

# Graphene

## Outline:

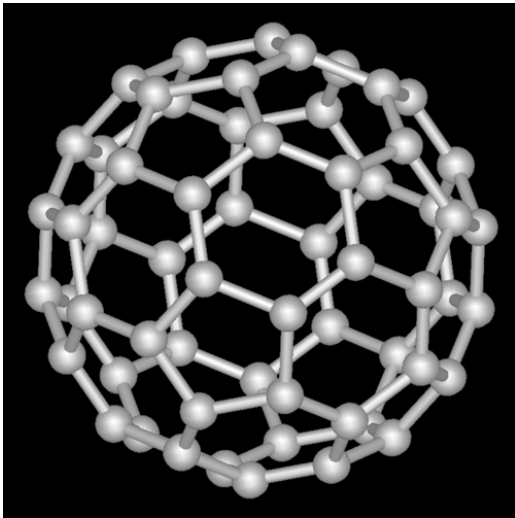
- Introduction (Making graphene, Applications, etc.)
- Band structure
- Physics of Dirac electrons (Berry phase, Klein tunneling)
- Half-Integer Quantum Hall Effect
- High quality graphene structures

## References:

- E. McCann Graphene monolayers Lancaster University, UK Tight-binding model, QHE
- C. Beenakker, Reviews of Modern Physics, 80, 1337 (2008)
- L. Tapasztó & J. Csértes, MAFIHE Teli Iskola a Grafenrol 2011, ELTE
- A. Geim talk, TNT Conference 2010  
[http://www.tntconf.org/2010/Presentaciones/TNT2010\\_Geim.pdf](http://www.tntconf.org/2010/Presentaciones/TNT2010_Geim.pdf)
- ...

# Graphene

**Fullerene**  
**0D**

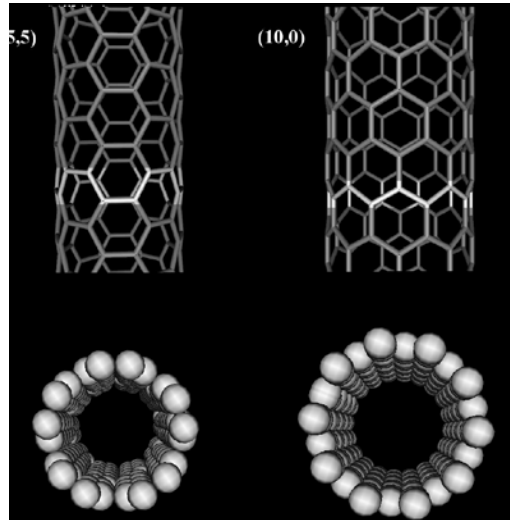


**1985**

H.W.Kroto

Mass spectrometer

**Nanotube**  
**1D**

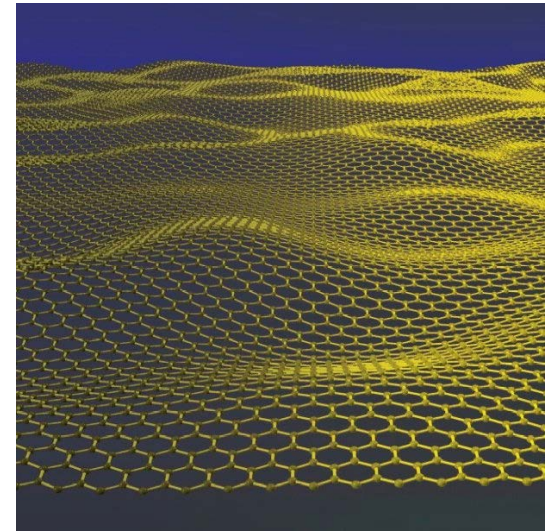


**1991**

S lijima

Electron microscope

**Graphene**  
**2D**



**2004**

K. S. Novoselov

Optical microscope

# Graphene – Nobel Prize in Physics 2010



**Andre Geim**



**Kostya Novoselov**

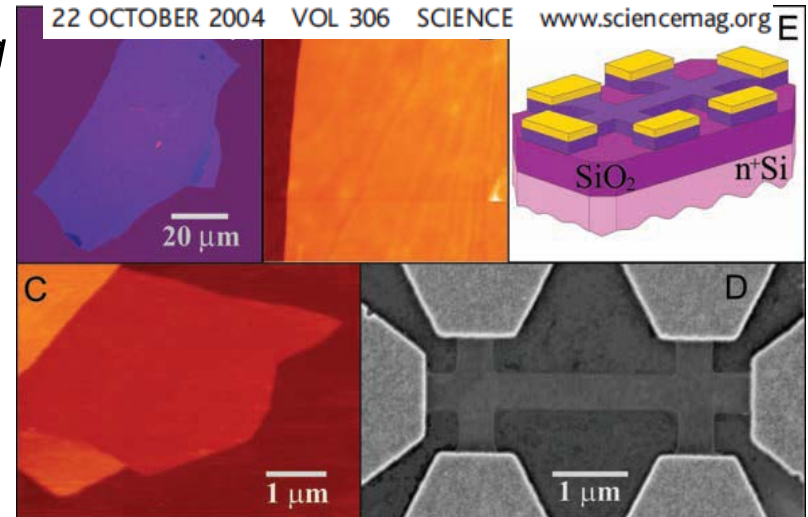
## Electric Field Effect in Atomically Thin Carbon Films

K. S. Novoselov,<sup>1</sup> A. K. Geim,<sup>1\*</sup> S. V. Morozov,<sup>2</sup> D. Jiang,<sup>1</sup>  
Y. Zhang,<sup>1</sup> S. V. Dubonos,<sup>2</sup> I. V. Grigorieva,<sup>1</sup> A. A. Firsov<sup>2</sup>

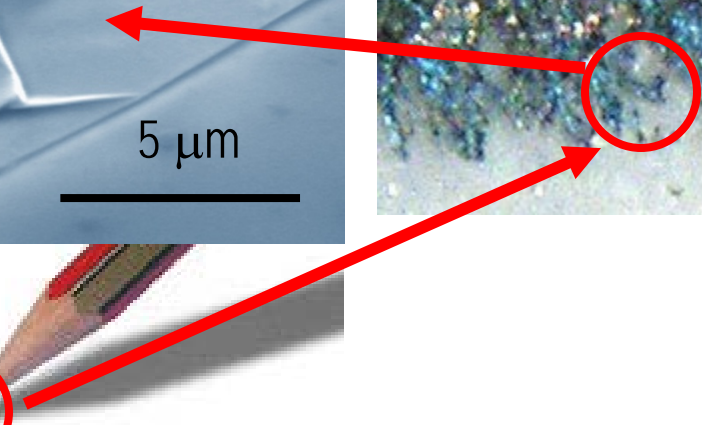
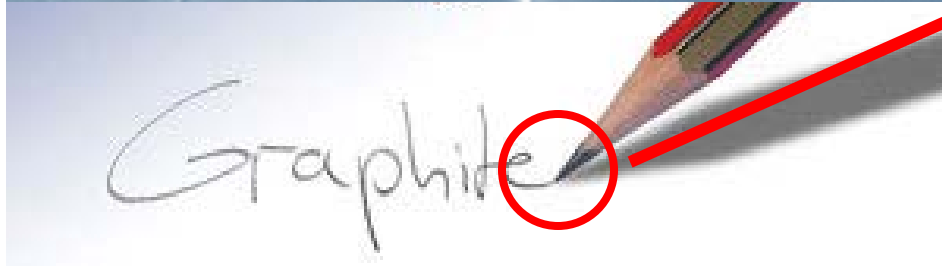
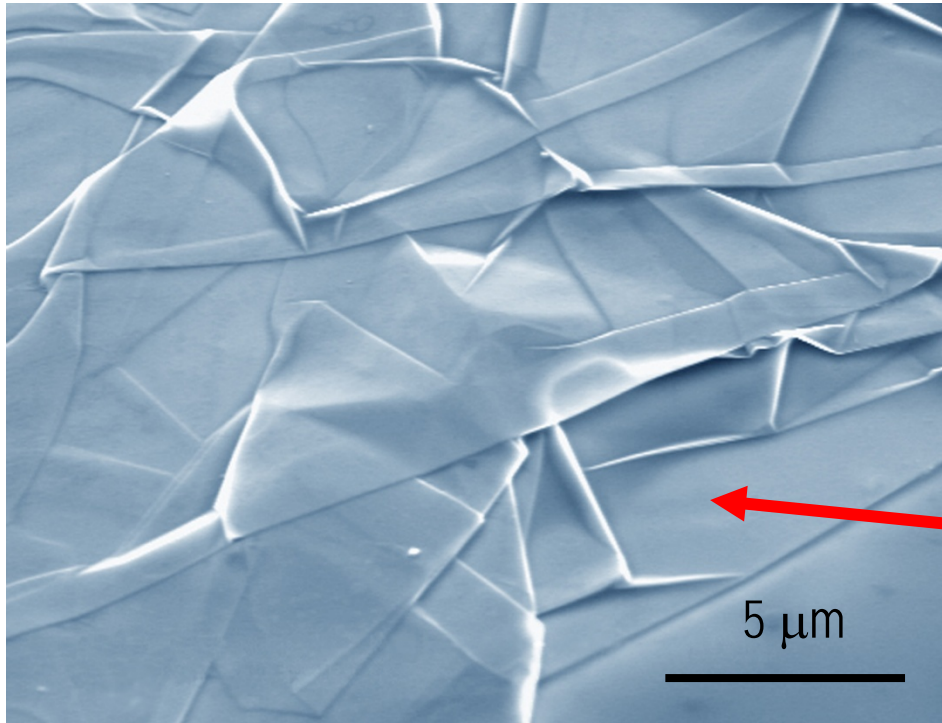
We describe monocrystalline graphitic films, which are a few atoms thick but are nonetheless stable under ambient conditions, metallic, and of remarkably high quality. The films are found to be a two-dimensional semimetal with a tiny overlap between valence and conduction bands, and they exhibit a strong ambipolar electric field effect such that electrons and holes in concentrations up to  $10^{13}$  per square centimeter and with room-temperature mobilities of  $\sim 10,000$  square centimeters per volt-second can be induced by applying gate voltage.

*“for groundbreaking experiments regarding the two dimensional material graphene”*

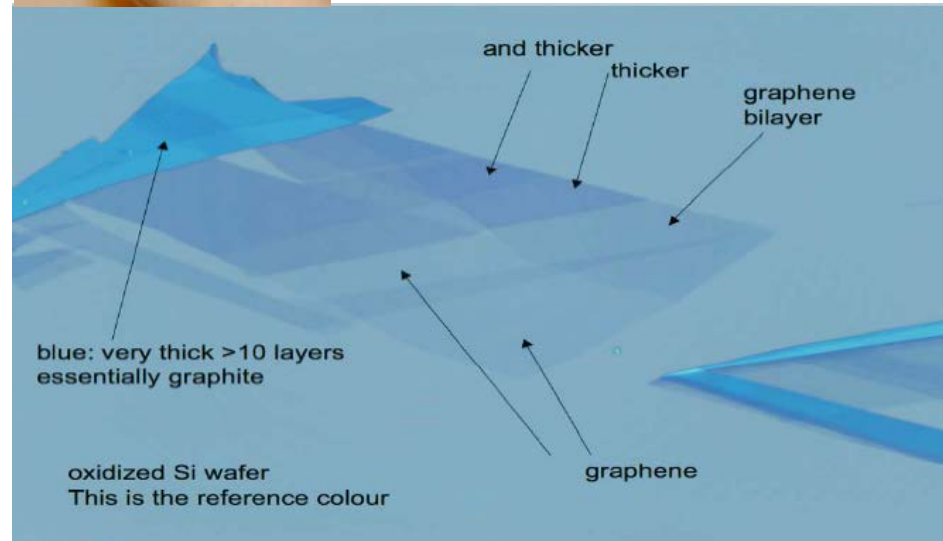
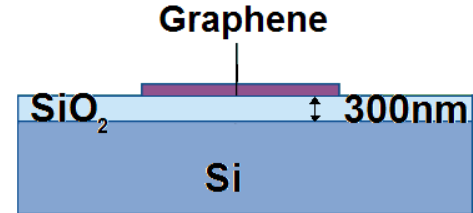
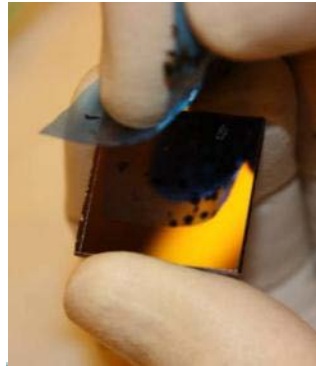
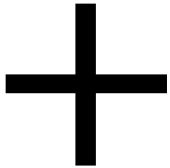
Surprising, since growth of macroscopic 2D objects is strictly forbidden due to phonons (Mermin Wagner - theorem)



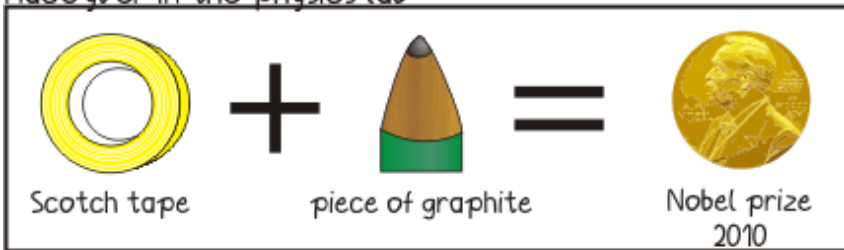
# How to make graphene?



# Mechanical exfoliation



MacGyver in the physics lab



www.strippedsience.com

For proper SiO<sub>2</sub> thickness interference makes it visible by optical microscope + Even size of 1mm, + high quality, - low yield

# Other methods

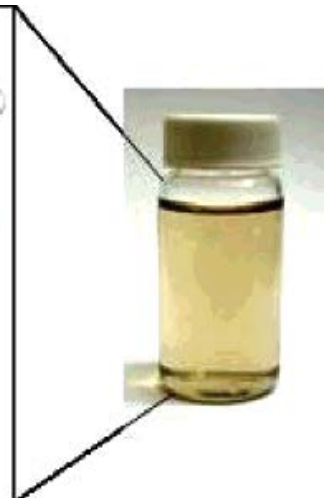
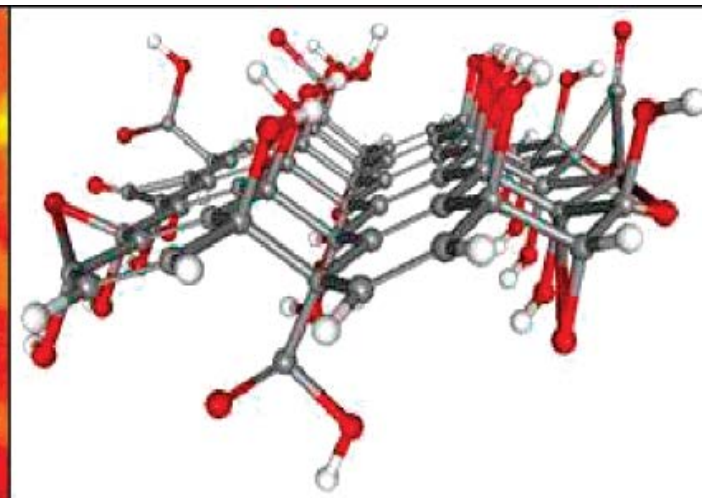
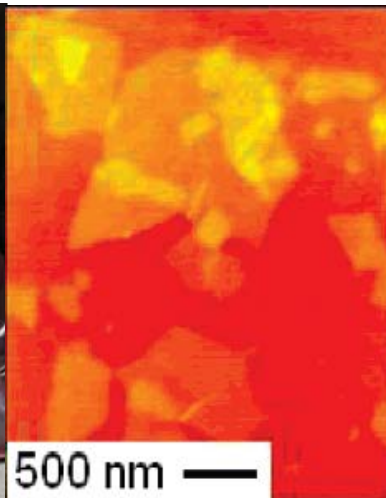
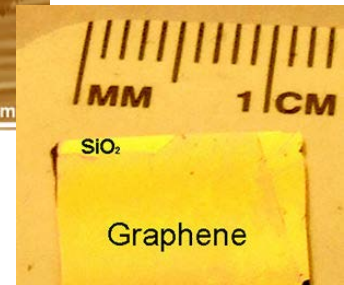
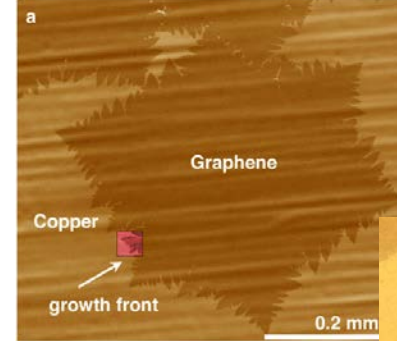
## Sonication + centrifugation, often intercalation

→ Submicrometer crystallites, mass production, industrial scale  
→ Good for polycrystalline films and composite materials.  
Suspension can be printed resulting highly conductive bendable film

## Growth of a monolayer of carbon

→ **CVD** on Cu, Ni (Lower figs.): T + gas flow. Self terminating process. Result: single layer, - polycrystalline, it follows the crystallites of the metal surface, Use e.g. HCl to remove substrate. (commercially available)

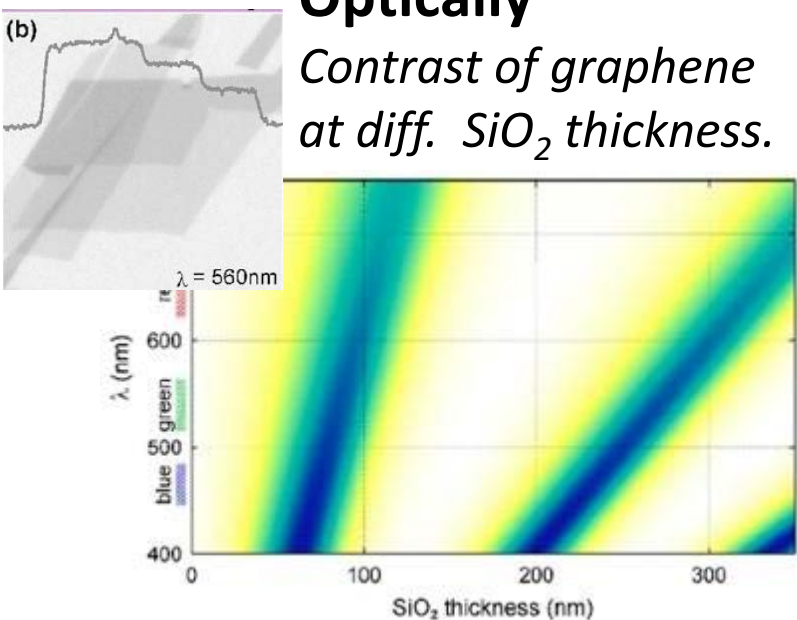
*Ruoff, Nature 2006, Manchester, Nanolett '08, Coleman et al, Nature Nano '08*



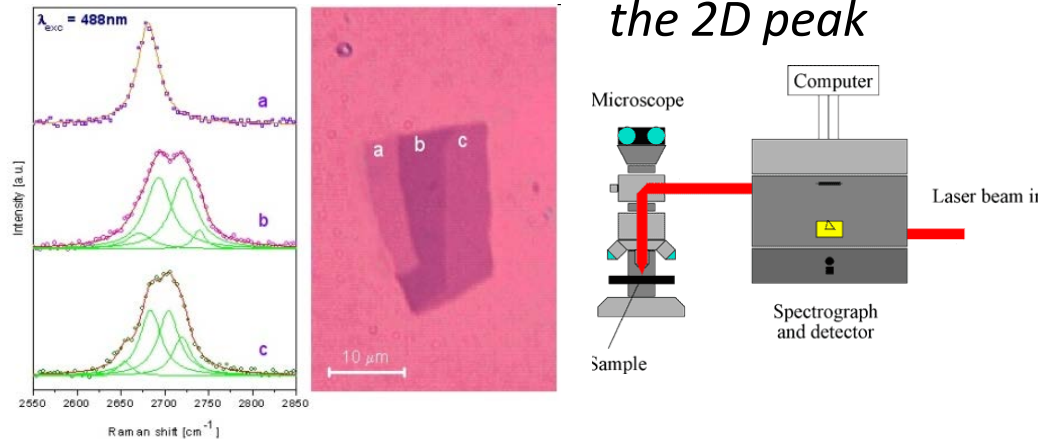
# Identification of graphene

## Optically

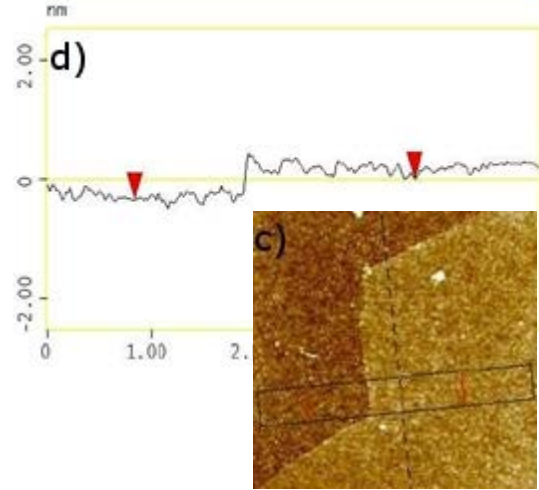
*Contrast of graphene at diff. SiO<sub>2</sub> thickness.*



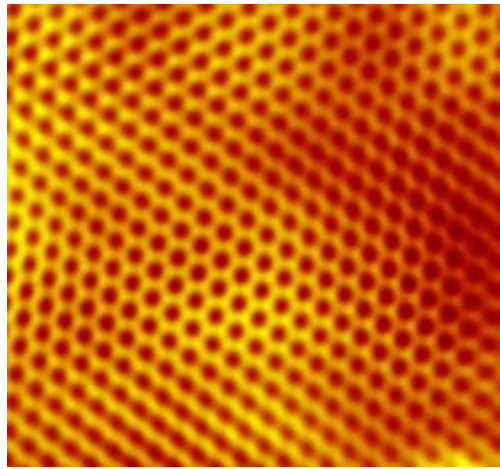
**Raman spectroscopy** *measure the energy difference of reflected laser light e.g. layer thickness can be determined from the 2D peak*



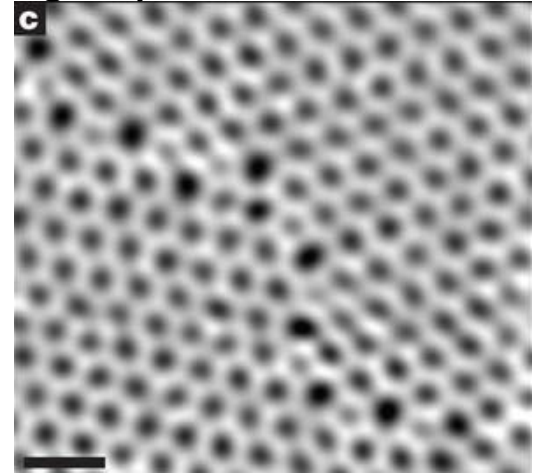
**AFM** *e.g. possible to determine thickness*



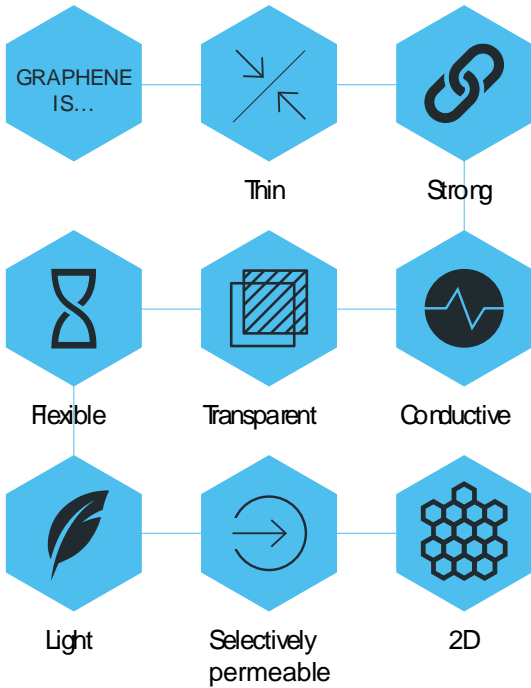
**STM** *e.g. exfoliated on metal substrate*



**TEM** *e.g. crystalite boarder SiC*

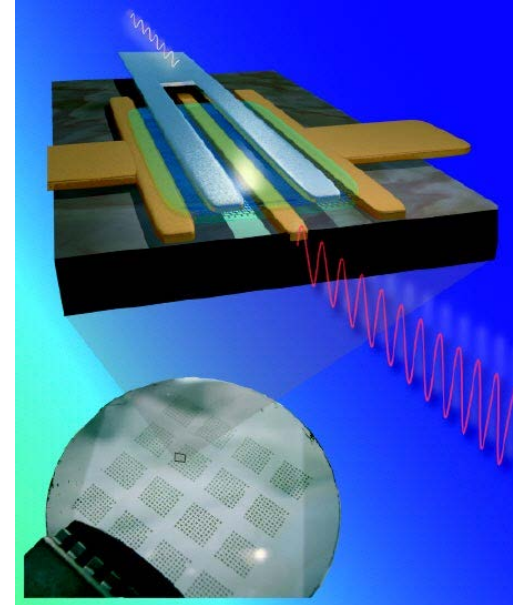


# Properties, applications



- Good electronic quality: submicrons without scattering mobility  $> 200000 \text{ cm}^2/\text{Vs}$  @ RT (Si:  $<1500 \text{ cm}^2/\text{Vs}$ )
- Quantum effect at RT
- Strongest material,
- Most stretchable material
- Impermeable to gases (also He)
- Strain sensors
- Hall sensors
- Conductive coatings etc.

## Ultra High Frequency Transistors

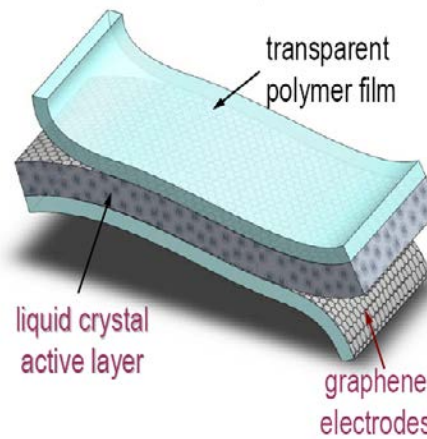


## Reinforcement

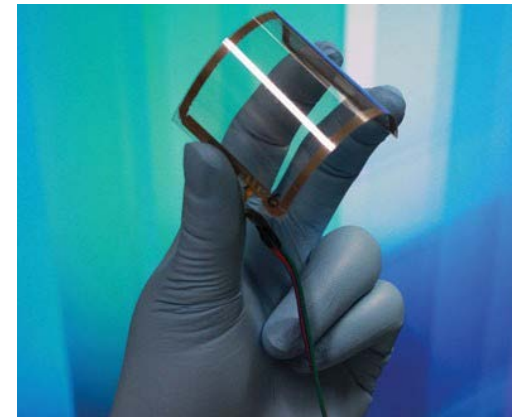
**SPORT BOOSTED WITH GRAPHENE**



2/3



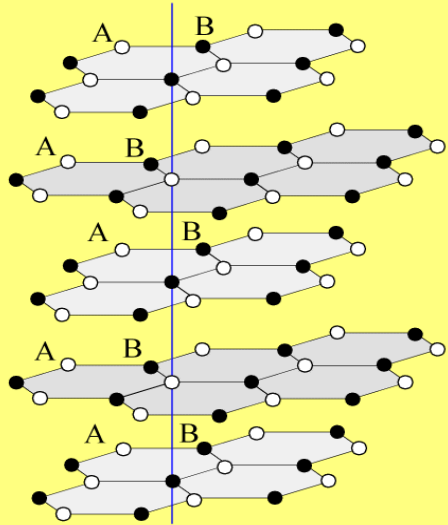
## Touch screen





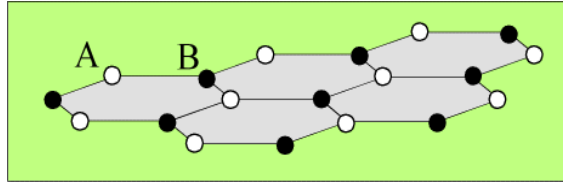
# Band structure of graphene

## Graphite



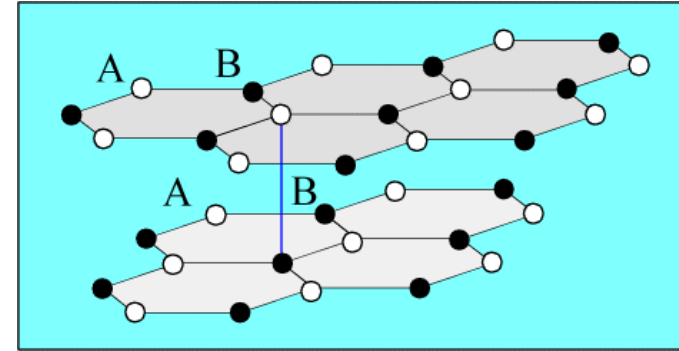
Three dimensional layered material with hexagonal 2D layers [shown here with Bernal (AB) stacking]

## Monolayer



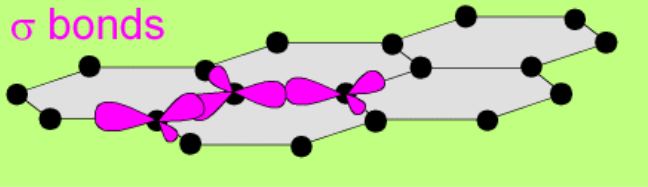
**Two dimensional material;**  
**zero gap semiconductor;**  
**Dirac spectrum of electrons**

## Bilayer



*Images: V. Falco, Lecture notes*

$\sigma$  bonds

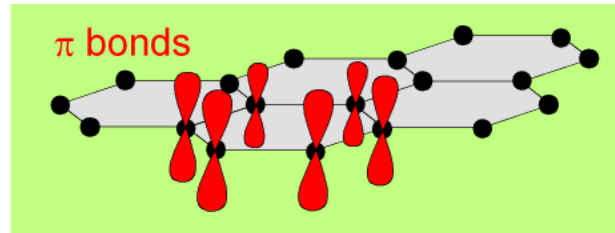


$sp^2$  hybridisation

- single 2s and two 2p orbitals hybridise forming three “ $\sigma$  bonds” in the x-y plane

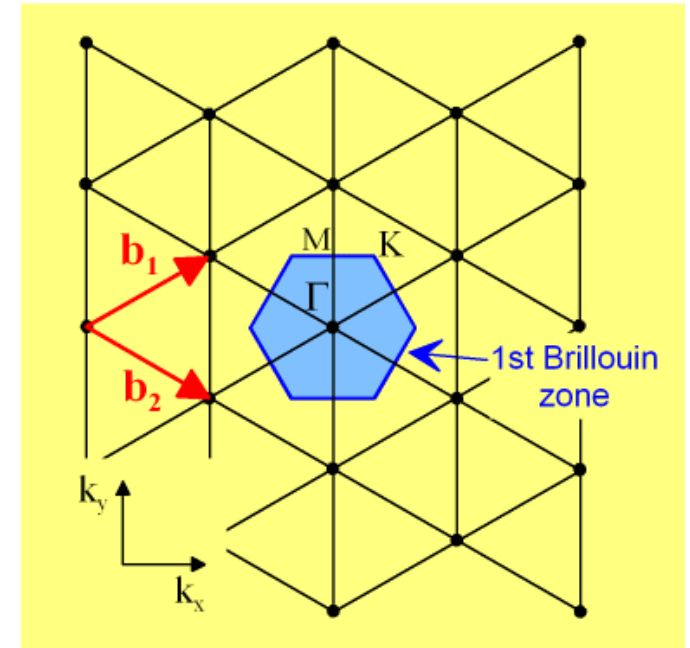
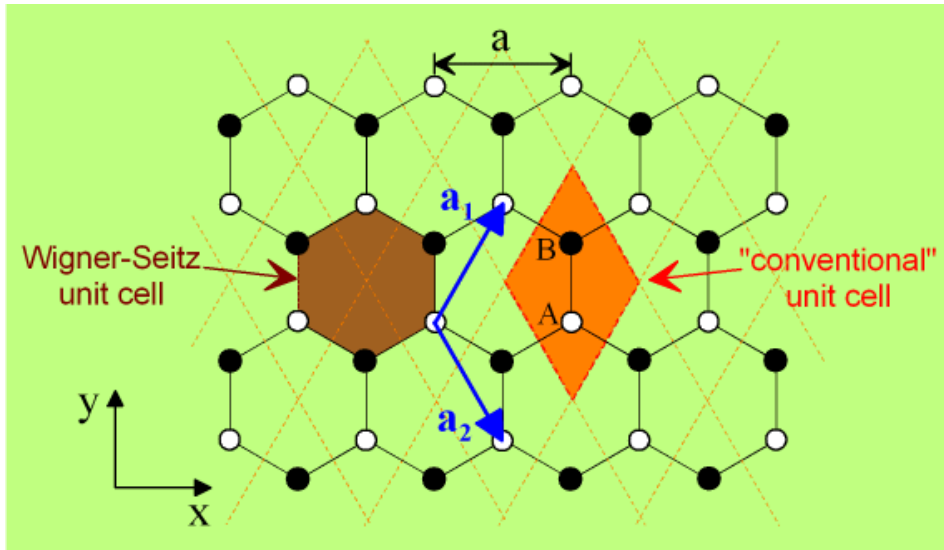
Carbon has 6 electrons: 2 core electrons, 4 valence electrons – one 2s and three 2p orbitals

$\pi$  bonds



- remaining  $2p_z$  orbital [“ $\pi$ ” orbital] exists perpendicular to the x-y plane, keep only this one orbital per site in the tight binding model

# Tight-binding model of graphene



**2 different atomic sites – 2 triangular sub-lattices**

We take into account one  $\pi$  orbital per site, so there are two orbitals per unit cell.

**Bloch functions**

$$\Phi_A(\vec{k}, \vec{r}) = \frac{1}{\sqrt{N}} \sum_{\vec{R}_A} e^{i\vec{k} \cdot \vec{R}_A} \varphi_A(\vec{r} - \vec{R}_A)$$

$$\Phi_B(\vec{k}, \vec{r}) = \frac{1}{\sqrt{N}} \sum_{\vec{R}_B} e^{i\vec{k} \cdot \vec{R}_B} \varphi_B(\vec{r} - \vec{R}_B)$$

sum over all type B  
atomic sites  
in N unit cells

**triangular reciprocal lattice  
– hexagonal Brillouin zone**

atomic wavefunction

# Tight-binding model of graphene

Bloch functions : label with  $j = 1$  [A sites] or  $2$  [B sites]

$$\Phi_j(\vec{k}, \vec{r}) = \frac{1}{\sqrt{N}} \sum_{\vec{R}_j} e^{i\vec{k} \cdot \vec{R}_j} \varphi_j(\vec{r} - \vec{R}_j)$$

**Eigenfunction  $\Psi_j$**  (for  $j = 1$  or  $2$ ) is written as a linear combination of Bloch functions:

$$\Psi_j(\vec{k}, \vec{r}) = \sum_{j'=1}^2 C_{jj'}(\vec{k}) \Phi_{j'}(\vec{k}, \vec{r})$$

**Eigenvalue  $E_j$**  (for  $j = 1$  or  $2$ ) is written as :

$$E_j(\vec{k}) = \frac{\langle \Psi_j | H | \Psi_j \rangle}{\langle \Psi_j | \Psi_j \rangle} \longrightarrow E_j(\vec{k}) = \frac{\sum_{i,l}^2 C_{ji}^* C_{jl} \langle \Phi_i | H | \Phi_l \rangle}{\sum_{i,l}^2 C_{ji}^* C_{jl} \langle \Phi_i | \Phi_l \rangle} \equiv \frac{\sum_{i,l}^2 H_{il} C_{ji}^* C_{jl}}{\sum_{i,l}^2 S_{il} C_{ji}^* C_{jl}}$$

**defining transfer integral matrix elements**

$$H_{il} = \langle \Phi_i | H | \Phi_l \rangle;$$

**and overlap integral matrix elements**

$$S_{il} = \langle \Phi_i | \Phi_l \rangle$$

# Tight-binding model of graphene

$$E_j(\vec{k}) = \frac{\sum_{i,l}^2 H_{il} C_{ji}^* C_{jl}}{\sum_{i,l}^2 S_{il} C_{ji}^* C_{jl}}$$

We can find the energy by minimising with respect

to  $C_{jl}^*$  :

$$\frac{\partial E_j}{\partial C_{jm}^*} = \frac{\sum_l^2 H_{ml} C_{jl}}{\sum_{i,l}^2 S_{il} C_{ji}^* C_{jl}} - \frac{\sum_{i,l}^2 H_{il} C_{ji}^* C_{jl} \sum_l^2 S_{ml} C_{jl}}{\left( \sum_{i,l}^2 S_{il} C_{ji}^* C_{jl} \right)^2}$$

$$\frac{\partial E_j}{\partial C_{jm}^*} = 0 \quad \Rightarrow \quad \sum_{l=1}^2 H_{ml} C_{jl} = E_j \sum_{l=1}^2 S_{ml} C_{jl} \quad S_{ii} \sim 1, S_{il} \sim 0$$

**Explicitly write out sums:**

$$m = 1 \quad \Rightarrow \quad H_{11} C_{j1} + H_{12} C_{j2} = E_j C_{j1}$$

$$m = 2 \quad \Rightarrow \quad H_{21} C_{j1} + H_{22} C_{j2} = E_j C_{j2}$$

**Write as a matrix equation:**

$$\begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} \begin{pmatrix} C_{j1} \\ C_{j2} \end{pmatrix} = E_j \begin{pmatrix} C_{j1} \\ C_{j2} \end{pmatrix}$$

$$H C_j = E_j C_j$$

**Secular equation gives the eigenvalues:**

$$\det(H - E) = 0$$

# Tight-binding model of graphene

## Diagonal matrix element

$$H_{AA} = \langle \Phi_A | H | \Phi_A \rangle = \frac{1}{N} \sum_{\vec{R}_{Ai}} \sum_{\vec{R}_{Aj}} e^{i\vec{k} \cdot (\vec{R}_{Aj} - \vec{R}_{Ai})} \langle \varphi_A(\vec{r} - \vec{R}_{Ai}) | H | \varphi_A(\vec{r} - \vec{R}_{Aj}) \rangle$$

## Same site only:

$$\begin{aligned} H_{AA} &= \frac{1}{N} \sum_{\vec{R}_{Ai}} \langle \varphi_A(\vec{r} - \vec{R}_{Ai}) | H | \varphi_A(\vec{r} - \vec{R}_{Ai}) \rangle \\ &= \langle \varphi_A(\vec{r} - \vec{R}_{Ai}) | H | \varphi_A(\vec{r} - \vec{R}_{Ai}) \rangle \\ &\equiv \varepsilon_0 \end{aligned}$$

$$\begin{aligned} S_{AA} &= \frac{1}{N} \sum_{\vec{R}_{Ai}} \langle \varphi_A(\vec{r} - \vec{R}_{Ai}) | \varphi_A(\vec{r} - \vec{R}_{Ai}) \rangle \\ &= \langle \varphi_A(\vec{r} - \vec{R}_{Ai}) | \varphi_A(\vec{r} - \vec{R}_{Ai}) \rangle \\ &\equiv 1 \end{aligned}$$

## A and B sites are chemically identical:

$$H_{AA} = H_{BB} = \varepsilon_0$$

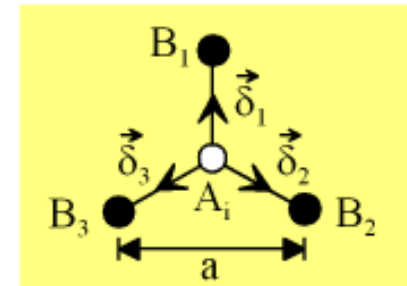
$$S_{AA} = S_{BB} = 1$$

## Off-diagonal matrix element

$$H_{AB} = \langle \Phi_A | H | \Phi_B \rangle = \frac{1}{N} \sum_{\vec{R}_{Ai}} \sum_{\vec{R}_{Bj}} e^{i\vec{k} \cdot (\vec{R}_{Bj} - \vec{R}_{Ai})} \langle \varphi_A(\vec{r} - \vec{R}_{Ai}) | H | \varphi_B(\vec{r} - \vec{R}_{Bj}) \rangle$$

## Every A site has 3 B nearest neighbours:

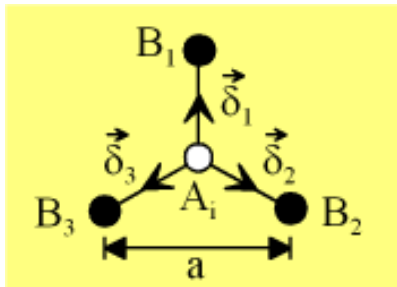
$$H_{AB} = \frac{1}{N} \sum_{\vec{R}_{Ai}} \left[ \sum_{\vec{\delta}_j=1}^3 e^{i\vec{k} \cdot \vec{\delta}_j} \langle \varphi_A(\vec{r} - \vec{R}_{Ai}) | H | \varphi_B(\vec{r} - \vec{R}_{Bj}) \rangle \right] = \sum_{\vec{\delta}_j=1}^3 e^{i\vec{k} \cdot \vec{\delta}_j} \langle \varphi_A(\vec{r} - \vec{R}_{Ai}) | H | \varphi_B(\vec{r} - \vec{R}_{Bj}) \rangle$$



# Tight-binding model of graphene

$$H_{AB} = \sum_{\vec{\delta}_j=1}^3 e^{i\vec{k}\cdot\vec{\delta}_j} \langle \varphi_A(\vec{r} - \vec{R}_{Ai}) | H | \varphi_B(\vec{r} - \vec{R}_{Bj}) \rangle$$

**Parameterise nearest neighbour transfer integral:**



$$\gamma_0 = -\langle \varphi_A(\vec{r} - \vec{R}_{Ai}) | H | \varphi_B(\vec{r} - \vec{R}_{Bj}) \rangle$$

$$\Rightarrow H_{AB} = -\gamma_0 f(\vec{k}); \quad f(\vec{k}) = \sum_{\vec{\delta}_j=1}^3 e^{i\vec{k}\cdot\vec{\delta}_j}$$

$$\vec{\delta}_1 = R_{B1} - R_{Ai} = \left( 0, \frac{a}{\sqrt{3}} \right);$$

$$\vec{\delta}_2 = R_{B2} - R_{Ai} = \left( \frac{a}{2}, -\frac{a}{2\sqrt{3}} \right);$$

$$\vec{\delta}_3 = R_{B3} - R_{Ai} = \left( -\frac{a}{2}, -\frac{a}{2\sqrt{3}} \right)$$

$$f(\vec{k}) = e^{ik_y a / \sqrt{3}} + 2e^{-ik_y a / 2\sqrt{3}} \cos\left(\frac{k_x a}{2}\right)$$

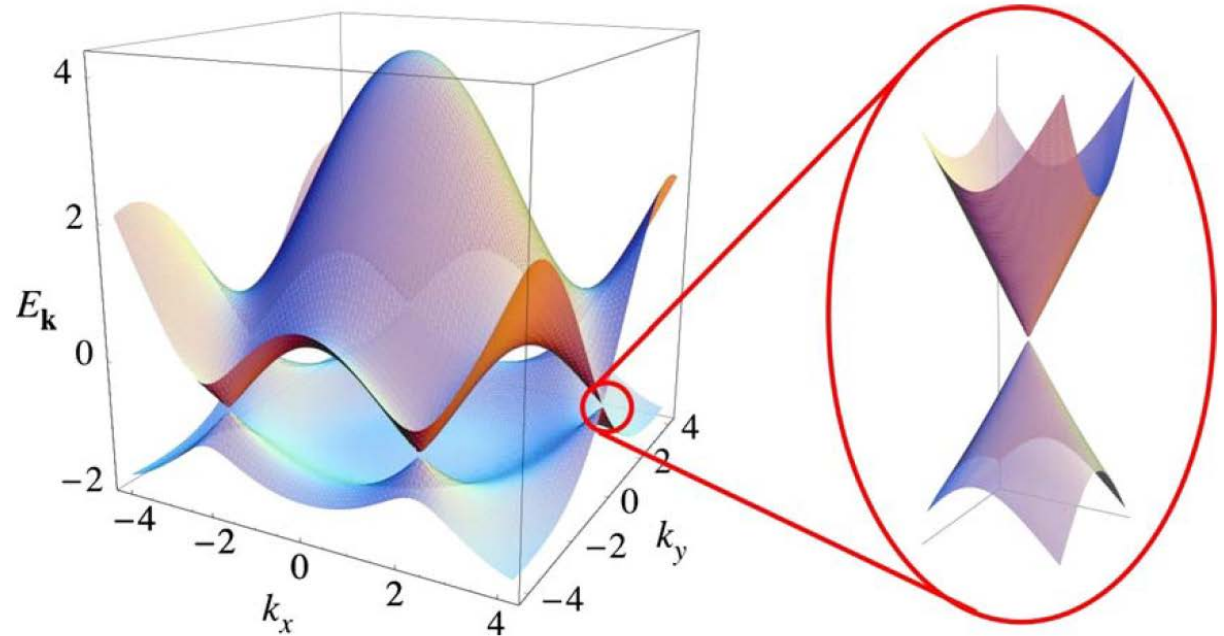
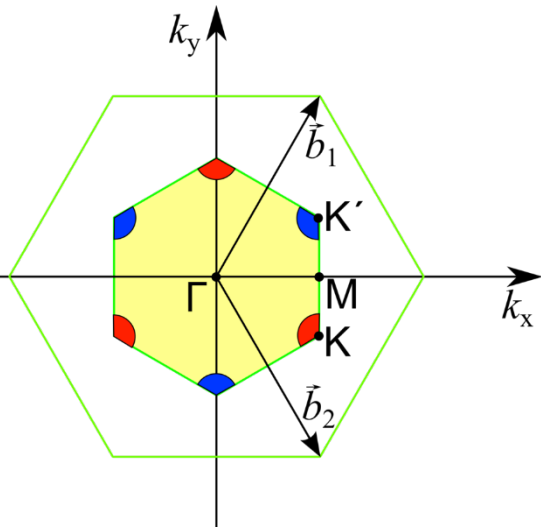
$$H = \begin{pmatrix} \varepsilon_0 & -\gamma_0 f(\vec{k}) \\ -\gamma_0 f^*(\vec{k}) & \varepsilon_0 \end{pmatrix};$$

$$E = \varepsilon_0 \pm \gamma_0 |f(\vec{k})|$$

# Tight-binding model of graphene

$$E = \varepsilon_0 \pm \gamma_0 |f(\vec{k})|$$

$$E(\mathbf{k}) = E_F \pm \gamma_0 \sqrt{1 + 4 \cos\left(\frac{\sqrt{3}k_x a}{2}\right) \cos\left(\frac{k_y a}{2}\right) + 4 \cos^2\left(\frac{k_y a}{2}\right)}$$



$$\varepsilon_0 = 0, \gamma_0 = 3.033\text{eV}, s = 0.129$$

→ Gapless semiconductor

- Two non-equivalent valleys:  $K$  and  $K'$ , where the dispersion is linear
- $E_f = 0$  for undoped graphene

# Tight-binding model of graphene

## Dispersion exactly at the K point

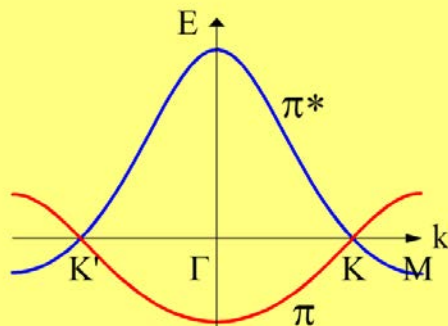
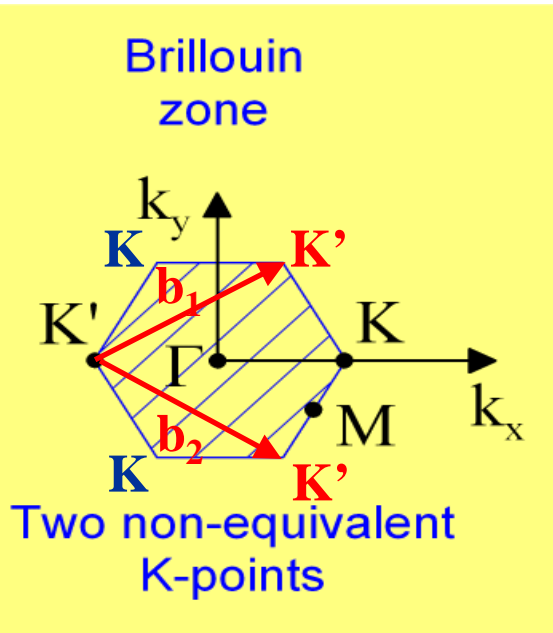
$$\vec{K} = \left( \frac{4\pi}{3a}, 0 \right); \quad \vec{K}' = \left( -\frac{4\pi}{3a}, 0 \right)$$

$$\vec{\delta}_1 = \left( 0, \frac{a}{\sqrt{3}} \right); \quad \Rightarrow \quad \vec{K} \vec{\delta}_1 = 0$$

$$\vec{\delta}_2 = \left( \frac{a}{2}, -\frac{a}{2\sqrt{3}} \right); \quad \Rightarrow \quad \vec{K} \vec{\delta}_2 = \frac{2\pi}{3}$$

$$\vec{\delta}_3 = \left( -\frac{a}{2}, -\frac{a}{2\sqrt{3}} \right); \quad \Rightarrow \quad \vec{K} \vec{\delta}_3 = -\frac{2\pi}{3}$$

$$f(\vec{K}) = \sum_{\vec{\delta}_j=1}^3 e^{i\vec{K} \cdot \vec{\delta}_j} = e^0 + e^{2\pi i/3} + e^{-2\pi i/3} = 0$$



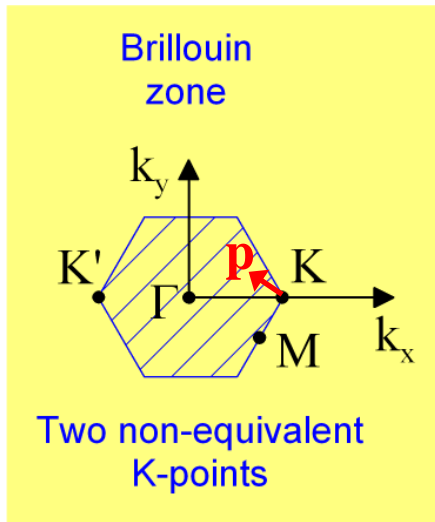
Two bands: no energy gap at the K-points

6 corners of the Brillouin zone (K points), but only two are non-equivalent

**K points also referred to as “valleys”**



# Tight-binding model of graphene



## Expansion near the K points

Consider two non-equivalent K points:

$$\vec{K}, \vec{K}' = \xi \left( \frac{4\pi}{3a}, 0 \right); \quad \xi = \pm 1$$

and small momentum near them:

$$\vec{k} = \xi \left( \frac{4\pi}{3a}, 0 \right) + \frac{\vec{p}}{\hbar}$$

Linear expansion in small momentum:

$$f(\vec{k}) = -\frac{\sqrt{3}a}{2\hbar} (\xi p_x - i p_y) + O(pa/\hbar)^2$$

$$H = \begin{pmatrix} 0 & -\gamma_0 f(\vec{k}) \\ -\gamma_0 f^*(\vec{k}) & 0 \end{pmatrix} \approx v \begin{pmatrix} 0 & \xi p_x - i p_y \\ \xi p_x + i p_y & 0 \end{pmatrix}$$

$$v_F = \frac{\sqrt{3}a\gamma_0}{2\hbar} \approx 10^6 \text{ m/s}$$

New notation for components on A and B sites

$$C_j = \begin{pmatrix} C_{j1} \\ C_{j2} \end{pmatrix} \Leftrightarrow \psi = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$$

$$HC_j = E_j C_j \Rightarrow v_F \begin{pmatrix} 0 & \xi p_x - i p_y \\ \xi p_x + i p_y & 0 \end{pmatrix} \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} = E \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$$

# Tight-binding model of graphene – Dirac equation

For one K point (e.g.  $\xi=+1$ ) we have a 2-component wave function:

$$\psi = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$$

Effective Hamiltonian:

$$H = v_F \begin{pmatrix} 0 & p_x - ip_y \\ p_x + ip_y & 0 \end{pmatrix} = v_F \begin{pmatrix} 0 & \pi^+ \\ \pi & 0 \end{pmatrix} = v_F (\sigma_x p_x + \sigma_y p_y) = v_F \vec{\sigma} \cdot \vec{p}$$

$$\begin{aligned} \pi &= p_x + ip_y = p e^{i\varphi} \\ \pi^+ &= p_x - ip_y = p e^{-i\varphi} \end{aligned}$$

Bloch function amplitudes on the AB sites ('pseudospin') mimic spin components of a relativistic Dirac fermion.

**Pseudospin** is an index that indicates on which of the two sublattices a quasi-particle is located

To take into account both K points ( $\xi=+1$  and  $\xi=-1$ ) we can use a 4-component wave function:

$$\psi = \begin{pmatrix} \psi_{AK} \\ \psi_{BK} \\ \psi_{AK'} \\ \psi_{BK'} \end{pmatrix} \longrightarrow H = v_F \begin{pmatrix} 0 & p_x - ip_y & 0 & 0 \\ p_x + ip_y & 0 & 0 & 0 \\ 0 & 0 & 0 & -p_x - ip_y \\ 0 & 0 & -p_x + ip_y & 0 \end{pmatrix}$$

**Isospin:** K and K' valleys are also called isospin.

# Dirac equation

$$H = v_F \begin{pmatrix} 0 & \pi^+ \\ \pi & 0 \end{pmatrix} = v_F \vec{\sigma} \cdot \vec{p} = v_F p \vec{\sigma} \cdot \vec{n}$$

Helicity:  $\vec{h} = \frac{1}{2} \frac{\vec{\sigma} \cdot \vec{p}}{|p|}$

**Chiral electrons/helical pseudospin direction is linked to an axis determined by electronic momentum.**

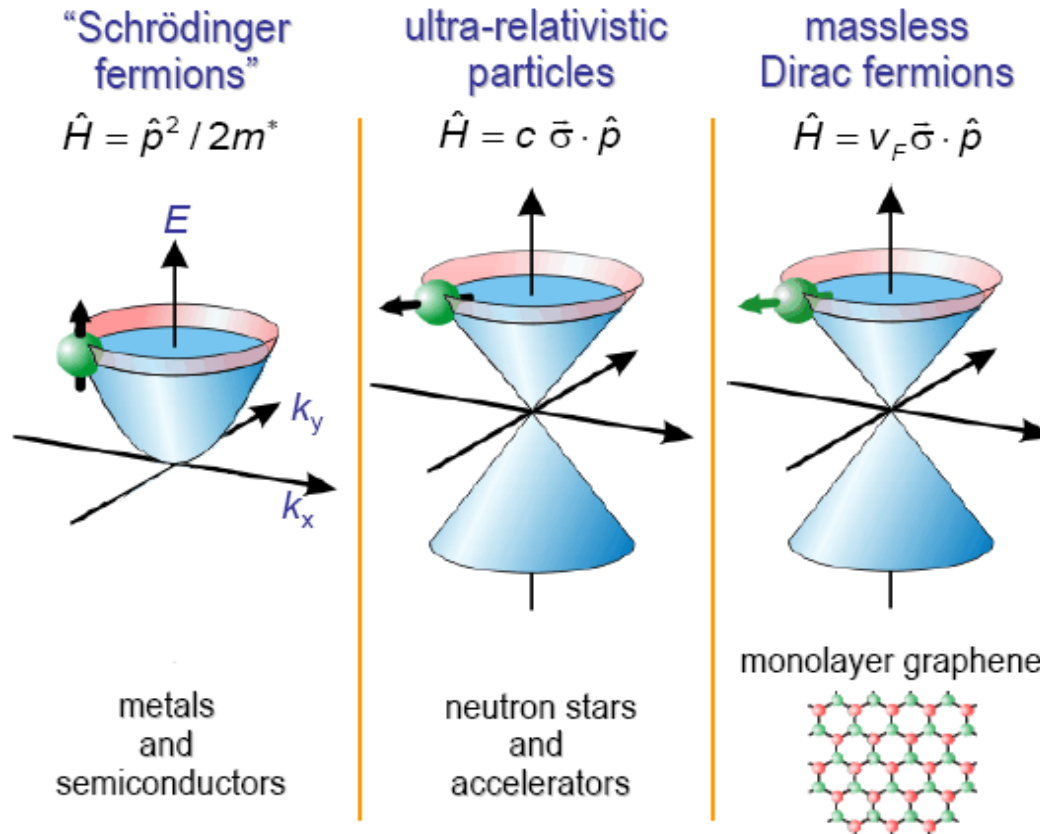
**for conduction band electrons,**

$$\vec{\sigma} \cdot \vec{n} = 1$$

**valence band ('holes')**

$$\vec{\sigma} \cdot \vec{n} = -1$$

It is due to symmetry of the honeycomb lattice



$$v_F = c / 300 = 10^6 \text{ m/s}$$

# Eigenfunctions

$$\psi = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$$

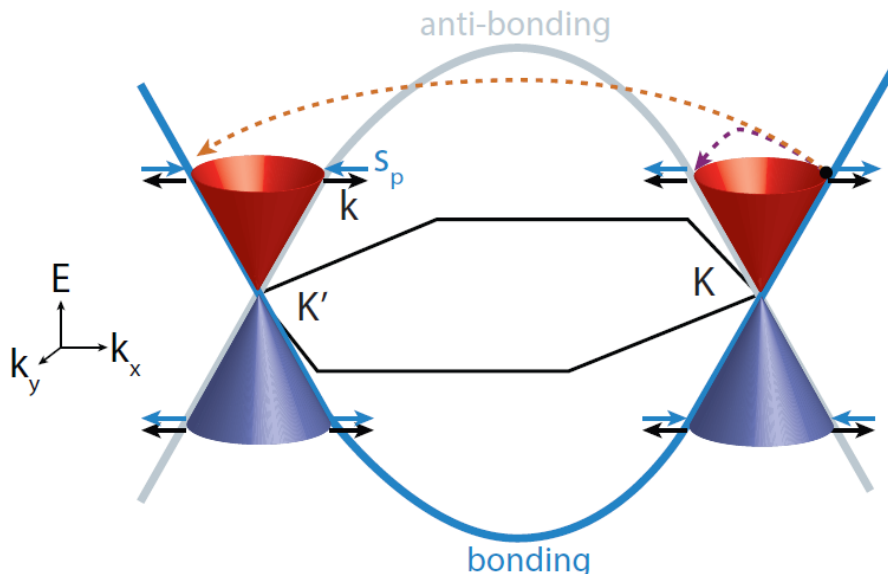
Effective Hamiltonian in K/K' valley ( $\xi = \pm$ ):

$$H = v_F \begin{pmatrix} 0 & \xi p_x - ip_y \\ \xi p_x + ip_y & 0 \end{pmatrix} = v_F p \begin{pmatrix} 0 & \pm e^{\mp i\varphi} \\ \pm e^{\pm i\varphi} & 0 \end{pmatrix} = v_F \boldsymbol{\sigma} \mathbf{p} \quad \sigma = \begin{pmatrix} \xi \sigma_x \\ \sigma_y \end{pmatrix}$$

$$E_{e/h} = \pm v |\mathbf{p}| \quad \psi_e(\varphi) = \frac{1}{\sqrt{2}} e^{ikr} \begin{pmatrix} e^{\mp i\varphi/2} \\ e^{\pm i\varphi/2} \end{pmatrix} \quad \psi_h(\varphi) = \frac{1}{\sqrt{2}} e^{ikr} \begin{pmatrix} e^{\mp i\varphi/2} \\ -e^{\pm i\varphi/2} \end{pmatrix}$$

$\varphi = \arctan(p_y/p_x)$   
Inverts for opposite momentum

In K valley conduction band  $\mathbf{k}$  parallel to pseudospin, in valance band it is opposite. It inverts in K valley. This prevents backscattering: pseudospin is conserved. Intervalley scattering needs large momentum.

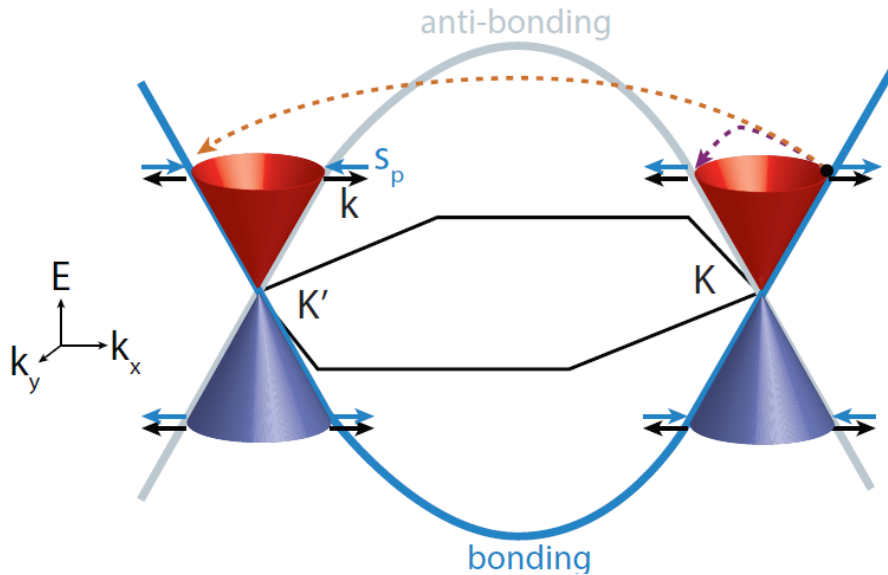


e.g.  $p_y = 0$ ,  $\psi_{B,K}(\varphi) = \frac{1}{\sqrt{2}} e^{ikx} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$   
 $\psi_{AB,K}(\varphi) = \frac{1}{\sqrt{2}} e^{-ikx} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$

Helicity eigenfunctions with  $\pm 1$  eigenvalues  $\psi_{B,K/K'}(\varphi)$  is an eigenfunction of  $\vec{\sigma}$  with  $\pm 1$  in K/K' valleys (blue arrows)  $\rightarrow$  P/AP to momentum (black arrows)

Same for anti-bonding wave-functions

# Eigenfunctions



If the scattering potential is pseudo-spin conserving, i.e. it does not contain  $\sigma$ :

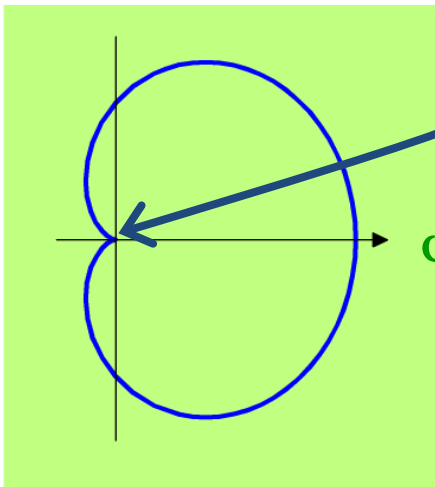
$$|\langle \psi(\phi) | V | \psi(\phi = 0) \rangle|^2 = |V|^2 |\langle \psi(\phi) | \psi(\phi = 0) \rangle|$$

$$\psi_{e,K}(\phi) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\phi/2} \\ e^{i\phi/2} \end{pmatrix}$$

$$\psi_{e,K}(\phi = 0) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$|\langle \psi(\phi) | \psi(\phi = 0) \rangle|^2 \sim \cos^2(\phi/2)$$

Scattering angular distribution



**under pseudospin conservation, helicity suppresses backscattering in a monolayer**

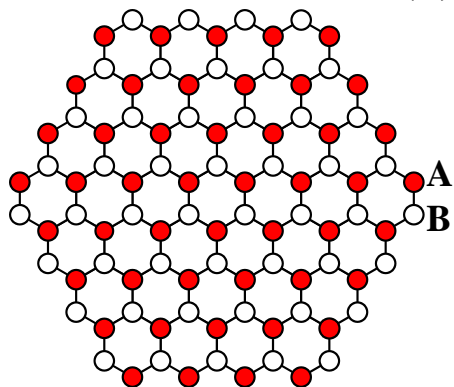
Since pseudo-spin is conserved intravalley backscattering is prohibited.

For intervalley scattering large momentum – atomic defects are required.

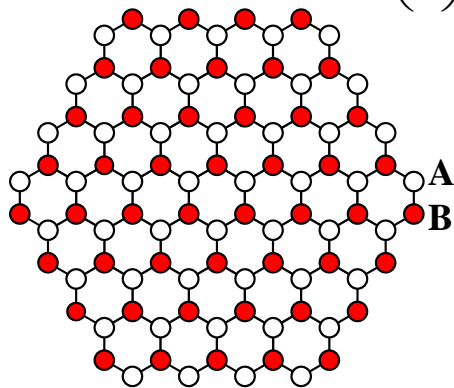
# Pseudospin

Visualization of the phase of the pseudospin on lattice

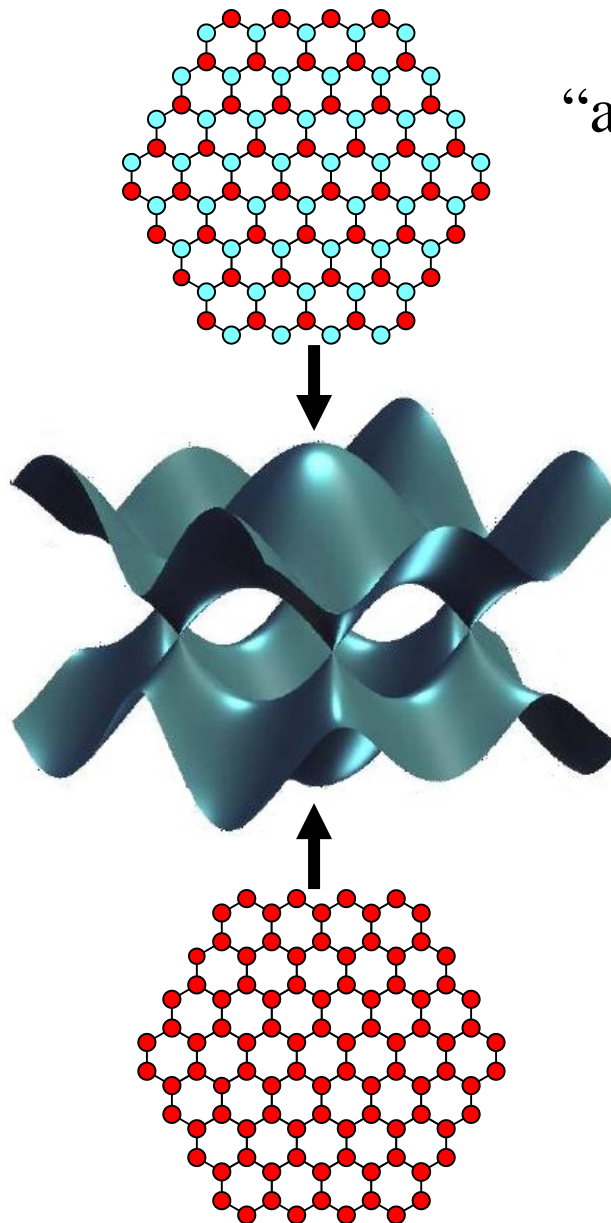
$$F_A(r), \text{ or } \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$



$$F_B(r), \text{ or } \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$



$\Gamma$  point:  
 $k = 0$



“anti-bonding”

$$E = +\gamma_0$$

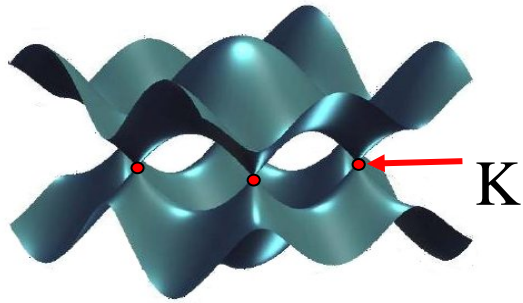
$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

“bonding”

$$E = -\gamma_0$$

$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

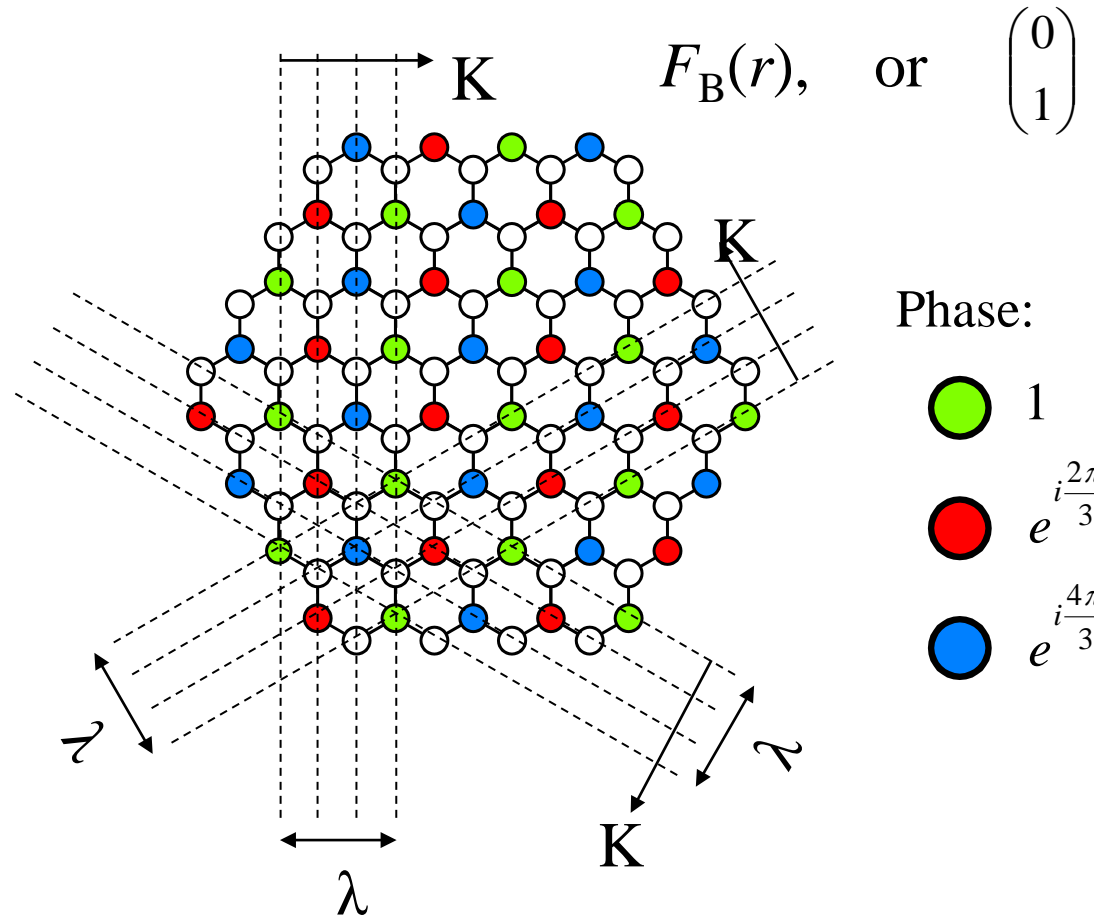
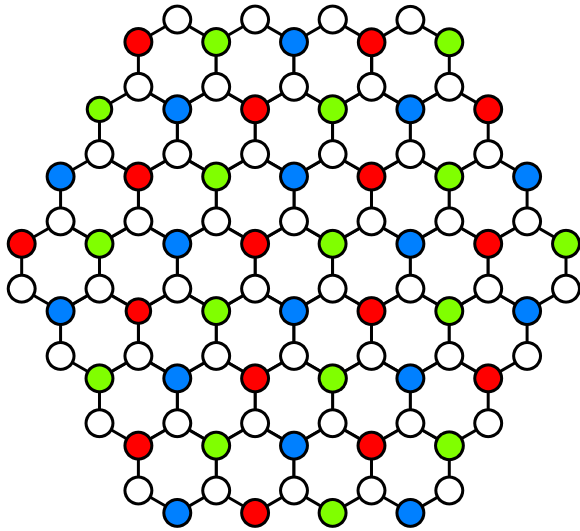
# Pseudospin



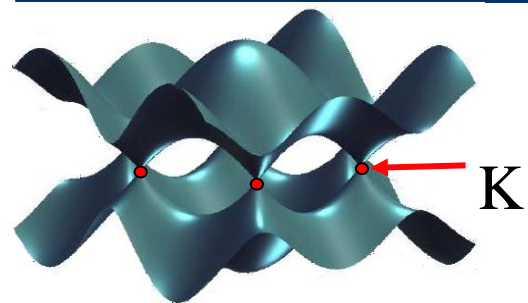
$$|\mathbf{K}| = \frac{4\pi}{3a} \longrightarrow \lambda = \frac{3a}{2}$$

The phase modulates on the lattice on short length scale due to  $e^{iKx}$  phase of the wavefunction

$$F_A(r), \text{ or } \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

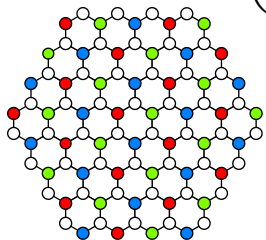


# Pseudospin

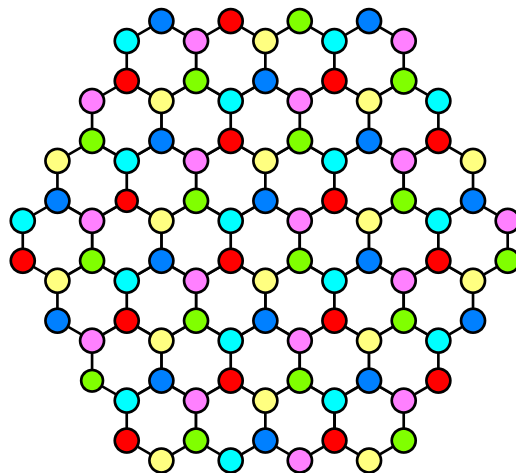
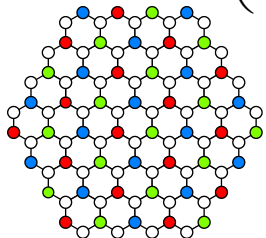


$$|\mathbf{K}| = \frac{4\pi}{3a} \longrightarrow \lambda = \frac{3a}{2}$$

$$F_A(r), \text{ or } \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$



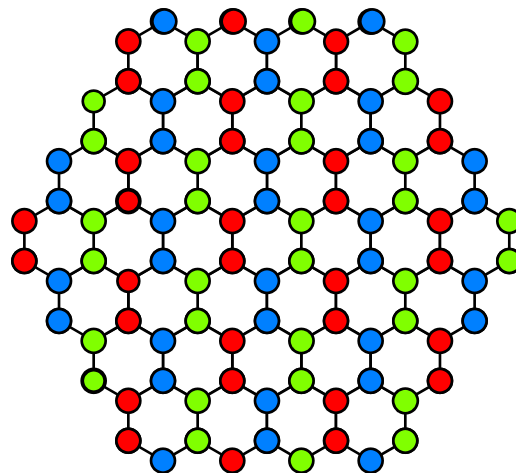
$$F_B(r), \text{ or } \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$



“anti-bonding”

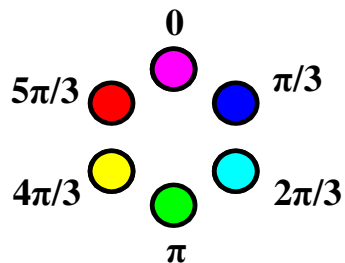
$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

**K** point:  
Bonding and anti-bonding  
are degenerate!



“bonding”

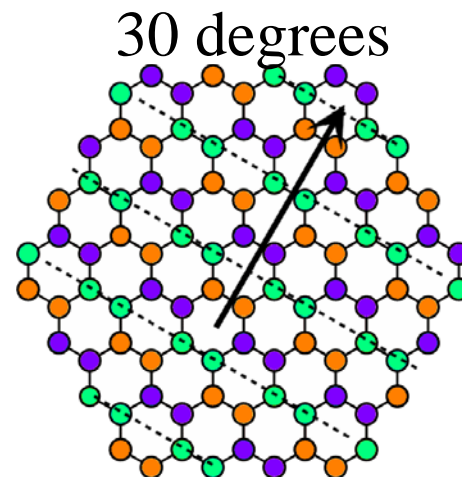
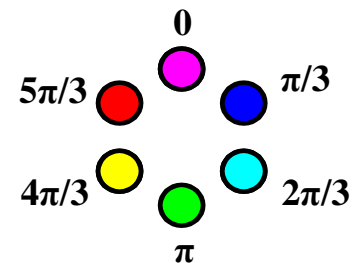
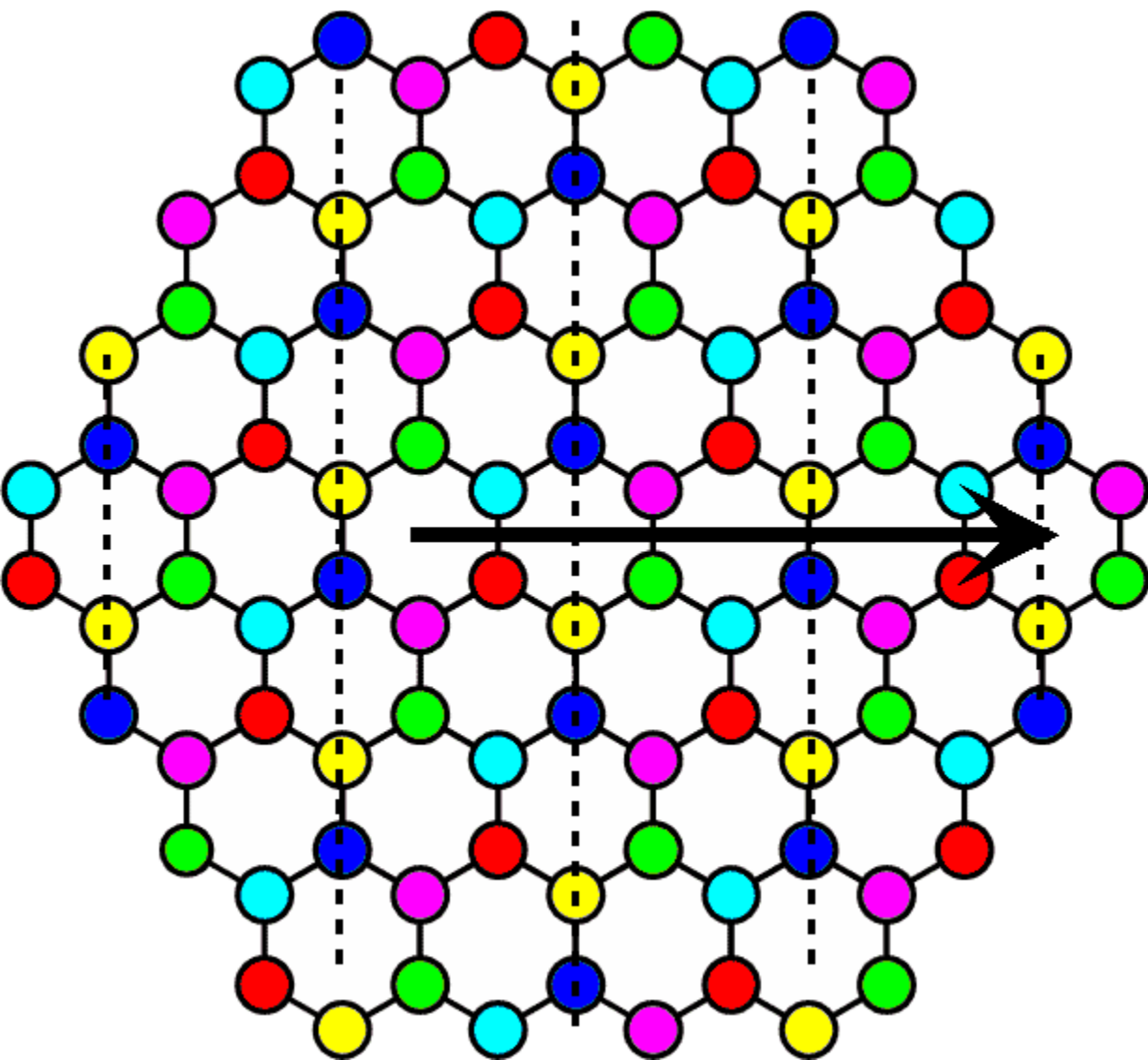
$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$



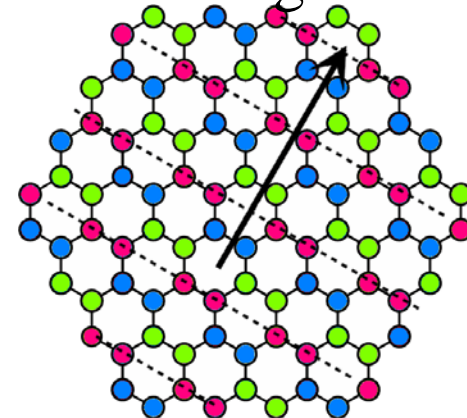
Visualization of the phase of  
the pseudospin on lattice



# Pseudospin



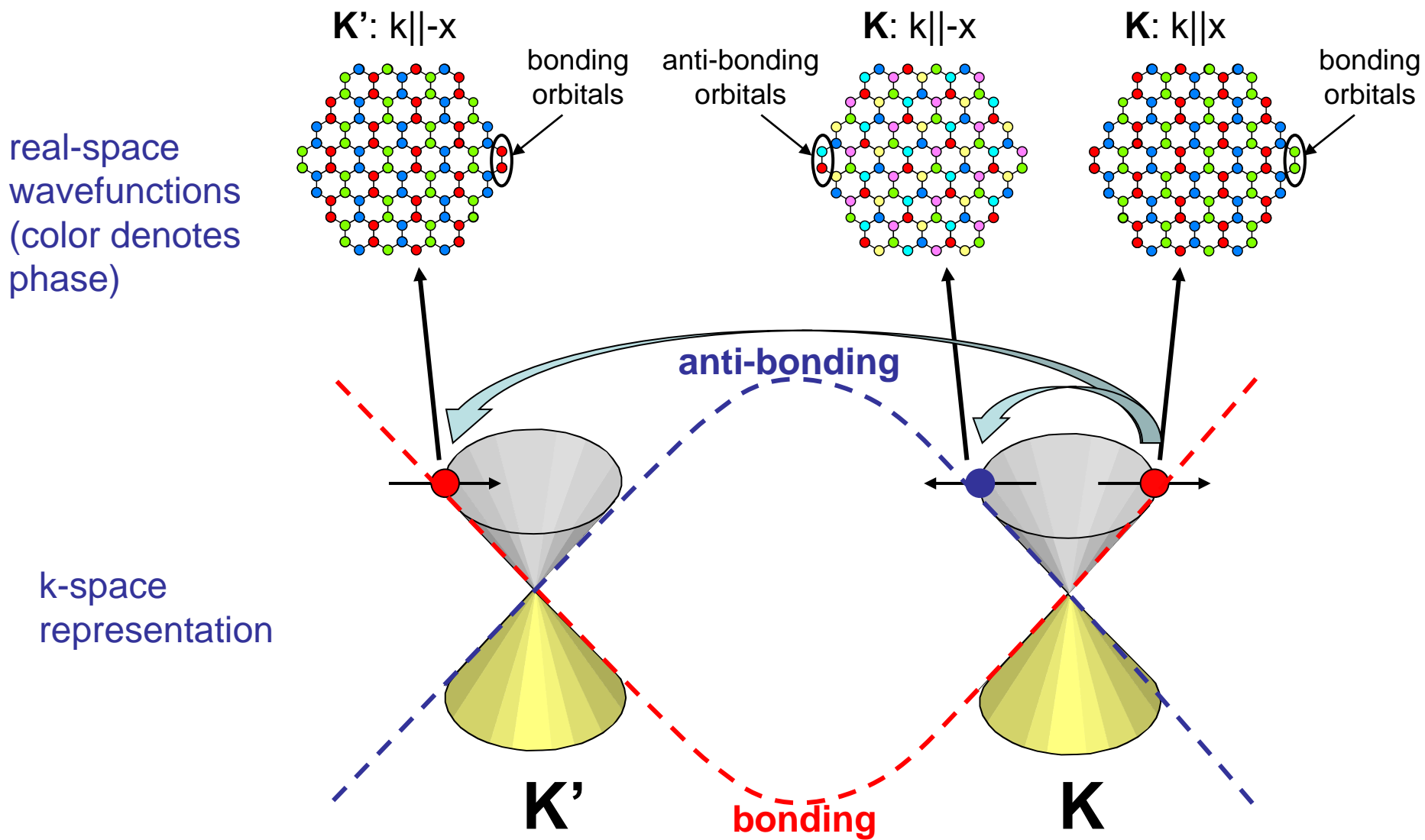
30 degrees



390 degrees

360 rotations does not give the same!

# Pseudospin



Intervalley: just a mirroring of phases, intravalley scattering should change relative amplitude on A and B

# Basic transport properties

## Measurement:

Graphene (blue) is etched to a Hall bar shape and contacted by metal leads (yellow). Si layer is doped, used as a backgate (G). By applying voltage on G the chemical potential of graphene can be varied.

Effect of gate voltage,  $V_g$ ?

$$N = C_g V_g / e \rightarrow n \sim V_g \rightarrow k_F \sim \sqrt{V_g}$$

## Drude model:

$$v_d \equiv \mu E, j \equiv env_d = en\mu E = \sigma E, \sigma = en\mu$$

$$\sigma = 1/\rho = \frac{e^2 n \tau}{m}, \quad \mu = \frac{e \tau}{m}, \quad R_H = \frac{V_y}{I} = \frac{E_y}{j_x} = -\frac{B}{ne}$$

Measurement of Hall resistance allows to determine  $n$ .

Combining it with  $\rho$ ,  $\mu$  can be derived.

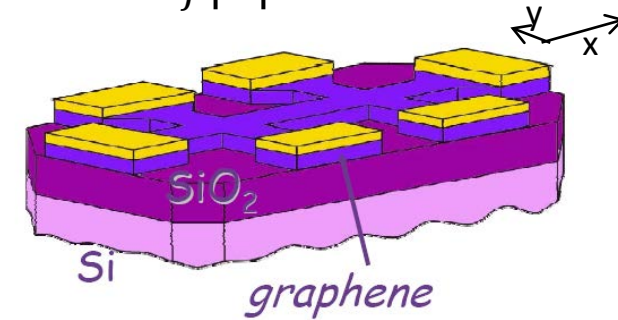
Fig. a: longitudinal resistance vs.  $V_g$ ,  $\Delta R \approx 100$  times!

Fig. b: mobility and charge carrier density vs.  $V_g$

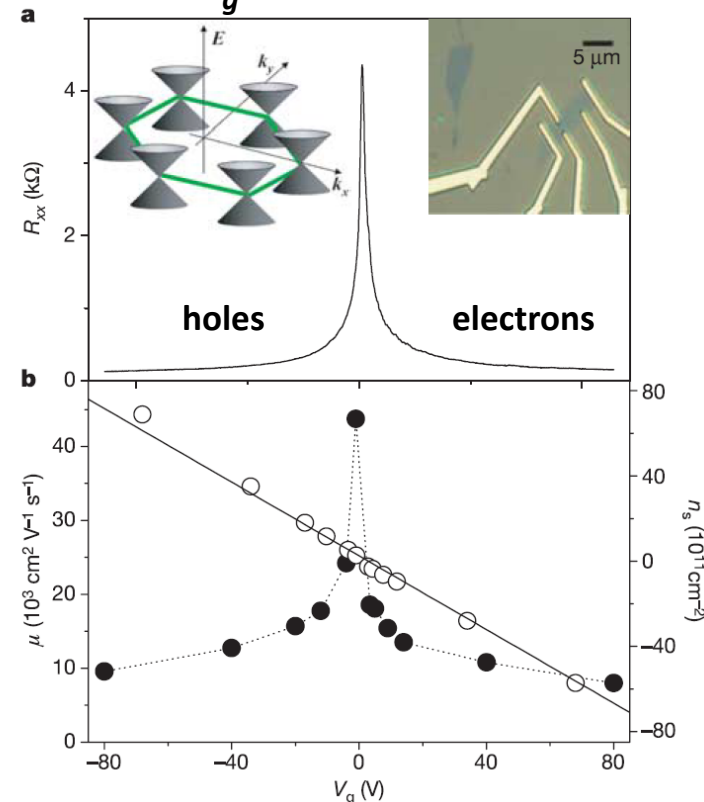
- At  $V_g = 0$ ,  $R_H$  (and  $n$ ) changes sign  $\rightarrow$  border between e and h bands

- If  $V_g \rightarrow 0$   $R \nearrow$ , however  $R$  is finite ( $\approx 4$  kOhm) at Dirac point although  $n=0$ . (No real OFF state.)

$$E = \pm \hbar v_f |\vec{k}|$$



## $R$ vs. $V_g$ characteristics



Nature **438**, 201 (2005)

# High-quality graphene structures - suspension

**Problem: charge traps in SiO<sub>2</sub> substrate decreases mobility of graphene** at low temperature (at high T phonons also play a role)

To improve mobility, eliminate the substrate. → Suspended graphene samples

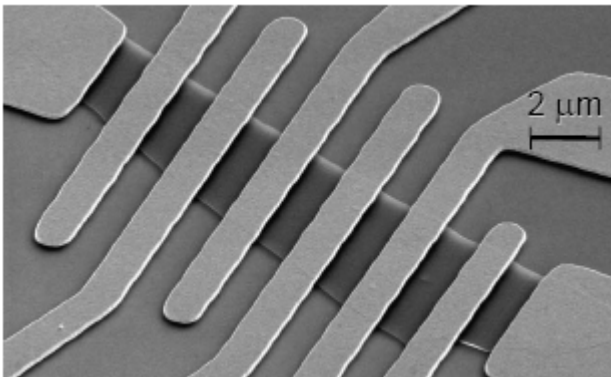
Two techniques:

- Etched SiO by BHF

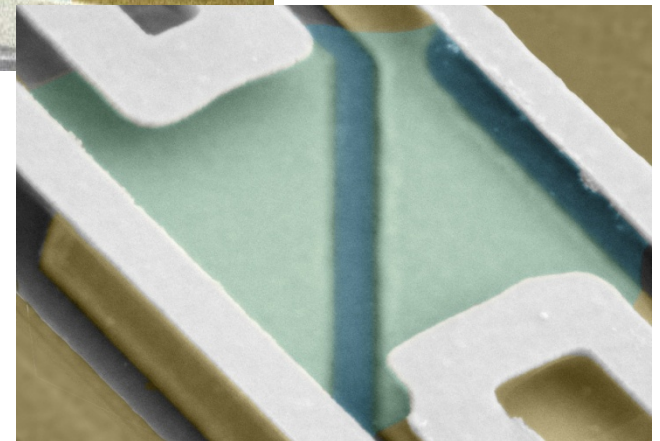
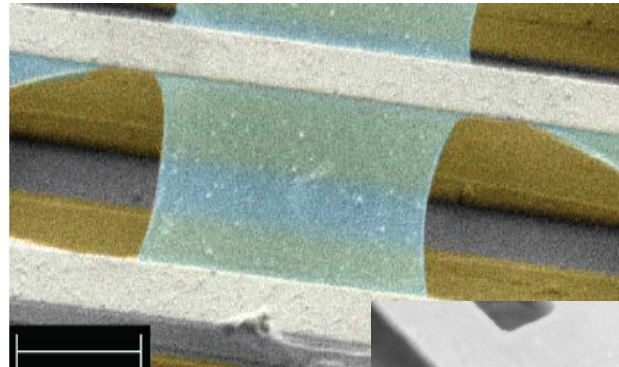
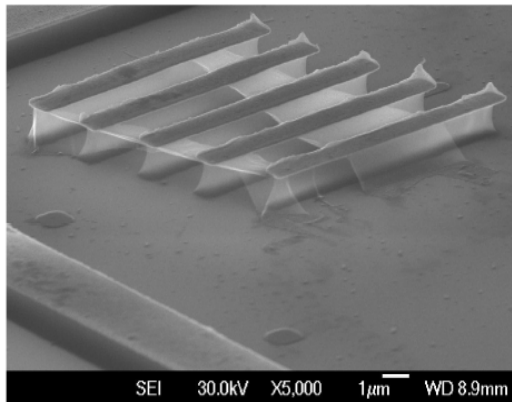
## Suspended devices

- Can have ultra-low residual disorder
- High mobility, electron optical experiments (also electro-mechanical)
- Fragile, have to be current annealed

Andrei, Kim & Yacoby  
also Manchester



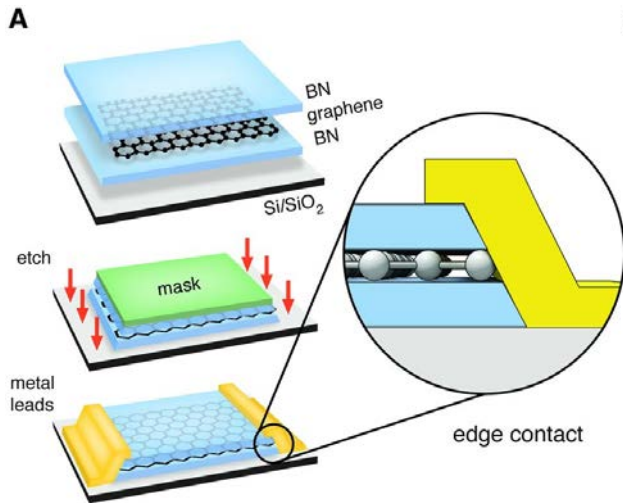
Use an organic polymer bellow, expose and dissolve



*R. Maurand, et al., Carbon 79, 486 (2014)*

N. Tombros [arXiv:1009.4213](https://arxiv.org/abs/1009.4213)

# High-quality graphene structures – hBN substrate

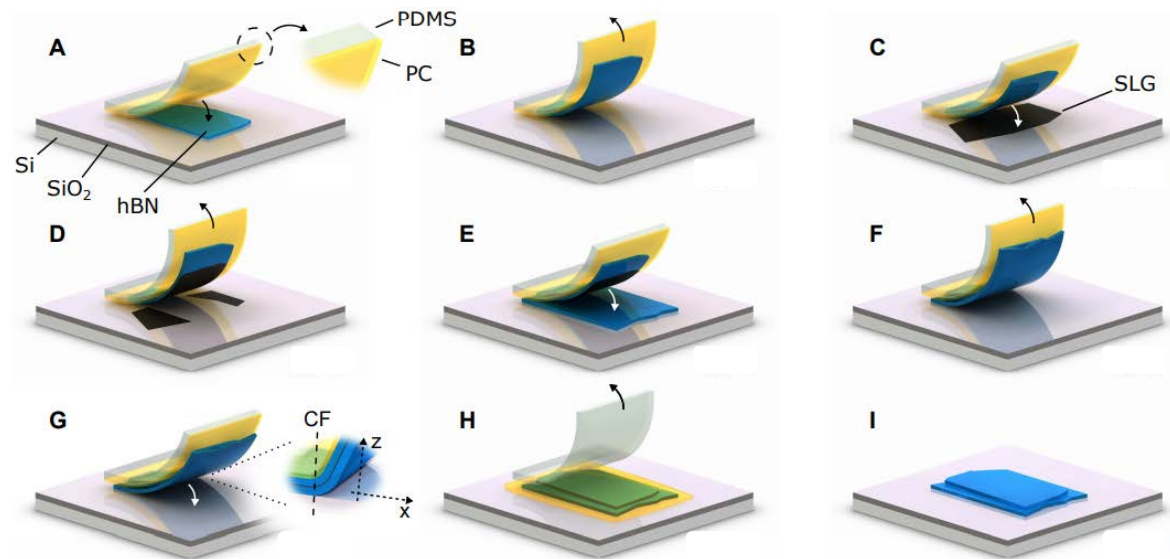
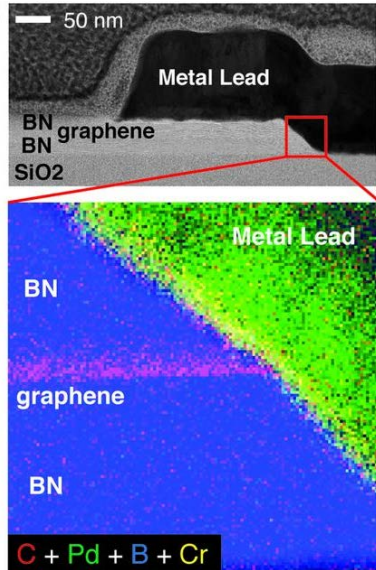


**E**

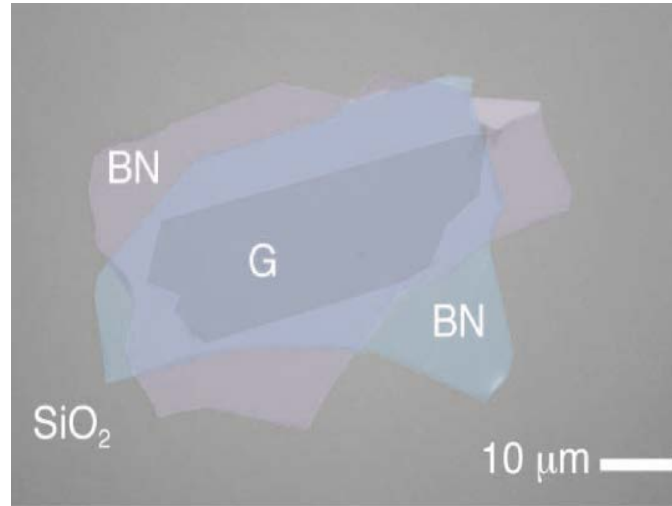
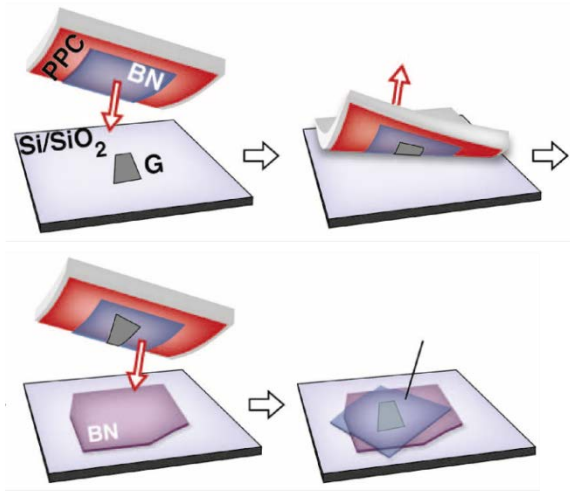
room-T mobility close to 100,000 cm<sup>2</sup>/V·s

## Advantages:

- Atomically smooth surface that is relatively free of dangling bonds and charge traps.
- Lattice constant similar to that of graphite and has optical phonon modes at large energy and has a large electrical bandgap.



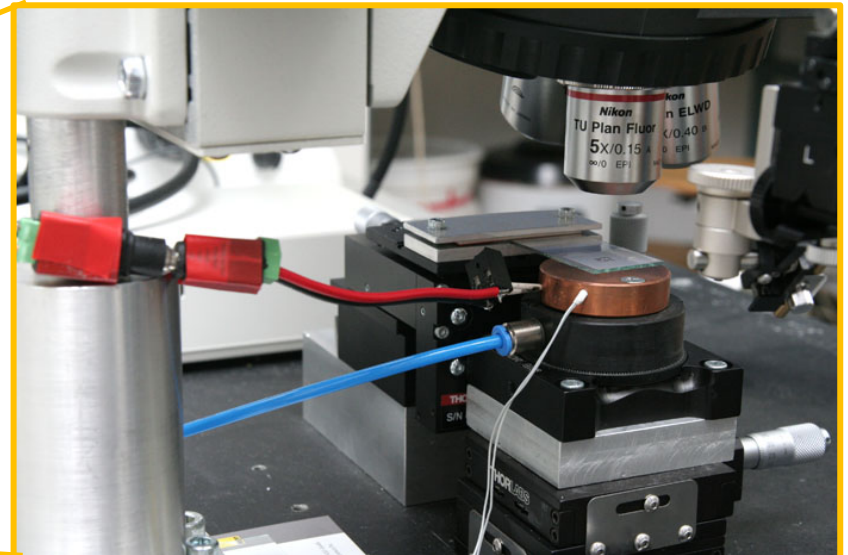
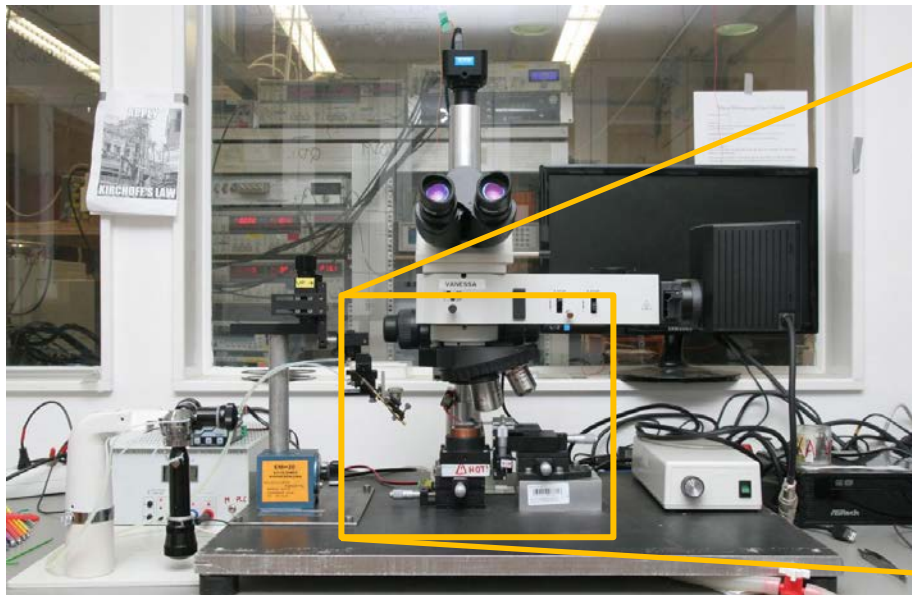
# High-quality graphene structures – hBN substrate



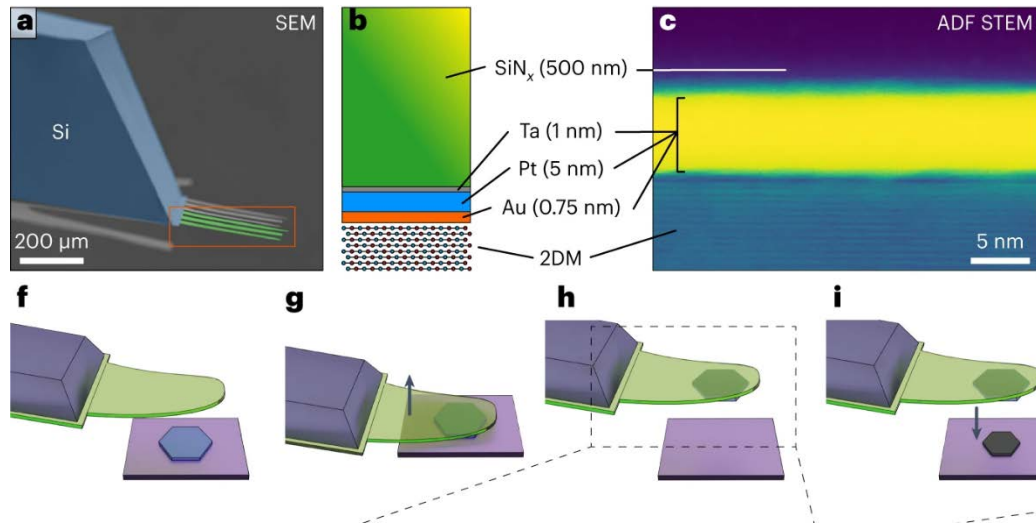
## Fabrication of encapsulated devices

- encapsulation in hBN using van der Waals pickup
- AFM to characterize the stack
- e-beam lithography and evaporation

*L. Wang et al., Science*  
342, 614 (2013)

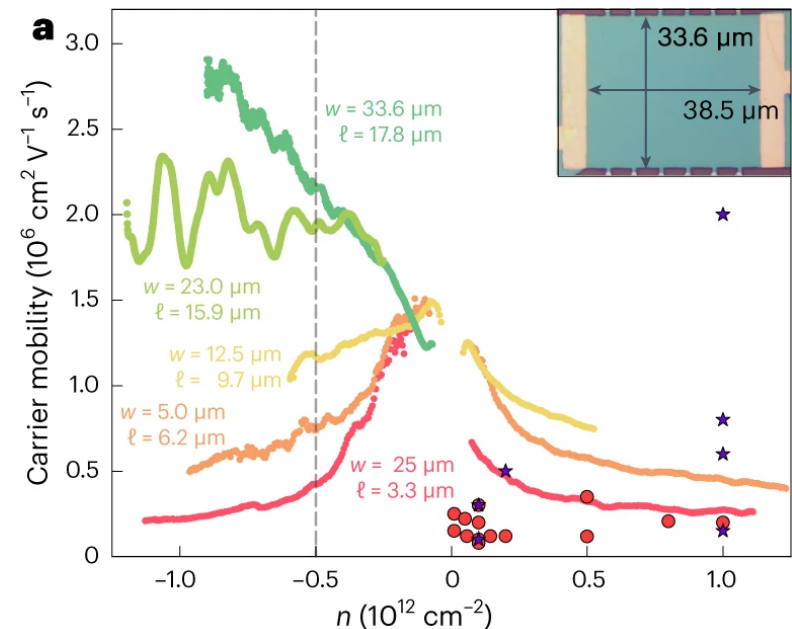


# High-quality graphene structures – hBN substrate

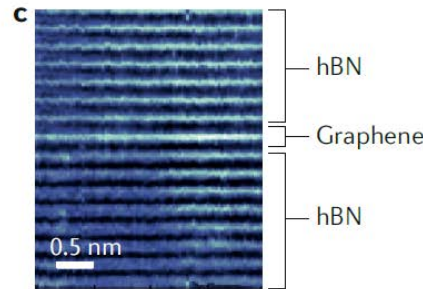
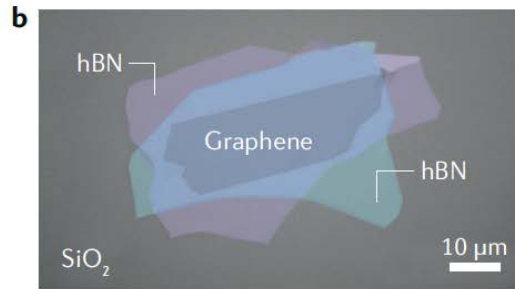
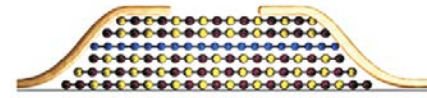
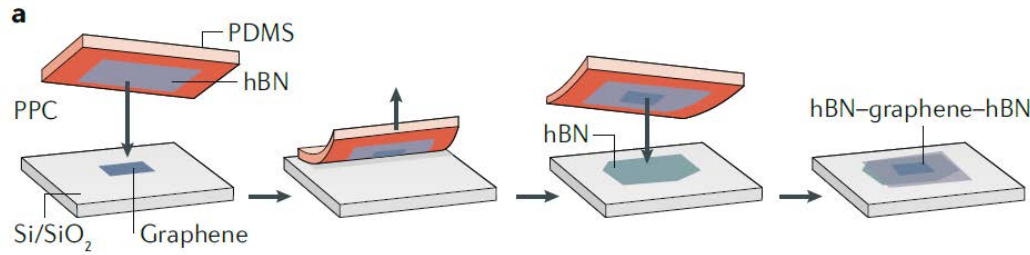


New technique with SiN<sub>x</sub> membrane

Ultra-clean assembly of devices  
Up to 20  $\mu\text{m}$  mean-free path ( $l$ ) can be achieved!

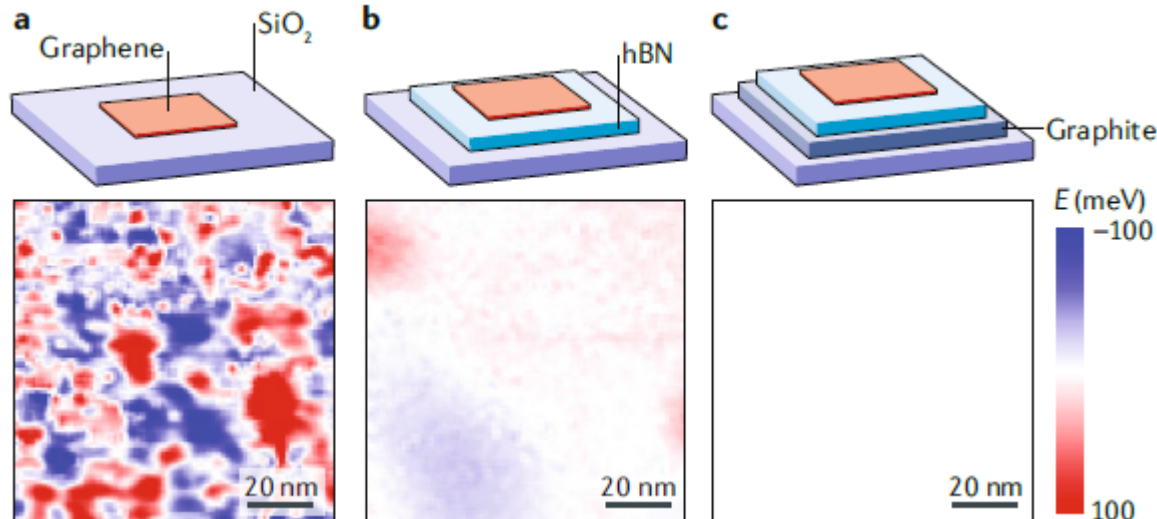


# Reduced disorder



hBN as an ideal substrate  
 Step forward: fully encapsulate graphene in hBN – high quality but hard to access – side contacts are needed  
 Clean interfaces (see next slide)

Higher quality since:  
 Reduced charge fluctuation  
 Measurement: STM spectroscopy measurement  
 Plotted is the spatial fluctuation of the CNP (measured by spectroscopy mode)  
 Graphite gate: flat surface and screens additional fluctuations



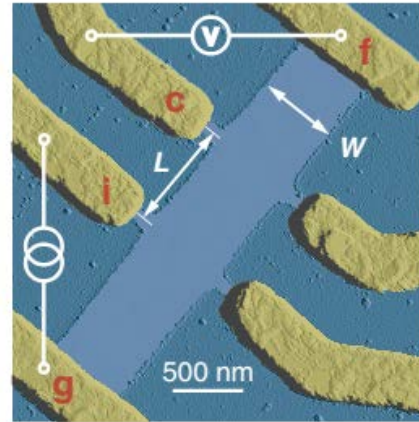


# Electron optics in graphene

High quality devices with sample size  $< L_e$   
 Ballistic electron trajectories, no scattering.  
 Similar motion as ray of light.  $\sim$  optics

## - Electrically tunable transverse magnetic focusing in graphene

Graphene stacked in hBN protection layers  
 Electron velocity and B field sets the radius of circular trajectories  
 Velocity opposite for electrons and holes (radially outward or inward, respectively)

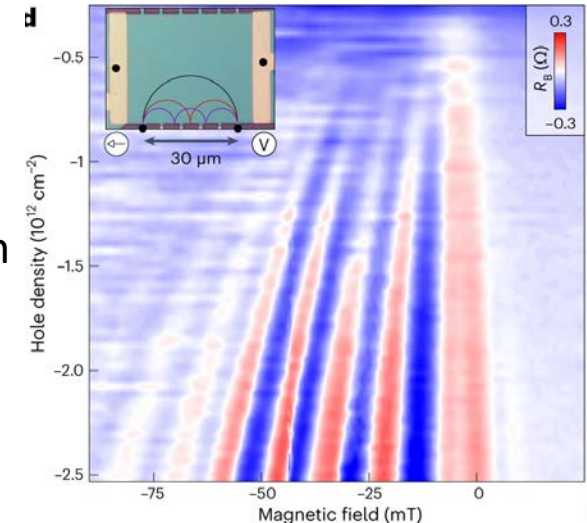
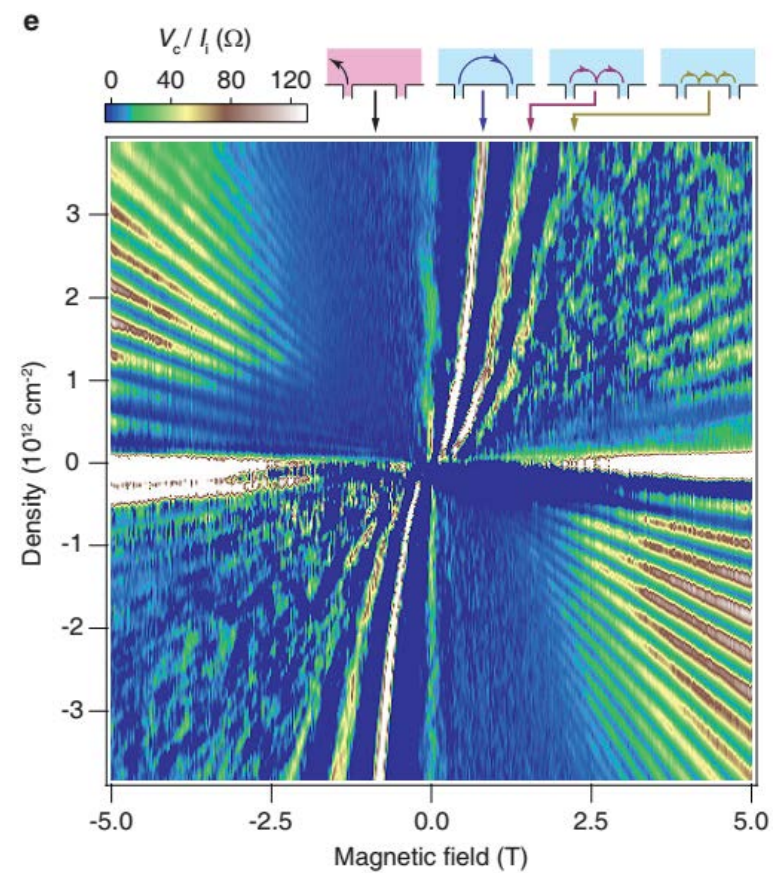


$$\dot{k} = -\frac{e}{\hbar}(E + \dot{r} \times B)$$

$$R_c = \frac{\hbar k_f}{eB} = \frac{\hbar \sqrt{n\pi}}{eB}$$

Novel, ultraclean devices: focusing on  $30 \mu\text{m}$  length scale

*W. Wang et al., Nature Electronics 6, 981–990 (2023)*



# Massless Dirac Fermions?

Consider Quasi Classical Dynamics of Dirac electrons (pos. sign)

$$\vec{v} \equiv \frac{1}{\hbar} \frac{\partial E}{\partial \vec{k}} = \frac{1}{\hbar} \hbar v_F \frac{\vec{k}}{|\vec{k}|} = v_F \vec{e}_{\vec{k}} = v_F^2 \frac{\vec{k}}{E}$$

$$\text{thus } |\vec{v}| = v_F, \vec{v} \parallel \vec{k}$$

→ Speed of e is constant independent of momentum, like photons ( $v_F \leftrightarrow c$ )

What is m, effective mass?

$$\frac{1}{m} = \frac{1}{m_{xx}} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k_x^2}$$

$$\text{For quadratic dispersion: } E = \frac{\hbar^2 k^2}{2m_{eff}}, m = m_{eff}$$

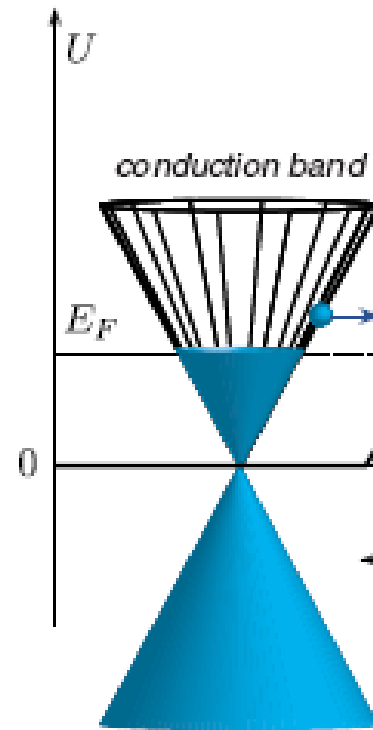
$$\text{For Dirac electrons, where } E(\vec{k}) = \hbar v_F |\vec{k}| \text{ ?}$$

Naively  $1/m = 0$ , but NOT. To calculate  $1/m$ :

$$\frac{\partial^2 |\vec{k}|}{\partial k_x^2} = \dots = \frac{k_y^2}{|\vec{k}|^3} \quad \rightarrow \quad \frac{1}{m_{xx}} = \frac{1}{\hbar} v_F \frac{k_y^2}{k^3}$$

$$\frac{\partial |\vec{k}|}{\partial k_x} = \frac{1}{2} \frac{2k_x}{|\vec{k}|} \rightarrow \text{Effective mass depends on } k$$

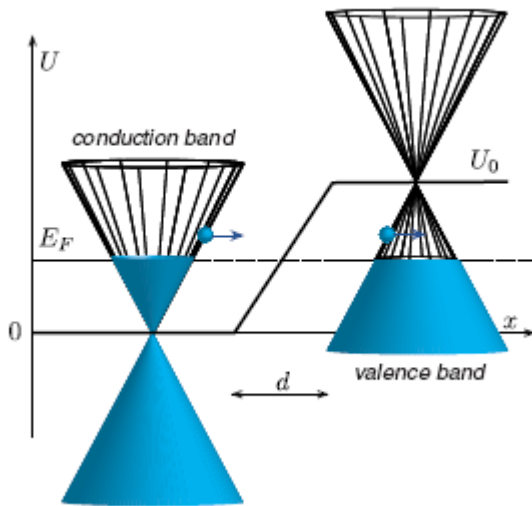
$$E = \pm \hbar v_f |\vec{k}|$$



$$\frac{1}{m_{xx}} = \frac{v_F}{\hbar} \frac{k_y^2}{|k|^3}$$

N-P junction:

Potential profile with a step of  $U_0$  at a distance  $d$



**Klein scattering:**

perfect transmission

at normal incident

This is again pseudo-spin conservation

Evolution of group velocity:

$$\frac{dv_x}{dt} \equiv \frac{1}{m_{xx}} F_x = \frac{1}{m_{xx}} (-e) E_0 \quad (*)$$

In linear electrostatic potential (e.g. slope in Figure) :

$$U = E_0 x, \quad E_x = E_0, \quad F_x = -e E_0$$

At normal incidence:  $k_y = 0 \rightarrow \frac{dv_x}{dt} = 0 \rightarrow$  backscattering is avoided. Electron can propagate through an infinite high potential barrier.

$$\hbar \dot{\vec{k}} \equiv \vec{F} = -e E_0 \vec{e}_x \quad (**)$$

Effect of the potential profile,  $U$  (see figure):

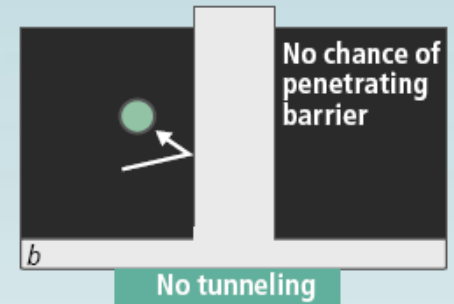
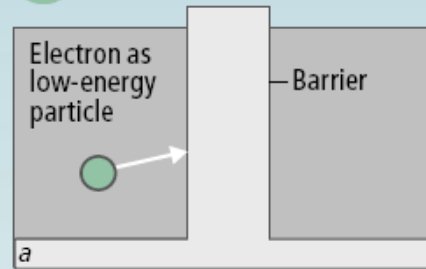
- $k$  decreases and changes sign (\*\*)
- based on (\*),  $\vec{v}$  stays constant, i.e.  $\vec{v} = v_F \vec{e}_x$ .
- $\rightarrow$  e ends up in the valence band

**Fermi surfaces**

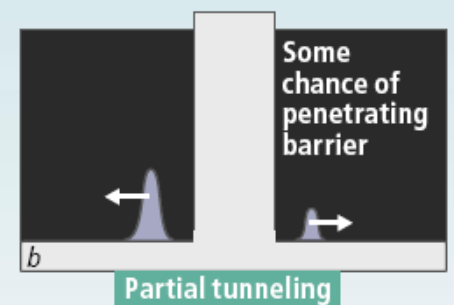
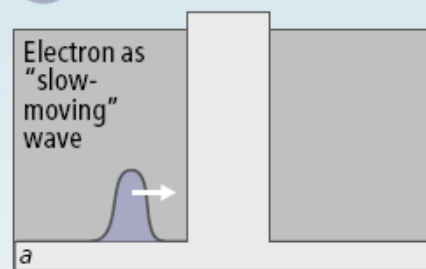
$$E = +\hbar v_f |\vec{k}| \quad \left( \begin{array}{c} \vec{v} \\ \vec{k} \end{array} \right) \quad \left( \begin{array}{c} \vec{k} \\ \vec{v} \end{array} \right) \quad E = -\hbar v_f |\vec{k}|$$

# Klein tunneling and backscattering

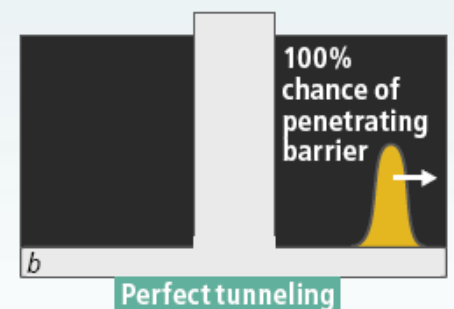
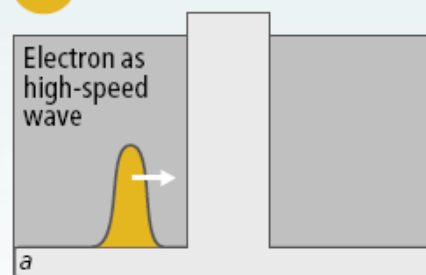
## 1 CLASSICAL PHYSICS



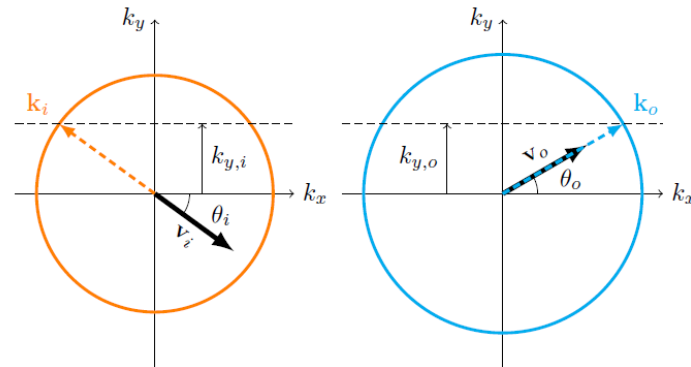
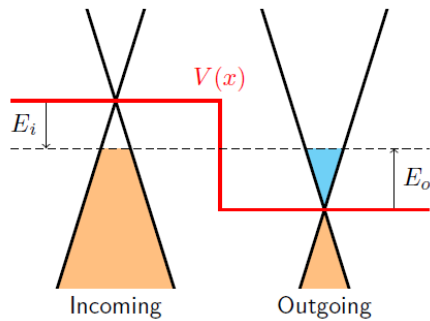
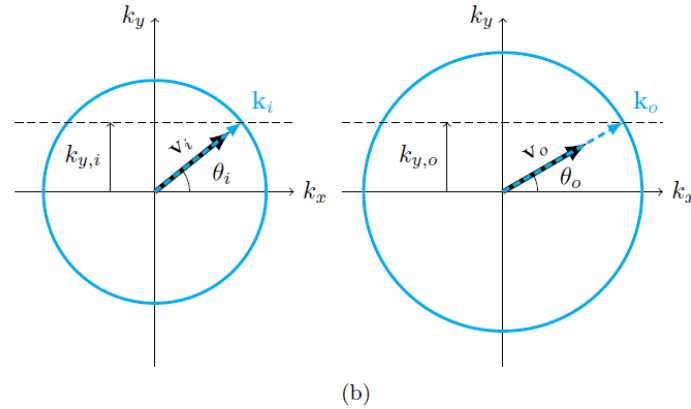
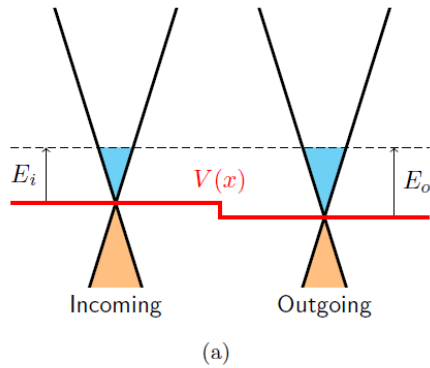
## 2 QUANTUM MECHANICS



## 3 QUANTUM ELECTRODYNAMICS



# Klein tunneling and backscattering



Electron reflection and refraction

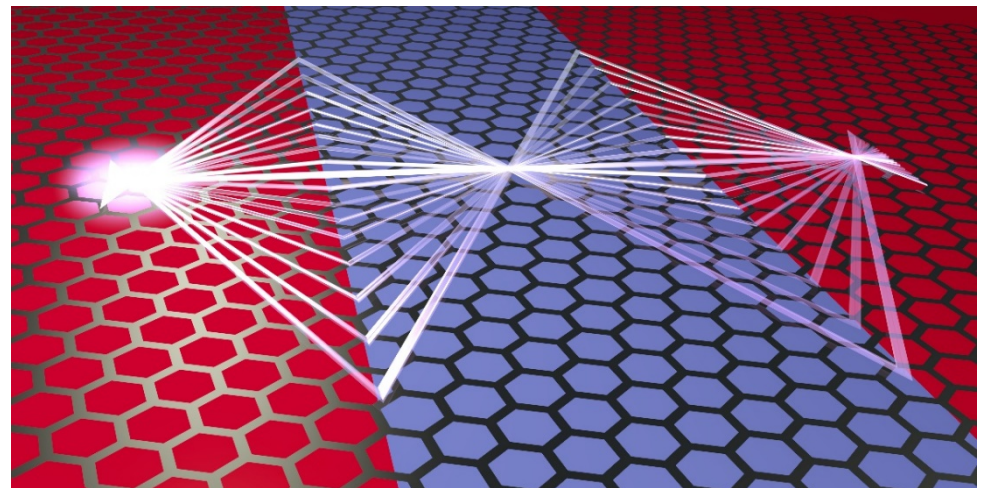
1D potential – invariant in the  $y$  direction,  $k_y$  is conserved

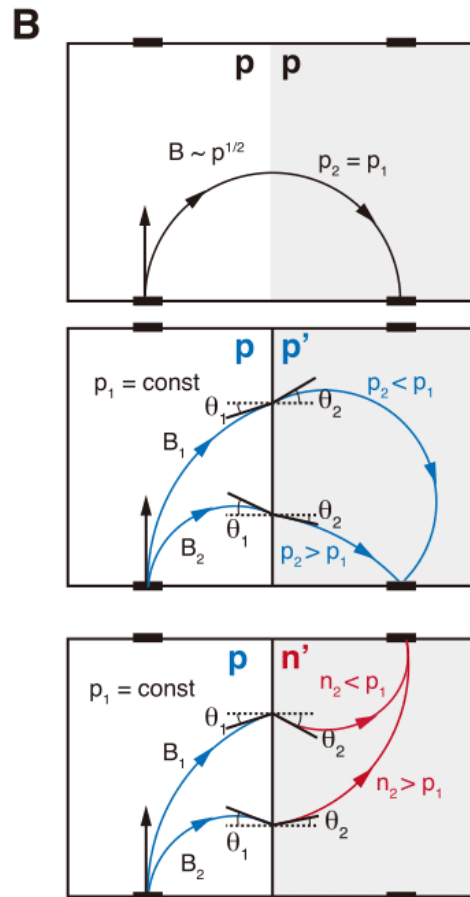
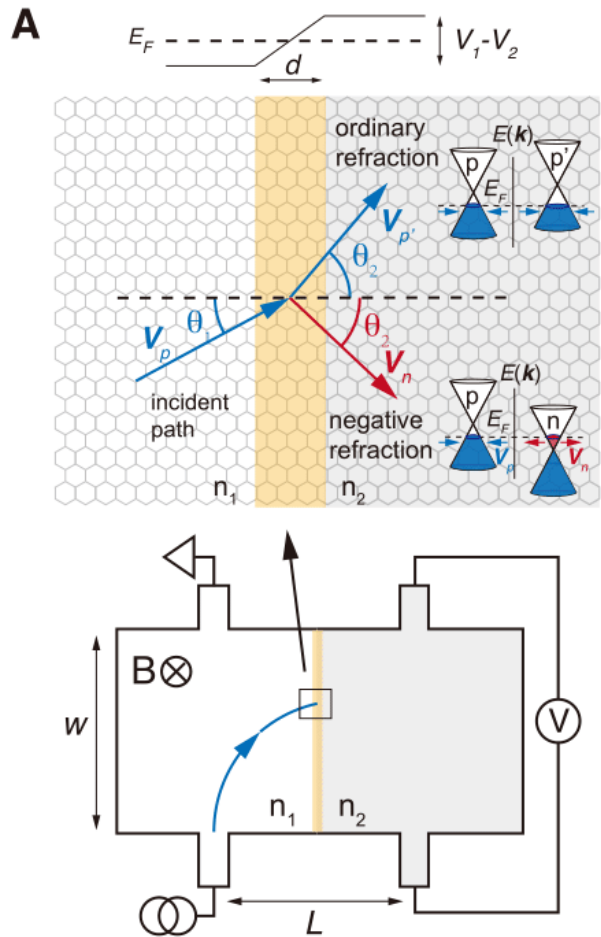
Snell's law can be derived - ratio of  $k$  vectors gives the refraction angles (densities).

For p-n junctions negative refraction!

## Idea: Veselago lens

Flat lens can be made for focusing

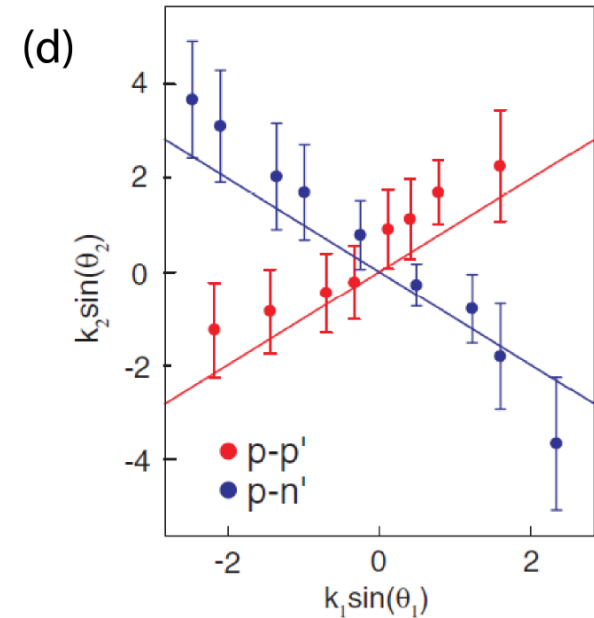




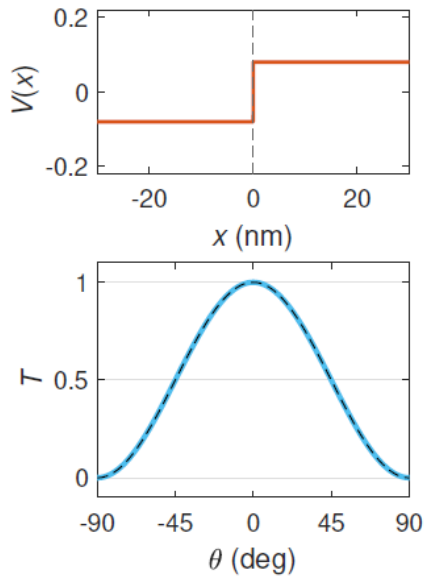
## - Negative refraction.

In p-n junctions the refraction is unconventional!

Can be seen e.g. in a focusing experiment.



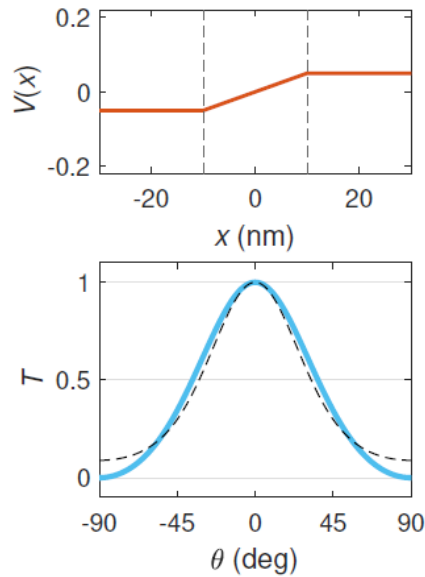
# Klein tunneling and backscattering



$$T(\theta) = \cos^2 \theta$$

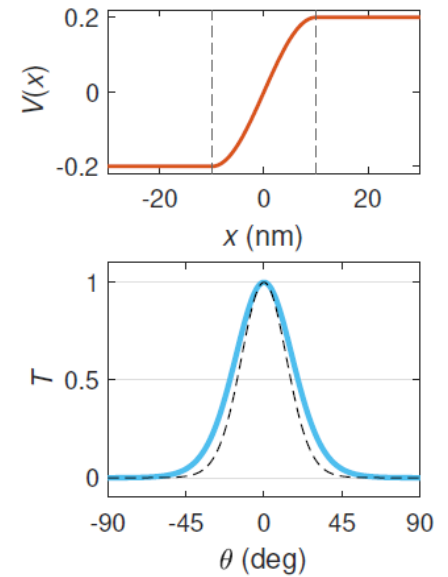
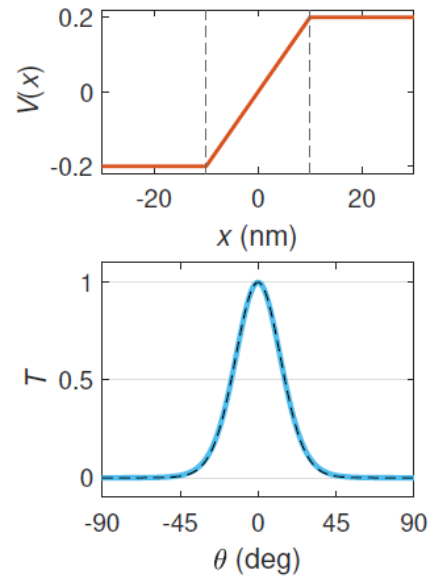
Sharp p-n junction

Smooth p-n junctions act as collimator  
(narrow angular distribution)

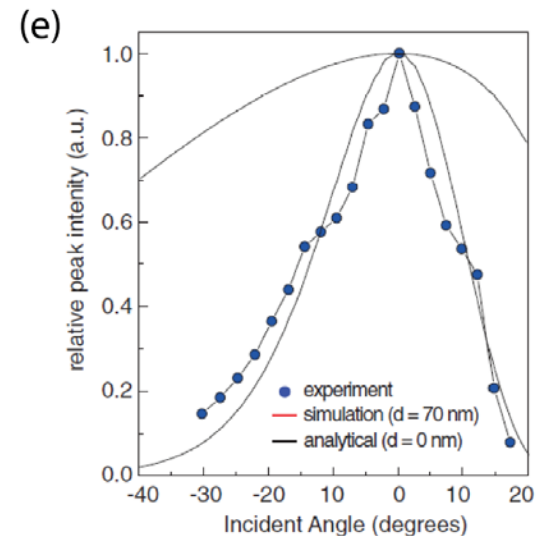


$$T(\theta) = \exp\left(-\pi \frac{k_F d}{2} \sin^2 \theta\right)$$

Smooth p-n junction



Dashed analytic,  
blue numerical



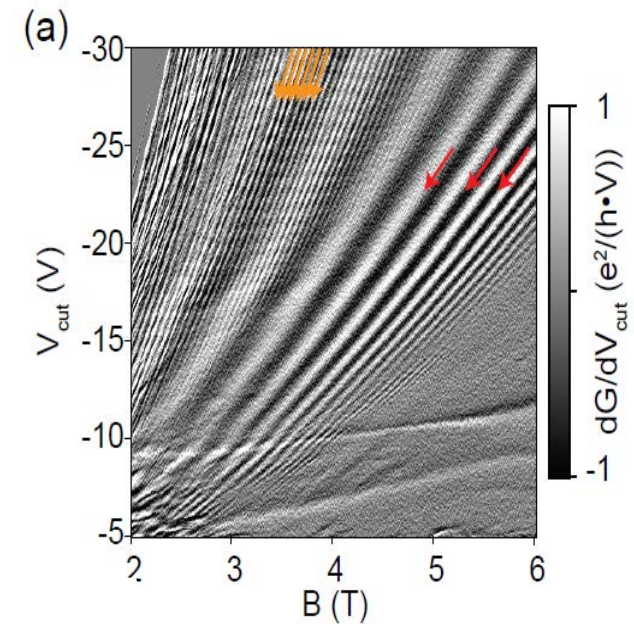
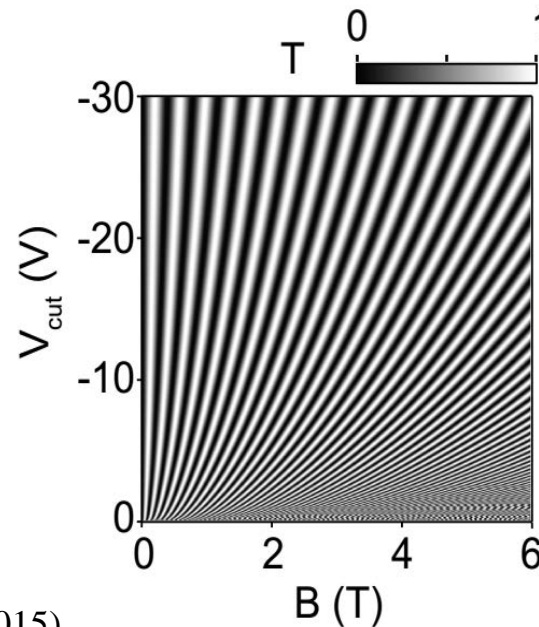
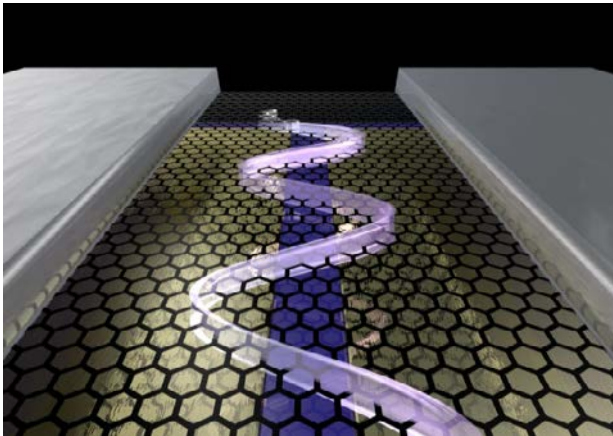
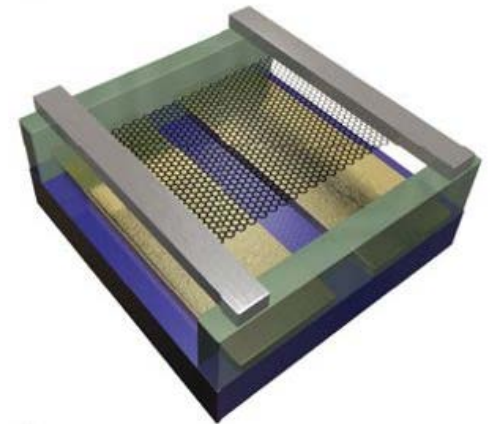
From focusing measurement  
on p-n junction:

# Snake states

Suspended graphene sample, with two gates bellow.  
 Half of the sample electron (red) and half of it hole (blue) doped.  
 Snake state propagates at the border.

$$R_C = \frac{\hbar\sqrt{n\pi}}{eB}$$

$$G(E) \sim \cos \left[ \pi \frac{W}{R_{C,p} + R_{C,n}} \right]$$



P. M., et al., PRB. 98, 035413 (2018)

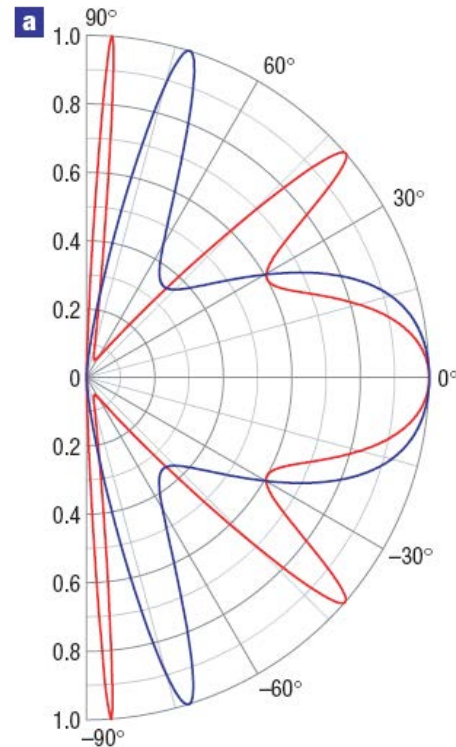
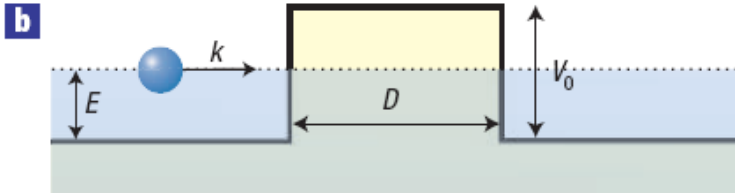
P. Rickhaus, et al. Nature Comm. 6, 6470 (2015)



# Klein tunneling and backscattering

## Result of proper calculation

Wave function matching

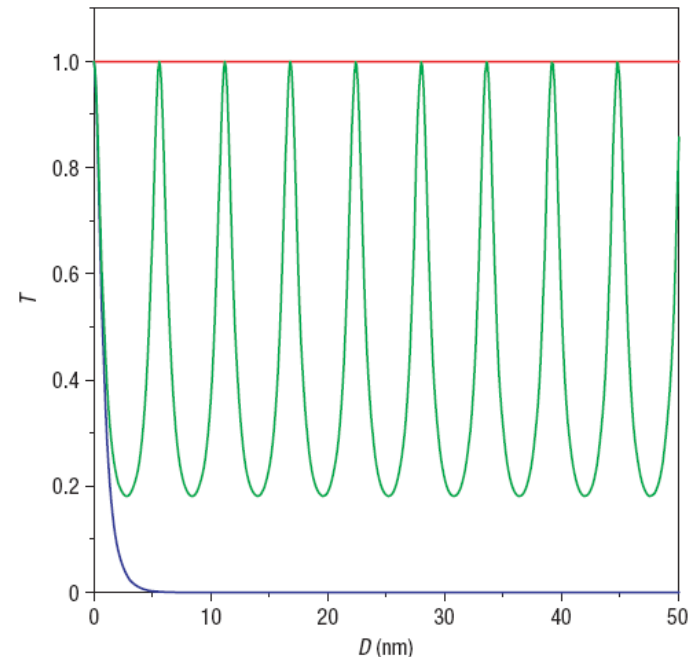


**Transmission probability T** through a 100-nm-wide barrier as a function of the incident angle, two different barrier height

## Transmission probability vs. D

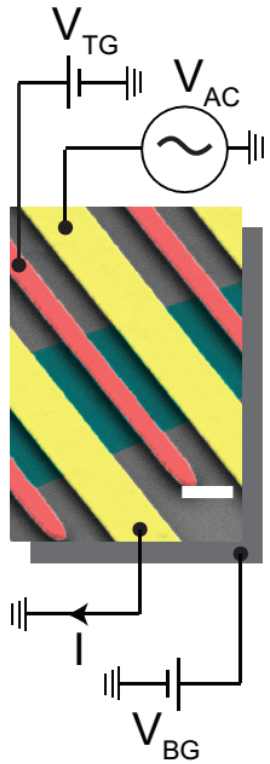
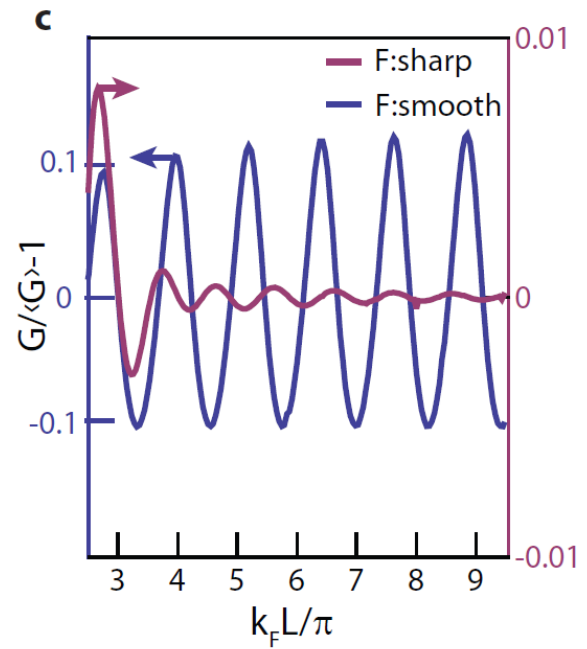
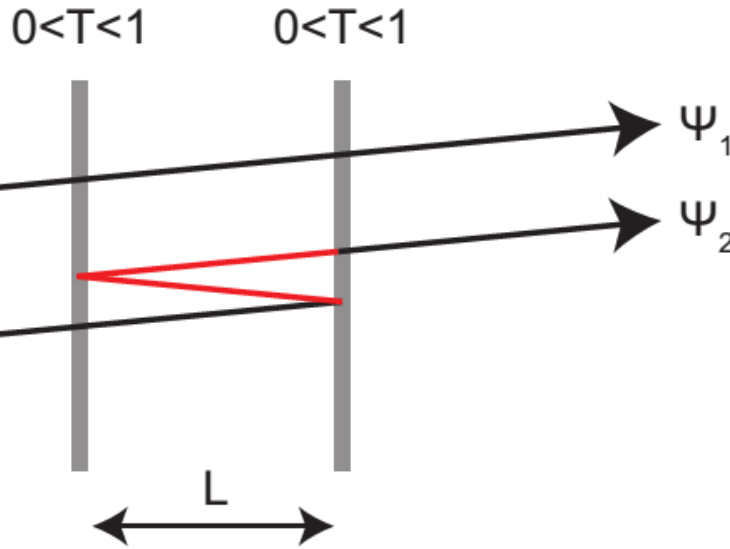
of normally incident electrons

- in single- and bi-layer graphene (red and blue curves, respectively) and in a non-chiral zero-gap semiconductor (green curve)



→ Difficult to measure whether it is 100%, since e-s out of normal incident also arrive

# Fabry-Perot interferences

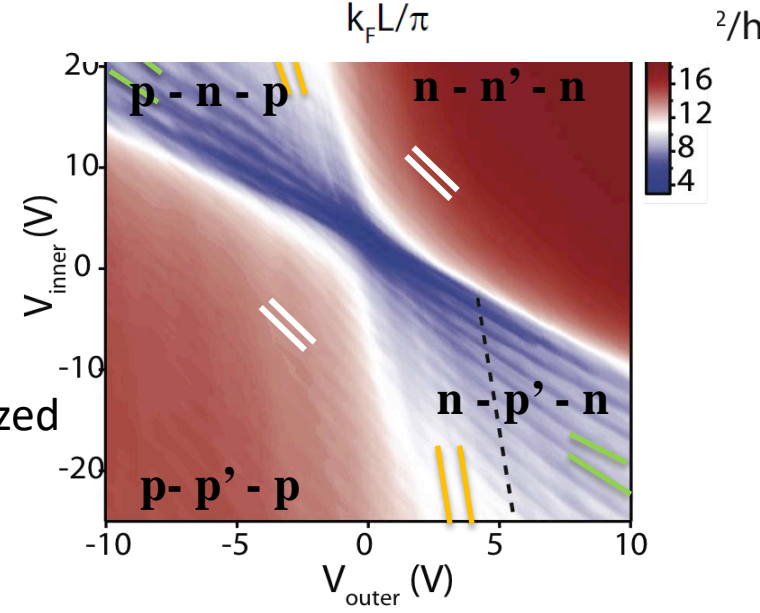


Positive interference:  

$$L = j \frac{\lambda}{2} \quad \text{where } j = 1, 2, 3, \dots$$
 For graphene:  

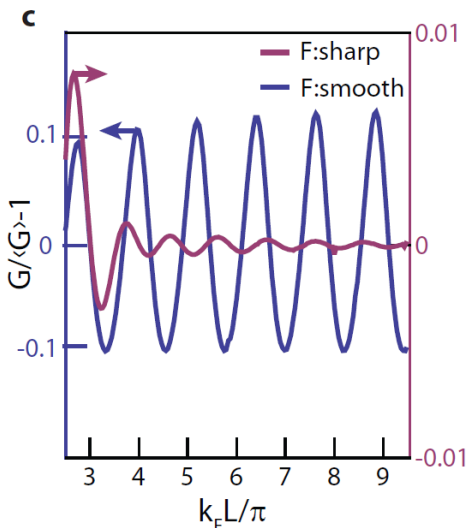
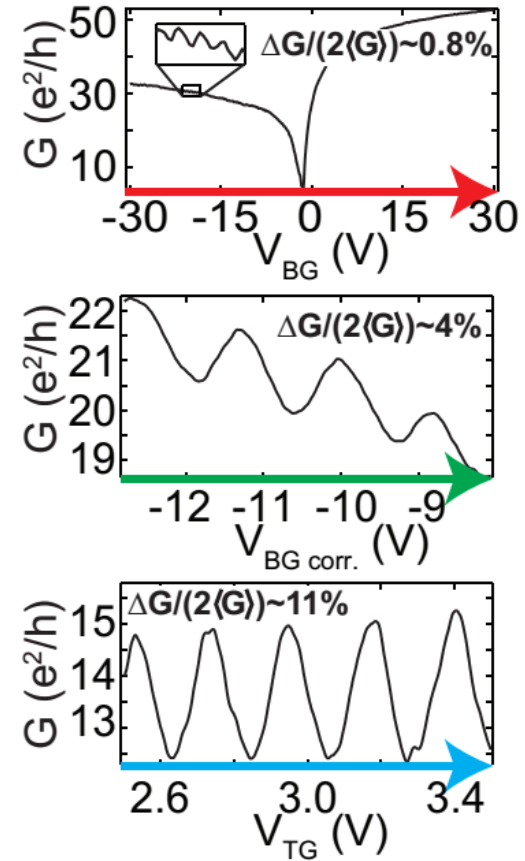
$$\lambda = \frac{2\pi}{\sqrt{n\pi}}$$

With two gate p-n-p junction can be realized  
 Lower conductance in bipolar regime.  
 Oscillations show up!



# Fabry-Perot interferences

Oscillations in  
different regimes  
Bipolar oscillations  
are the most visible  
(blue)



Filtering of trajectories: only close to perpendicular trajectories are important in the oscillation