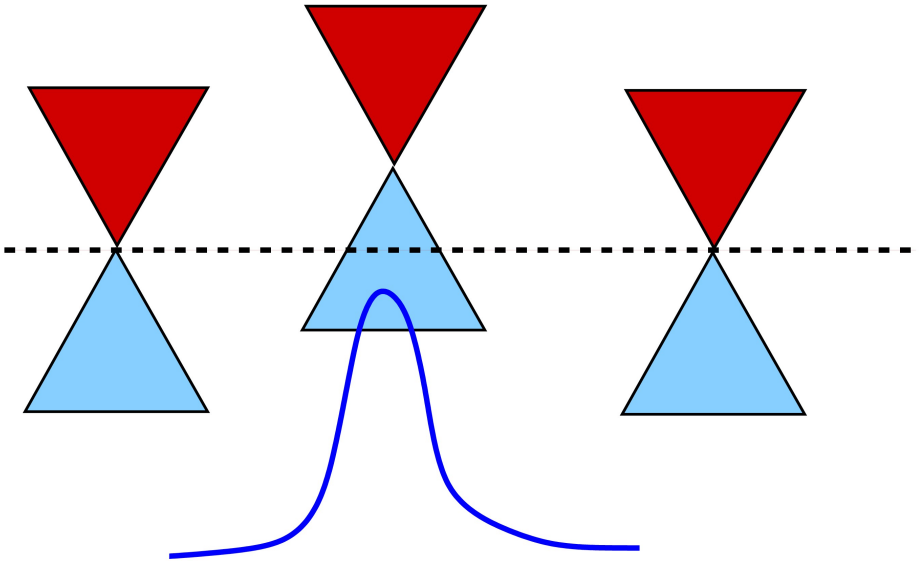
$$\sigma = \begin{cases} 0 & \text{Intervalley scattering} \\ \infty & \text{Disorder that does not mix the valleys} \\ \dfrac{4e^2}{\pi h} & \text{In absence of any disorder} \end{cases}$$

Experimentally: σ is a sample dependent constant !

# Effect of disorder



Scattering



Shifts bottom of the band ⟷ shift of Fermi energy

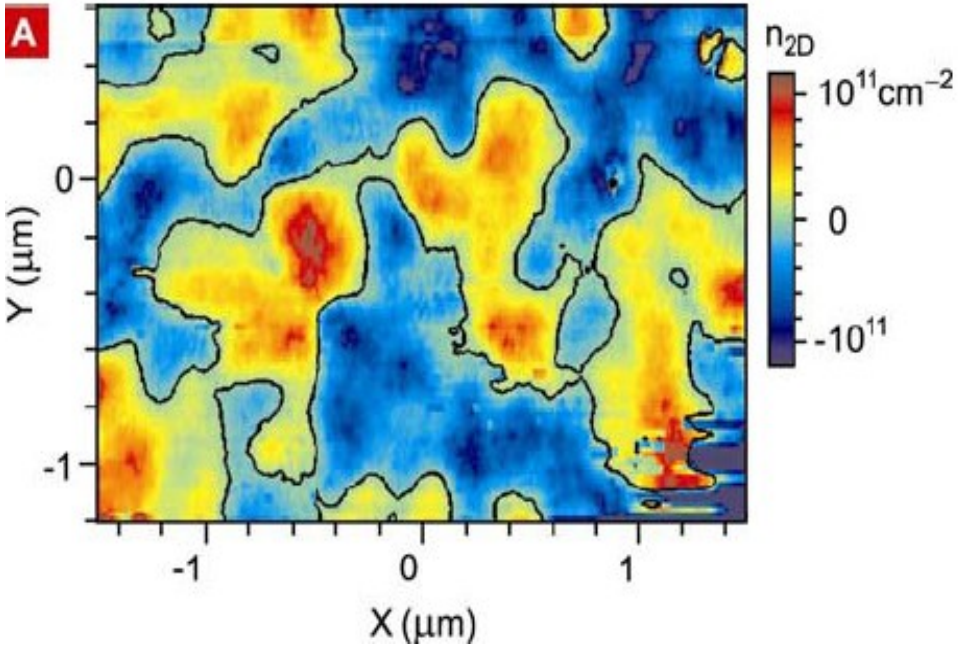
At the Dirac point disorder induces electron-hole puddles

Suggested theoretically :

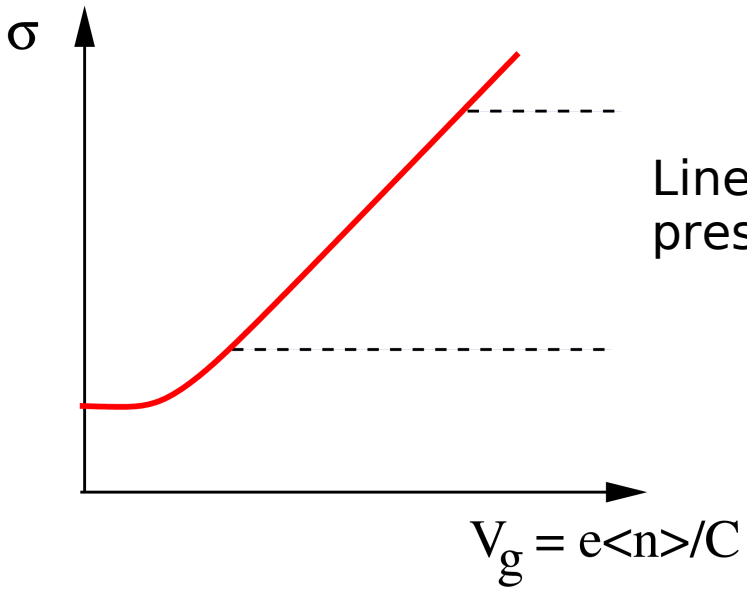
E.H. Hwang, S. Adam, S. Das Sarma., PRL, **98**, 186806 (2007).

Observed experimentally:

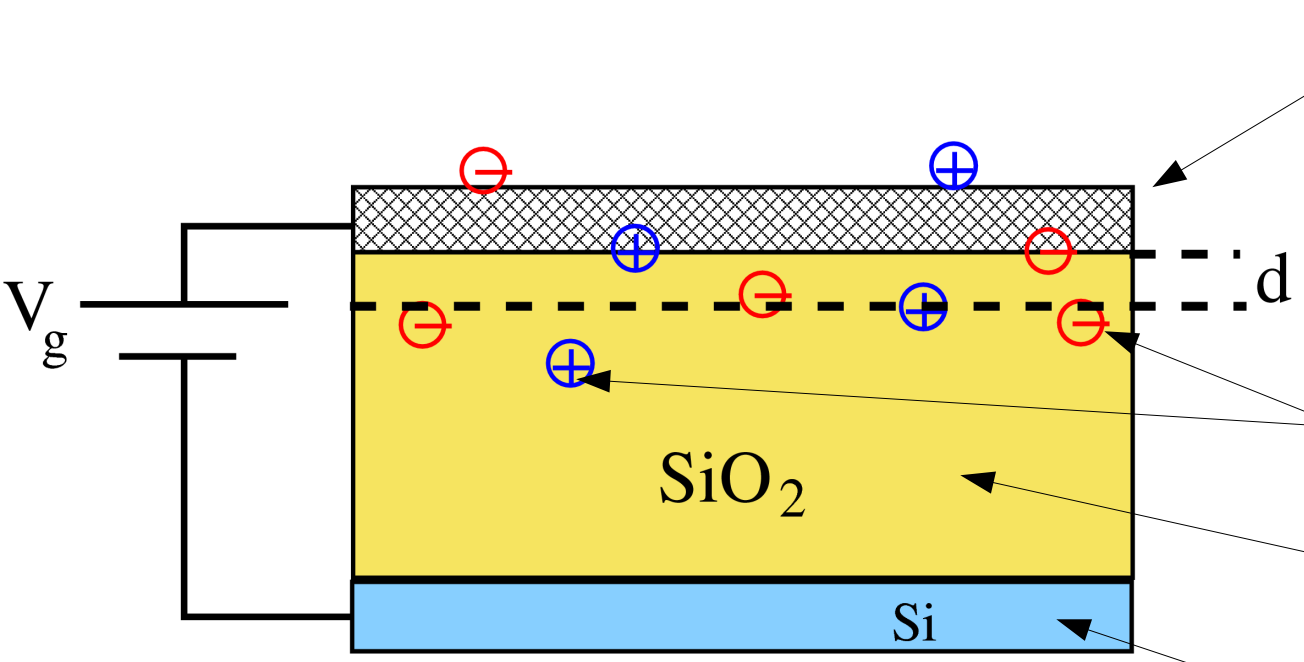
J. Martin et al., Nature Physics, **4**, 144 (2008)



# System




Linear scaling region well explained by presence of random charged impurities




Average distance of impurities from the graphene layer

# Thomas-Fermi-Dirac theory

Start from the energy functional E[n] and then minimize it with respect to the electron density n. In presence of disorder for the total energy we have:

$$E[n] = E_{kin}[n(\mathbf{r})] + E_H[n(\mathbf{r})] + E_{exch}[n(\mathbf{r})] - \int_A \mathbf{V_D} n(\mathbf{r}) d^2r - \mu \int_A n(\mathbf{r}) d^2r$$

and then:

$$\frac{\delta E}{\delta n} = 0$$

$$\hbar v_F \mathrm{sign}(n)\sqrt{\pi n} + \frac{e^2}{2\epsilon_0}\int d^2r' \frac{n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} + \Sigma(n) - \mathbf{V_D} - \mu = 0$$

Where Σ is the exchange self energy:

$$\Sigma \approx r_s \sqrt{|n|}\ln|n|\ ;$$

The correlation energy contribution is quite smaller and scales as the self energy :

$$\frac{\delta E_c}{\delta n} \approx F[r_s]\sqrt{|n|}\ln|n|$$

$$F[r_s] < r_s$$

and of opposite sign

# Construction of disorder potential

- We assume charge distribution with zero average. A nonzero average it simply translates in a voltage gate off-set.

$$\langle C(\mathbf{r}) \rangle = 0$$

- We assume the charge positions to be uncorrelated.

$$\langle C(\mathbf{r}_1) C(\mathbf{r}_2) \rangle = n_{\mathrm{imp}} \delta(\mathbf{r}_2 - \mathbf{r}_1)$$

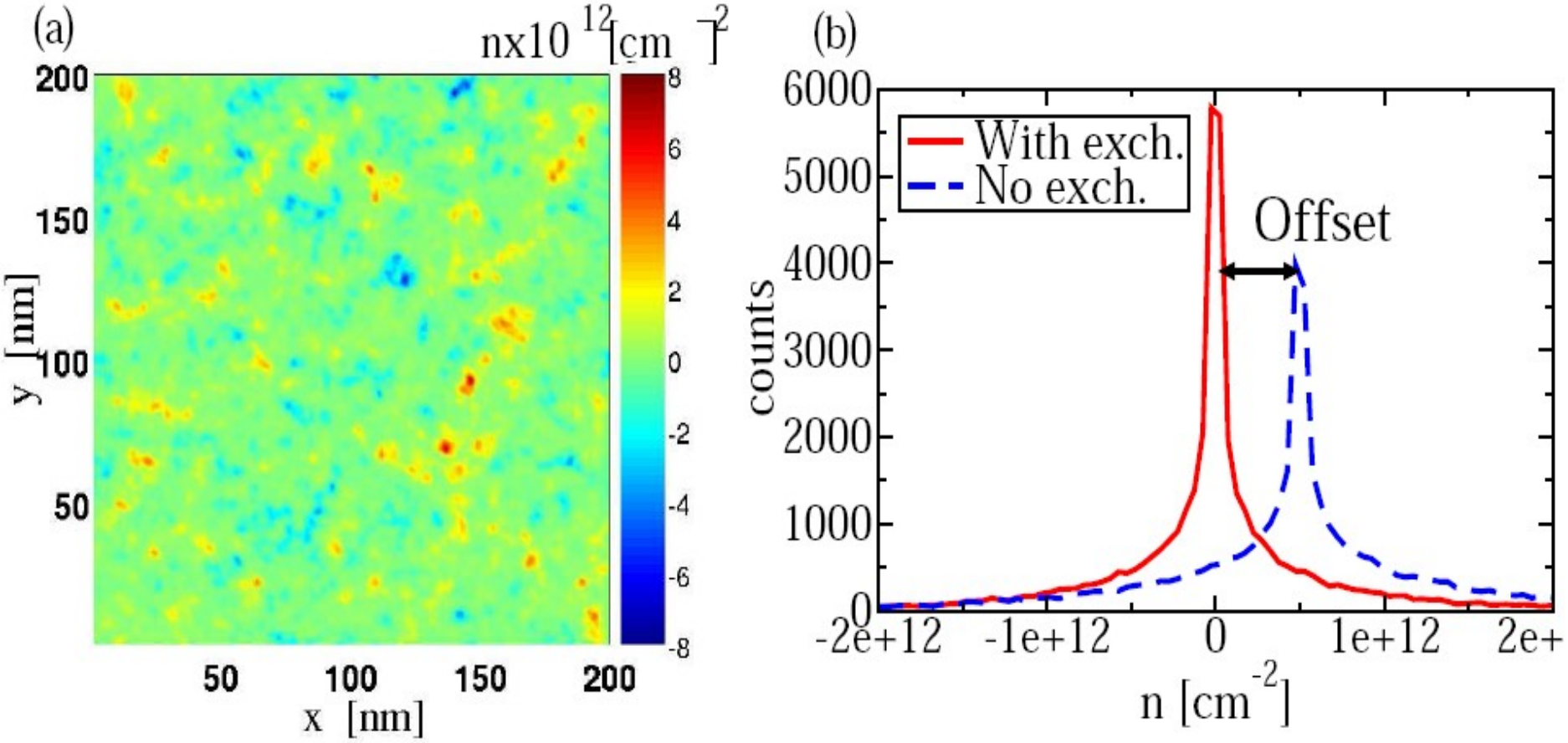
$$\langle C(\mathbf{q}) \rangle = 0$$
$$\langle C^2(\mathbf{q}) \rangle = n_{\mathrm{imp}}$$

- We then calculate C(q) using random number with Gaussian distribution and variance equal to impurity density.

- Assuming the impurities to be in a layer at distance d we finally calculate $V_D$

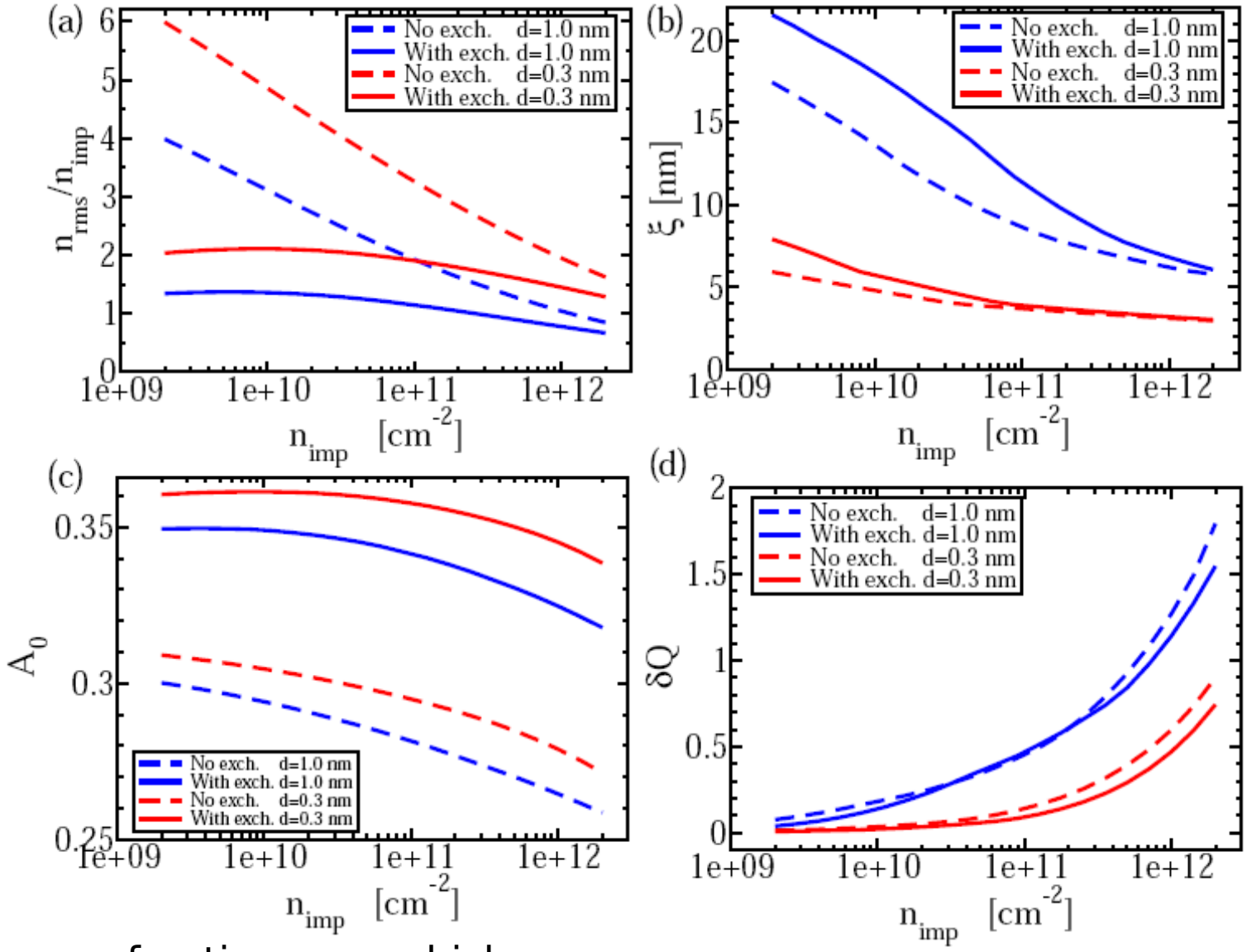
$$V_D(\mathbf{q}) = 2\pi \frac{e^{-qd}}{q} C(q)$$

# Dirac point: single disorder realization




We can see that many-body effects, exchange, tend to suppress the density fluctuations as it can be seen from the “histogram” plot of the density distribution.

# Density rms and correlation length, as function of impurity density



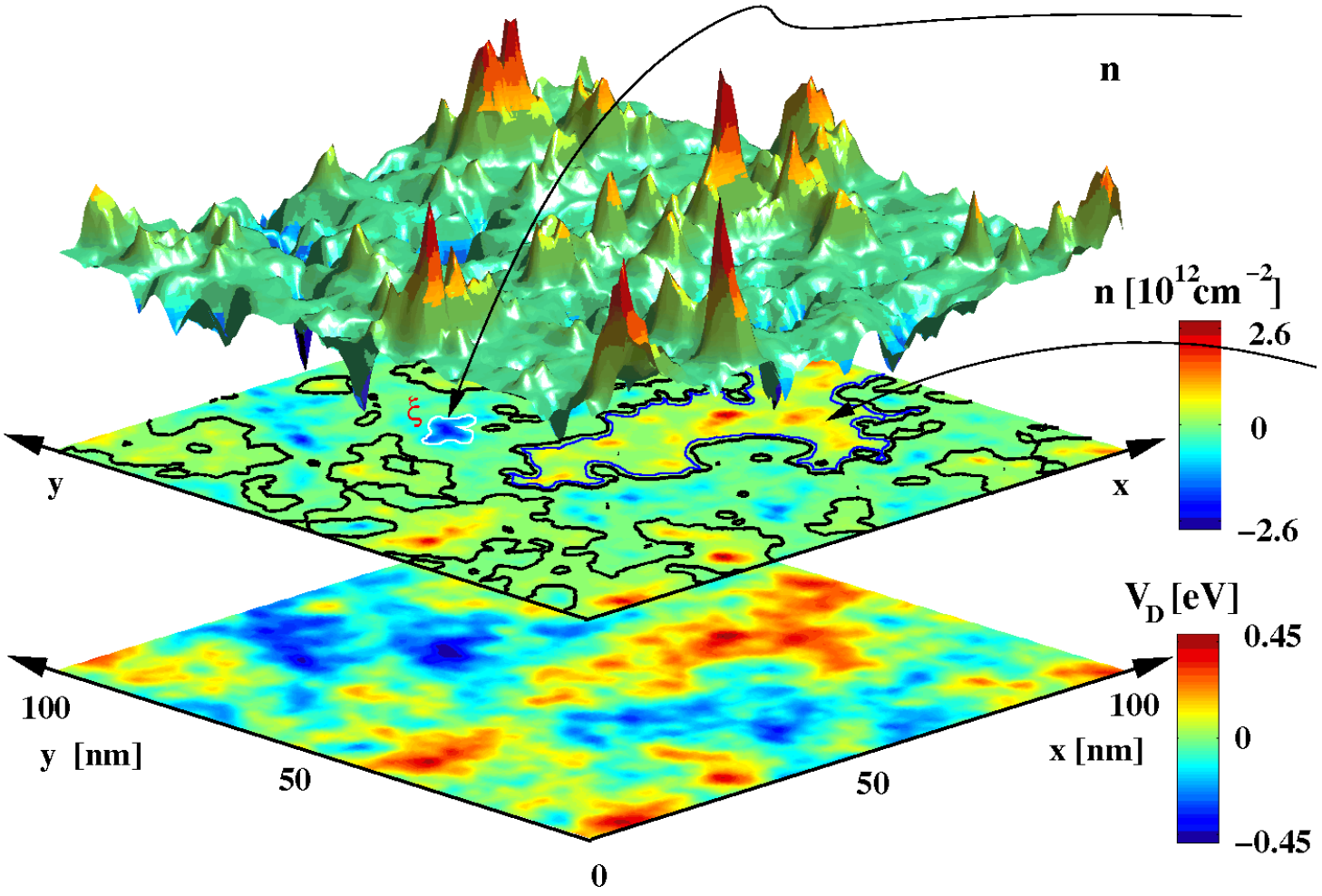

$A_0$ : area fraction over which

$|n(\mathbf{r}) - \langle n \rangle| < n_{rms}/10$

$$\delta Q \equiv n_{rms} \pi \xi^2$$

*ER and S. Das Sarma, Phys. Rev. Lett. (2008)*

# Carrier density properties

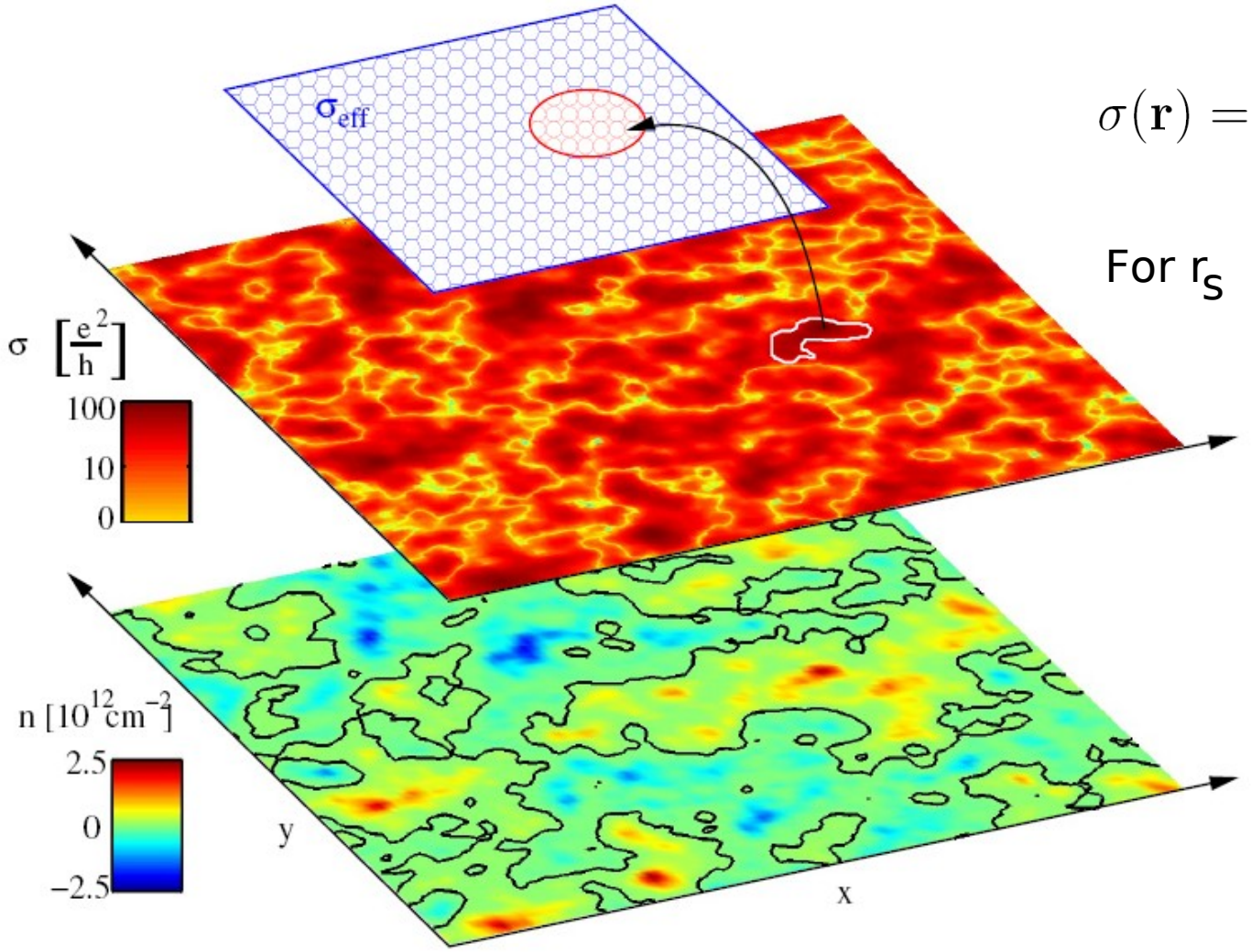



Small region of size ξ, ~10 nm, fixed by non-linear screening, and high density. δQ ~ 2e. Result in agreement with recent STM experiment [V. Brar et al. unpublished]

Wide regions of size ~ L (sample size) and low density. δQ ~ 10e.

# Inhomogeneous conductivity

The inhomogeneous character of the n will be reflected in inhomogeneous transport properties such as the conductivity, σ, and the mean free path, l. Because in presence of disorder the density is strongly inhomogeneous, and different from zero almost everywhere, we assume the RPA-Boltzmann expression [Ando J. Phys. Soc. (2006); Nomura & MacDonald, PRL (2006); Hwang, Adam, Das Sarma, PRL (2007); Cheianov & Falko, PRL (2006), Adam et al. PNAS (2007)] to be valid locally also at the Dirac point:




$$\sigma(\mathbf{r}) = F(r_s)\frac{2e^2}{h}\frac{|n(\mathbf{r})|}{n_{imp}}$$

For $r_s$ =0.8 is $F(r_s)$ = 10.

# Effective medium theory

We use the Landauer-Bruggeman [Bruggeman Ann. Phys (1935), Landauer J. Appl. Phys. (1952)] Effective Medium Theory. In this approach an effective medium conductivity, $\sigma_{eff}$ , is calculated requiring that the spatial average of the electric field fluctuations induced by the inhomogeneity of σ is equal to zero. In 2D this requirement translates into the equation:

$$\int d^2r \frac{\sigma(\mathbf{r}) - \sigma_{\rm eff}}{\sigma(\mathbf{r}) + \sigma_{\rm eff}} = 0$$

For graphene this equation, after disorder averaging, takes the form:

$$\left\langle \int d^2r \frac{\sigma(\mathbf{r}) - \sigma_{\rm eff}}{\sigma(\mathbf{r}) + \sigma_{\rm eff}} = 0 \right\rangle \Longleftrightarrow \int dn \frac{\sigma_0 \frac{|n|}{n_{imp}} - \sigma_{\rm eff}}{\sigma_0 \frac{|n|}{n_{imp}} + \sigma_{\rm eff}} P(n) = 0$$

$$\sigma(\mathbf{r}) = F(r_s)\frac{2e^2}{h}\frac{|n(\mathbf{r})|}{n_{imp}}$$

We know P(n): obtained using the Thomas-Fermi-Dirac approach.

*ER, S. Adam, S. Das Sarma, arxiv:0809.1425*

# Effective medium theory: regime of validity

The Effective Medium Theory is valid when:

a) $$l \ll \left[\frac{\nabla\sigma}{\sigma}\right]^{-1} \longleftrightarrow l \ll \left[\frac{\nabla n}{n}\right]^{-1}$$

From Boltzmann-RPA result

In general we have seen that ξ is ~10 nm, smaller than the typical l. However:

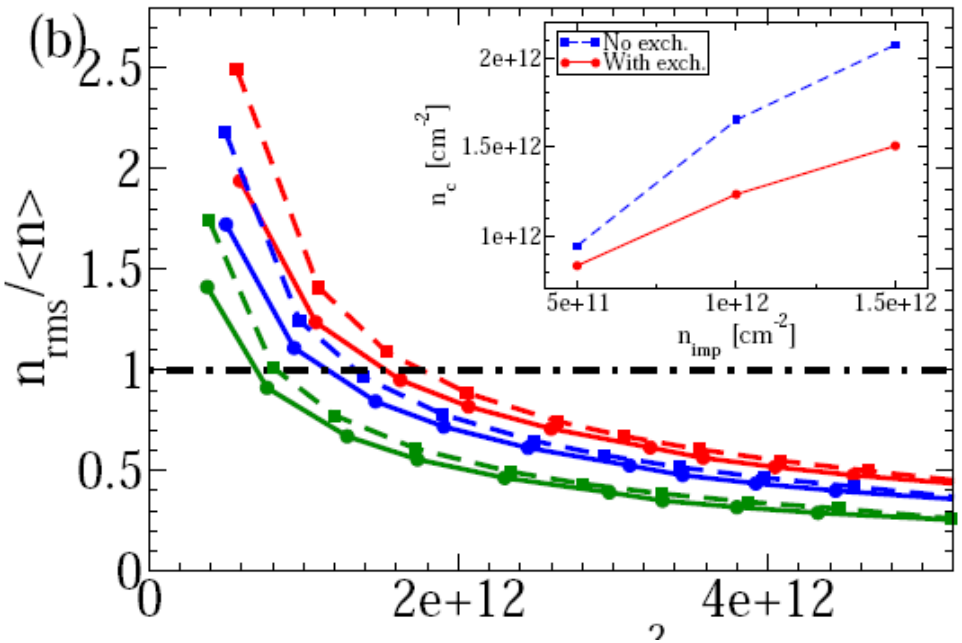
• ξ characterizes small regions that are quite sparse and, in first approximation, we can assume their contribution to the conductivity to be small;

• Close to the Dirac point most of the sample is characterized by wide regions with small density. Because is $l(\mathbf{r}) = \sigma(\mathbf{r})/\sqrt{\pi n(\mathbf{r})}$; in this regions l is quite smaller than the length scale over which n varies.

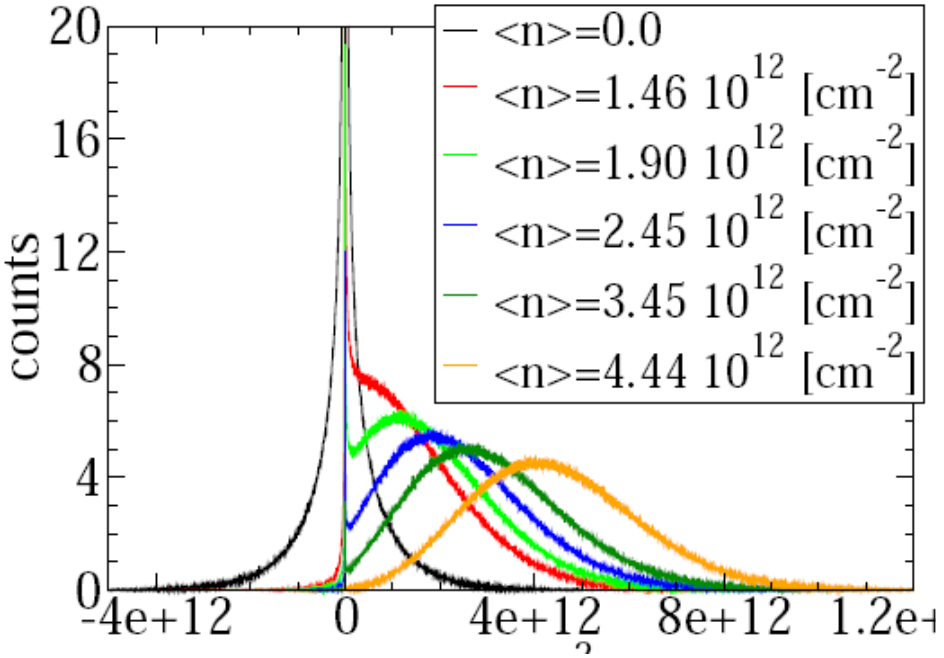
b) Resistive contribution due to boundaries between e-h puddles is small., [Cheianov & Falko, PRB (2006); Cheianov et al, PRL (2007); Fogler et al. PRB (2008)].

This contribution becomes less important with the size of the e-h puddles.

# Results away from the Dirac point.



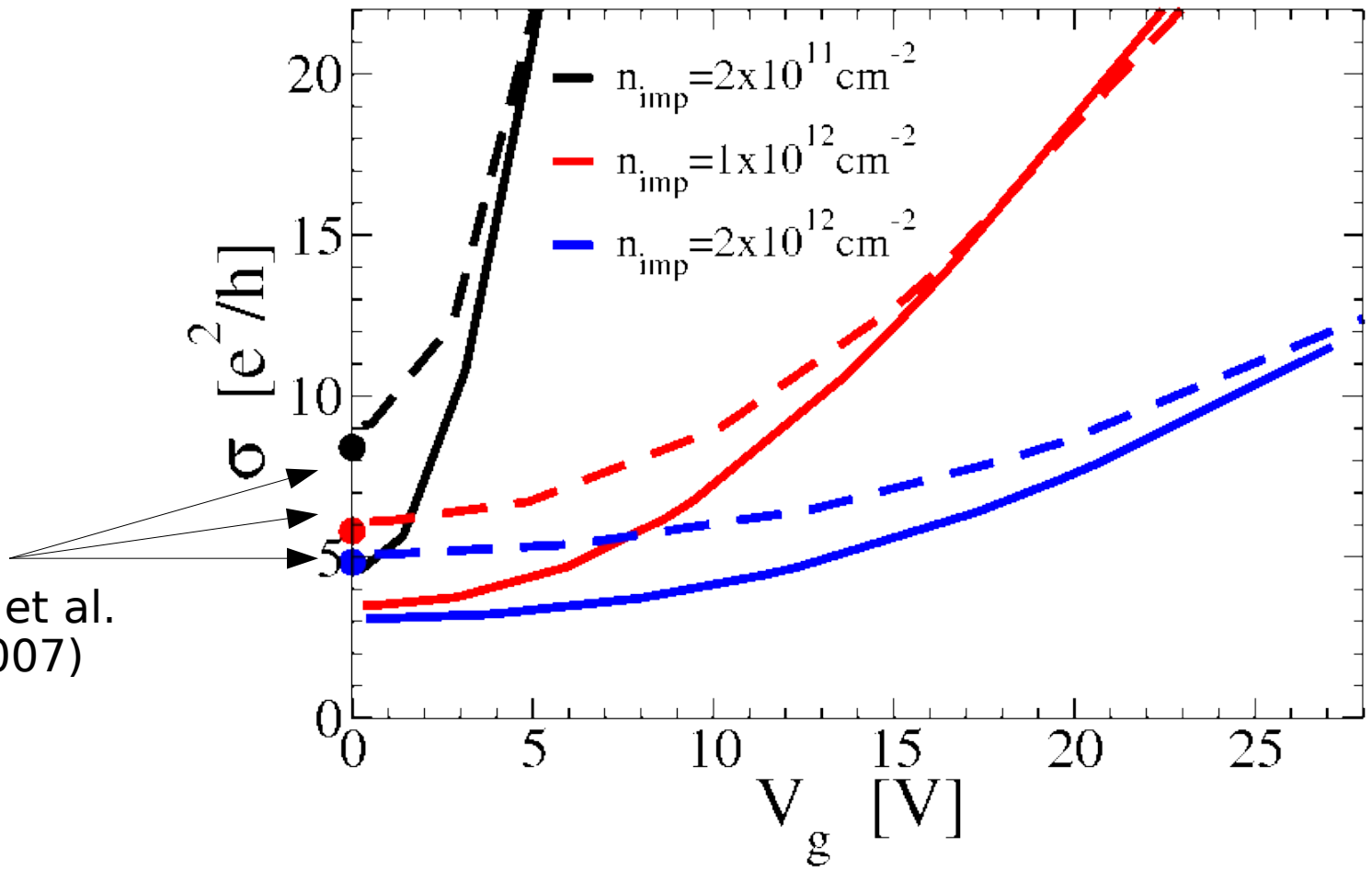

Up to high carrier densities densities fluctuations dominate




The density probability distribution has bimodal character

Dirac-point physics dominates over finite range of gate voltages

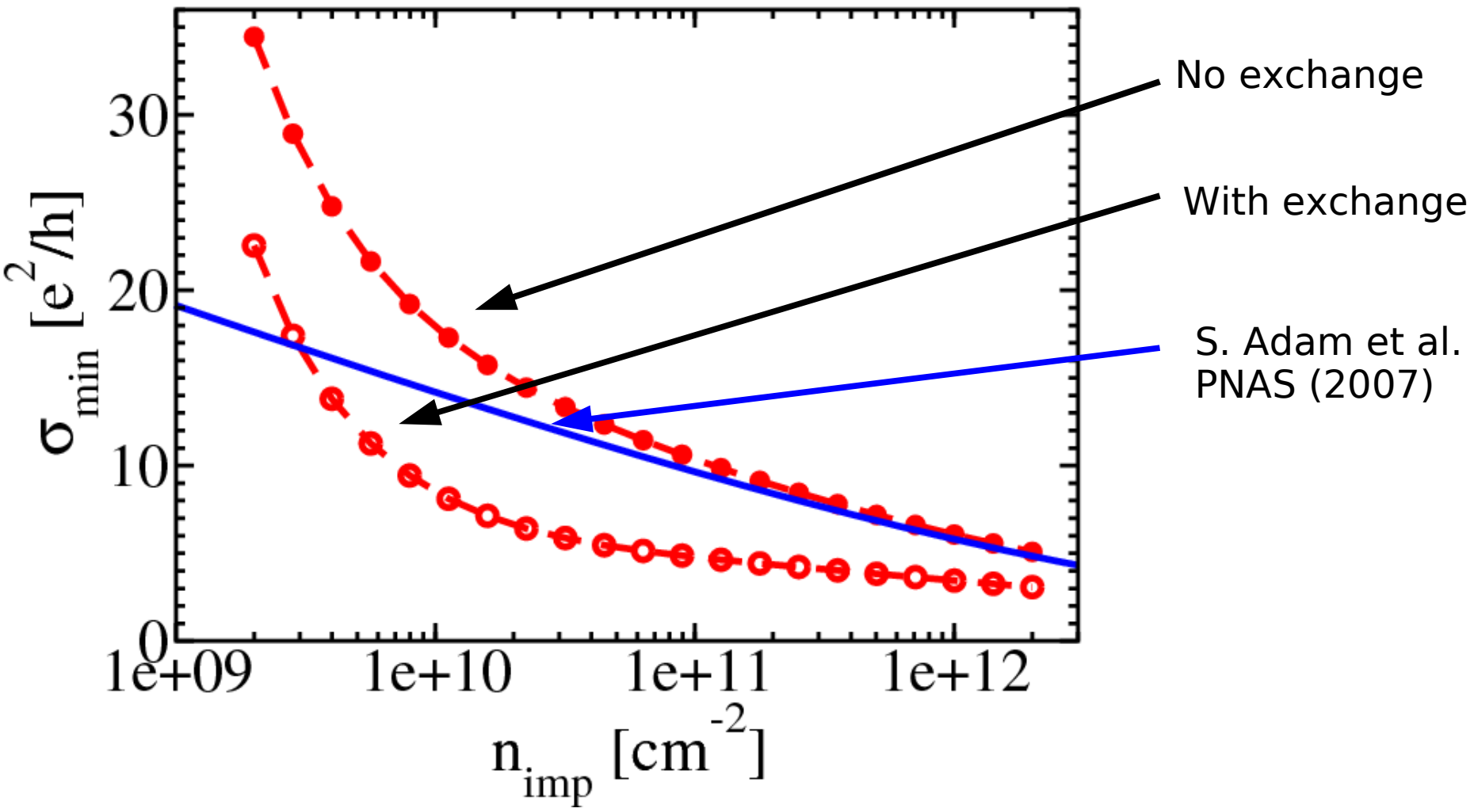
# EMT: conductivity vs. gate voltage




S. Adam et al.
PNAS (2007)

- Finite value of the conductivity at Dirac point;
- Recovers linear behavior at high gate voltages;
- Describes crossover;
- Shows importance of exchange-correlation at low voltages.

# EMT: minimum conductivity vs. impurity density



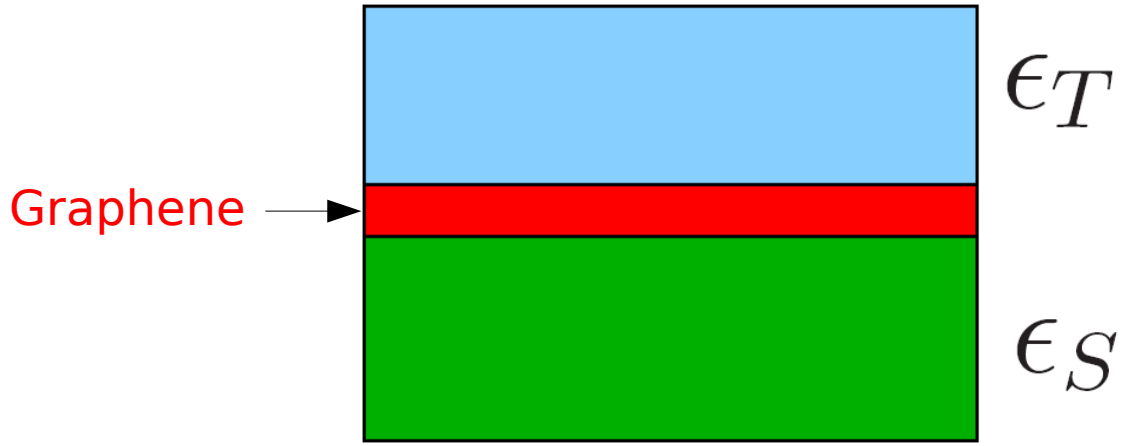

**Dependence of conductivity on impurity density in qualitative and quantitative agreement with experiments.**

# Tuning $r_s$

C. Jang et al. PRL (2008)

$$r_s = \frac{e^2}{\hbar v_F \bar{\epsilon}}$$

$$\bar{\epsilon} = \frac{\epsilon_T + \epsilon_S}{2}$$




$$\epsilon_S = 3.9$$

**Vacuum**

$$\epsilon_T = 1$$

$$r_s = 0.81$$

**Ice**

$$\epsilon_T = 3.2$$

$$r_s = 0.56$$

# How $r_s$ enters the theory

- $r_s$ affects the ground-state carrier distribution:

$$\frac{1}{\hbar v_F}\frac{\delta E}{\delta n} = \mathrm{sign}(n)\sqrt{\pi n} + \mathbf{r_s}\int d^2r' \frac{n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} + \mathbf{r_s}\hat{\Sigma}(n) - \mathbf{r_s}\hat{V}_D - \mu$$

- $r_s$ controls the scattering time:

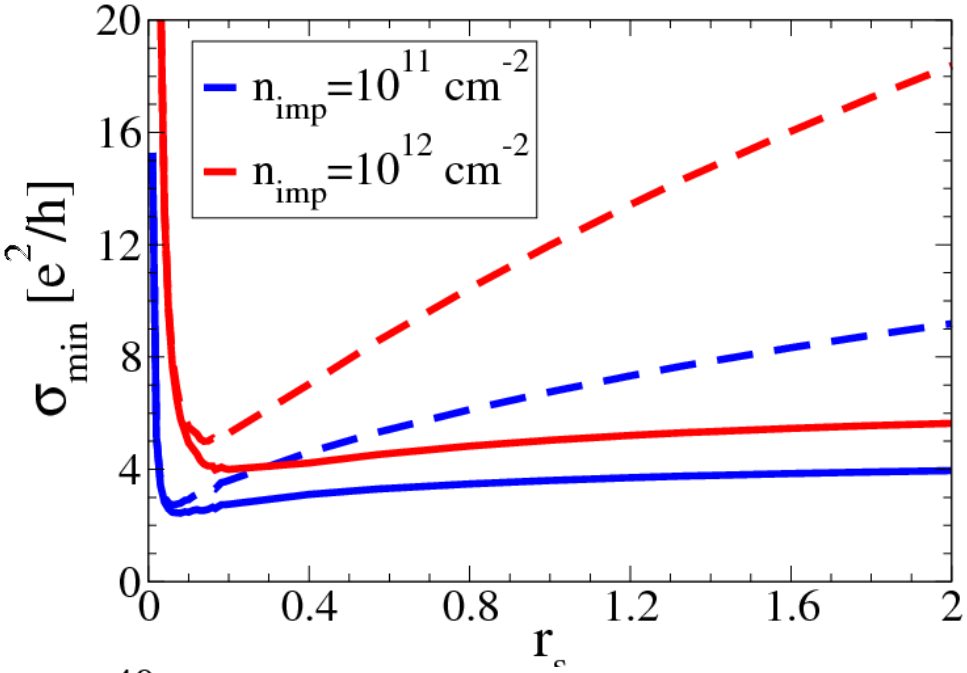
$$\frac{1}{\tau} = \frac{\sqrt{\pi} v_F n_{imp}}{\hbar\sqrt{n}} F(\mathbf{r_s})$$

S. Adam et al. PNAS (2008).
E. Hwang et al. PRB (2008).

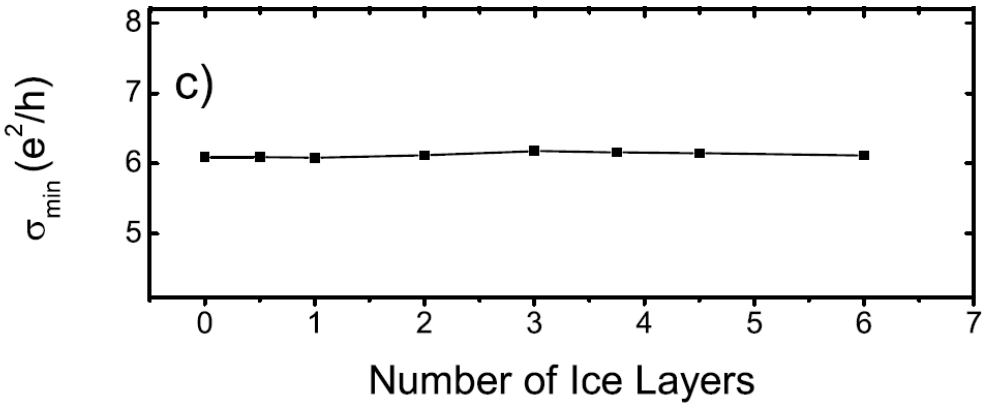
and therefore the local value of the conductivity

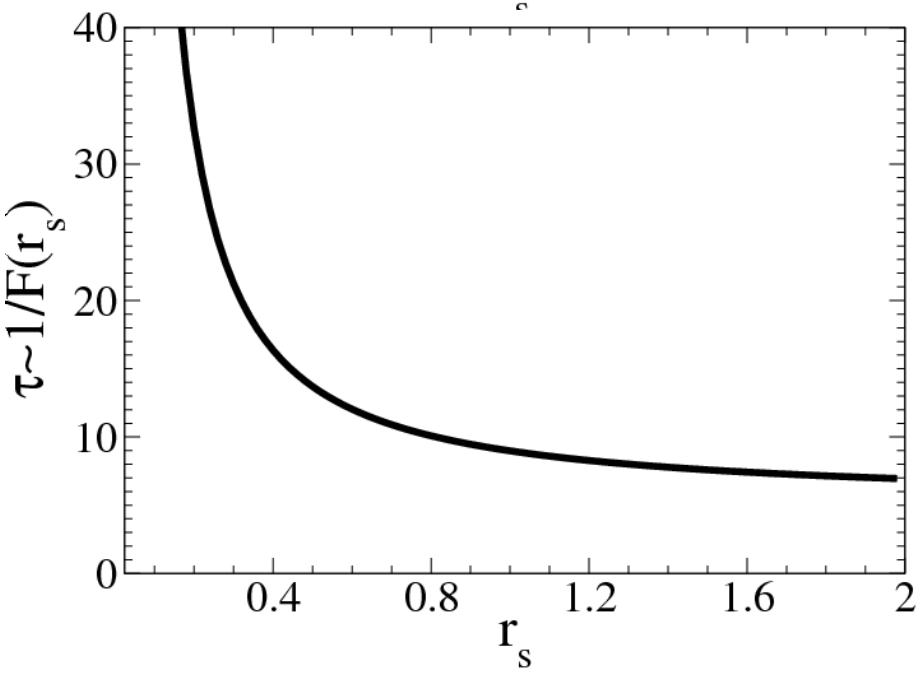
$$\sigma = 2\frac{e^2}{h}E_F\tau = 2\frac{e^2}{h}\frac{n}{n_{imp}}\frac{1}{F(\mathbf{r_s})}$$

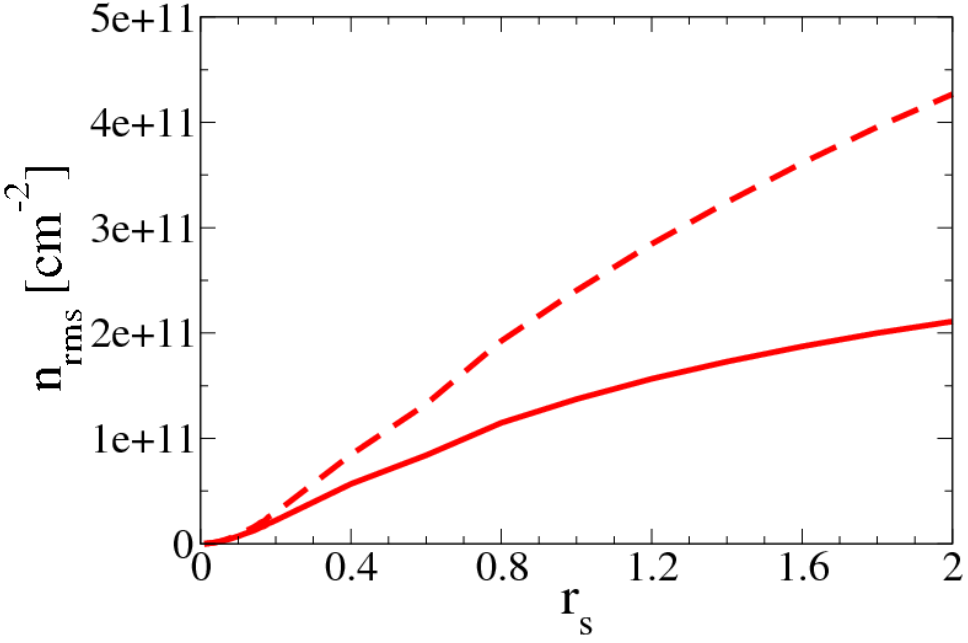
# EMT: $r_s$ dependence of the minimum conductivity




Experiment: C. Jang et al PRL (2008)



# Conclusions

- Graphene is interesting.
- Close to the Dirac-point, disorder induced density inhomogeneities are extremely important to understand graphene properties, especially transport.
- We understand transport in current samples close to Dirac point;
- Interactions not strong enough to cause long-range order but essential to understand transport close to the Dirac point;
- Many things not covered and still largely unexplored: bilayers; graphene nanostructures, ...