Exotic electronic phases in graphene nanostructures

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Physics Today, 2001

1. Are there reasons why the fundamental dimensionless parameters have the values they do?
2. What role did quantum gravity play in the Big Bang?
3. What is the lifetime of the proton?
4. Is supersymmetry a broken symmetry of nature?
5. Why is spacetime apparently four-dimensional?
6. What is the value of the cosmological constant, and is it really constant?
7. Does M-theory describe nature?

REFERENCE FRAME

What's Wrong with These Questions?

N. David Mermin

6. Tell me about a collective state of matter, unimagined in the year 2000, that is as remarkable as, for example, superconductivity, superfluidity, or the fractionally quantized Hall effect seemed to be at the end of the 20th century.

Who could have imagined such phenomena in 1900? Surely the extraordinary capacity of bulk matter to behave in ways that transcend anything one could possibly have guessed from studying its constituents, will produce many comparably unimaginable things in the next 100 years.

http://phy.ntnu.edu.tw/~changmc/Teach/Translation/Mermin.pdf

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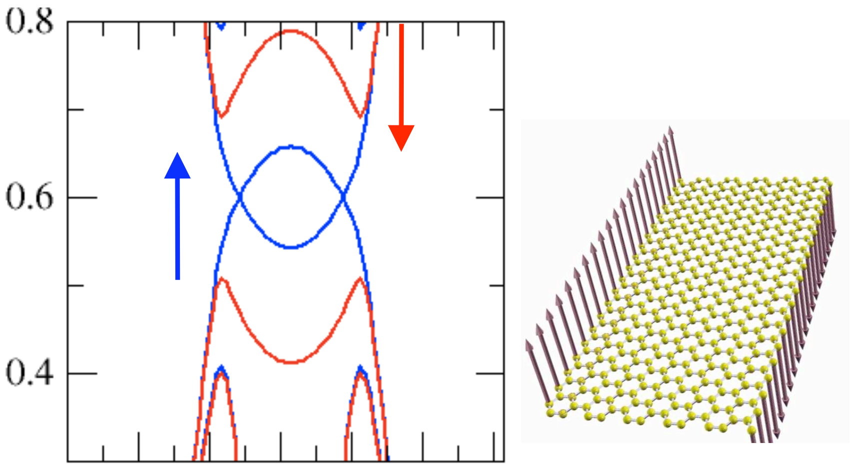
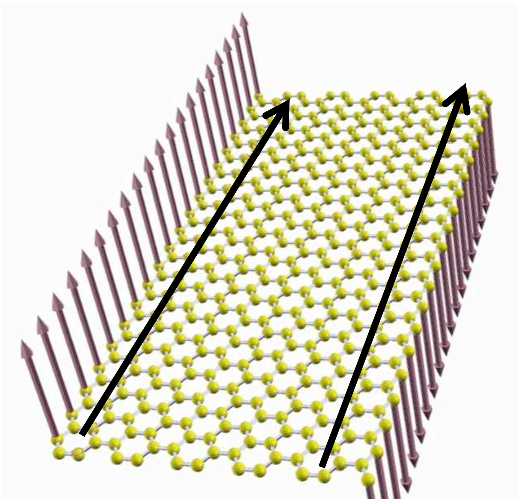
1. Intro. to Graphene
2. Exotic electronic phases in graphene nanostructures
    1. Edge Magnetism
    2. Edge magnetism with broken sublattice symmetry
    3. Graphene as a topological insulator
    4. Combined action of SO and e-e in graphene ribbons

-

AF Half metal



Persistent charge currents



Collaborators

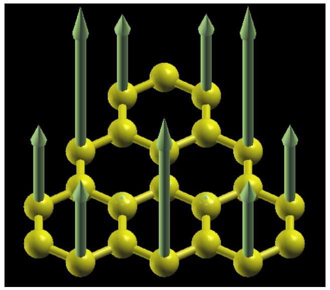
Fede Muñoz

Dani Gosalbez

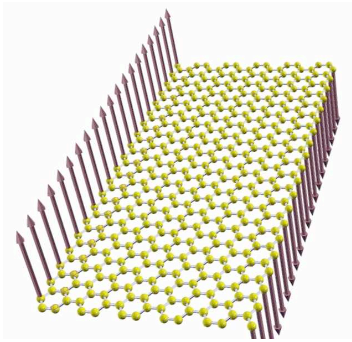
David Soriano

Juanjo Palacios

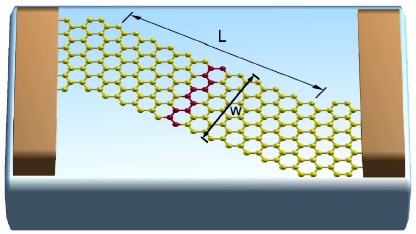
Luis Brey



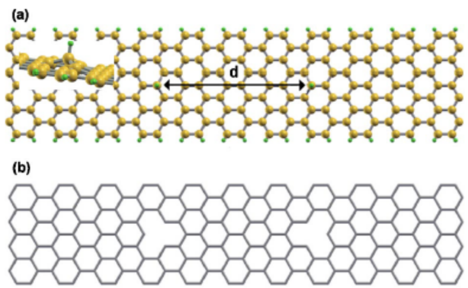
JFR, J.J. Palacios, PRL **99**, 177204 (07)



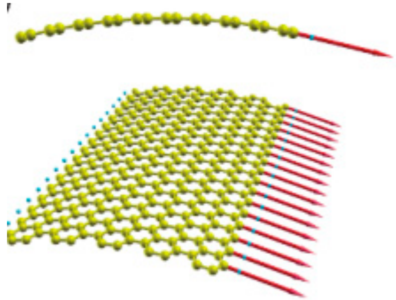
JFR, PRB **77**, 075430, (08)



F. Muñoz, JFR, J. J. Palacios PRL **102,** 136810 (09)



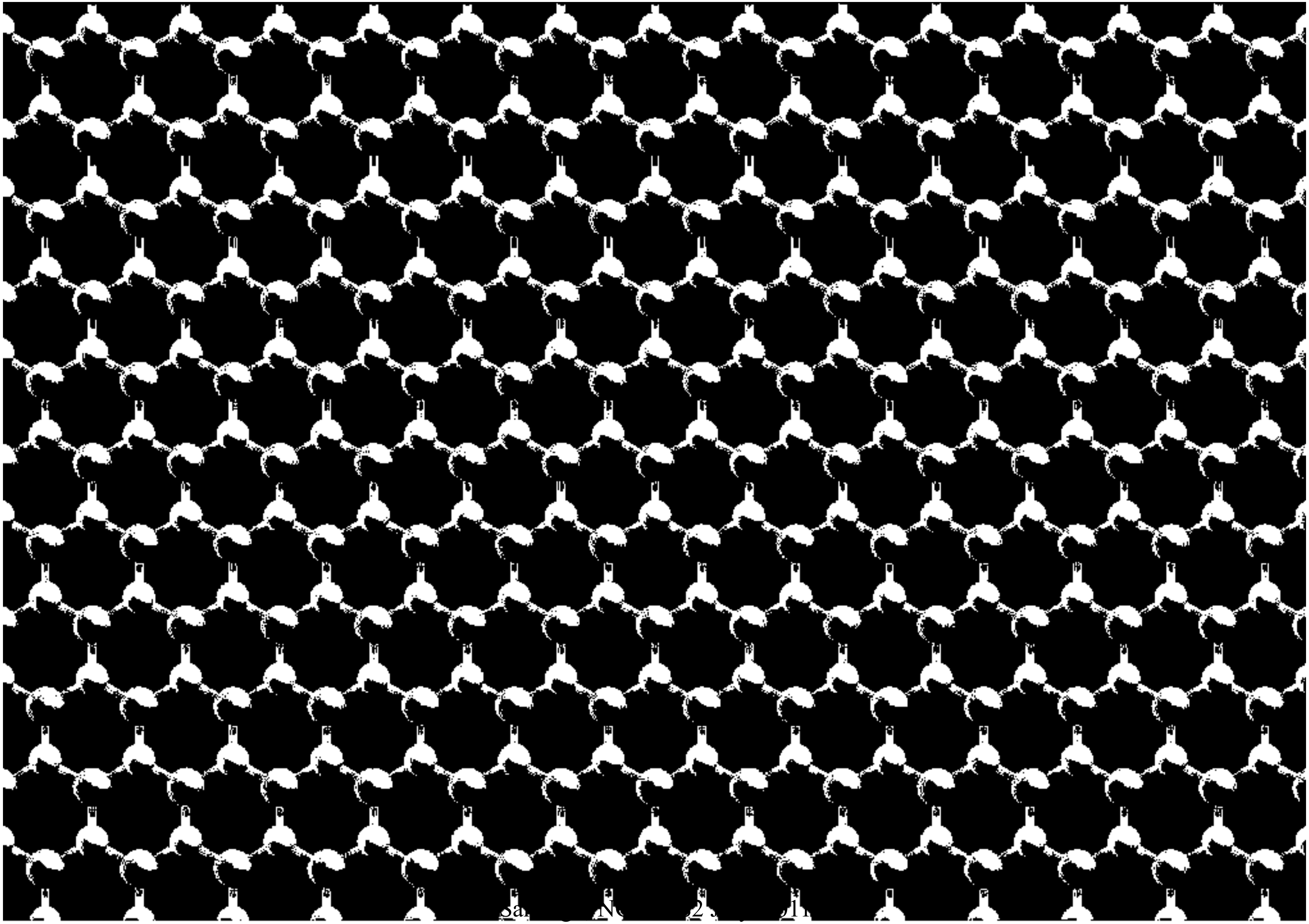
D. Soriano, FMR, JFR,JJP PRB 2010



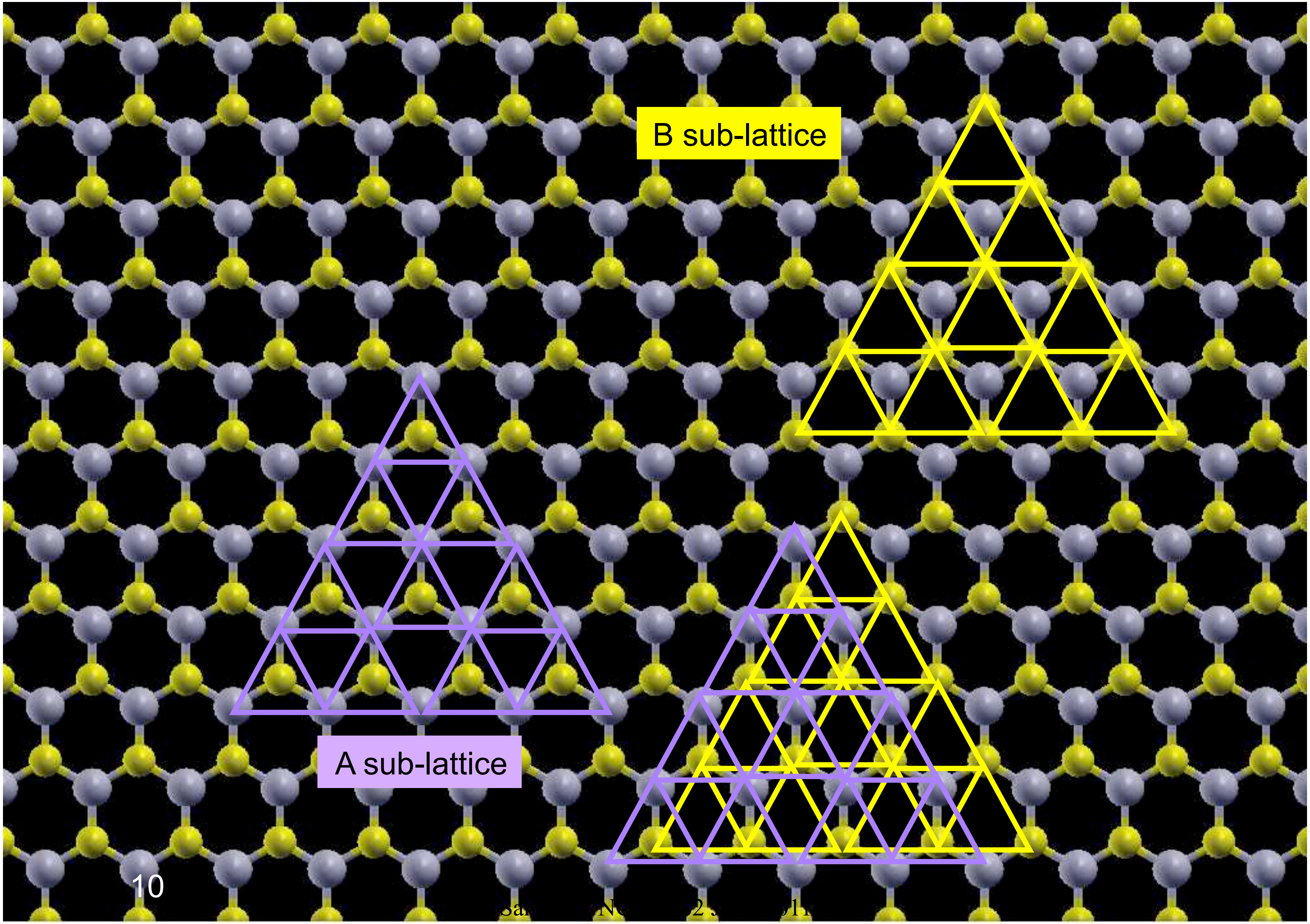
D. Gosálbez, JFR, PRB 2011

Graphene: a short intro

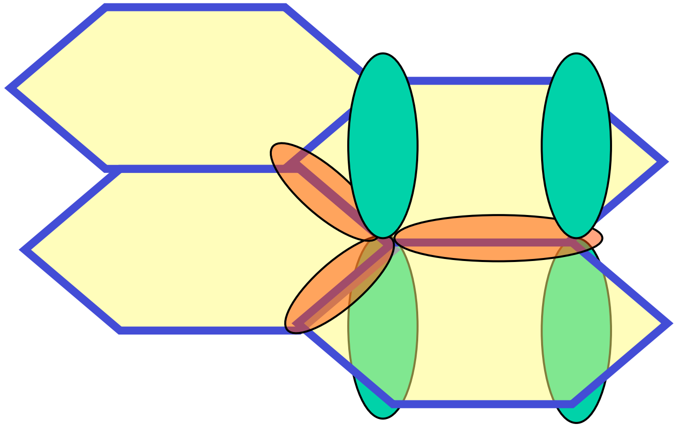
Honeycomb lattice of carbon atoms



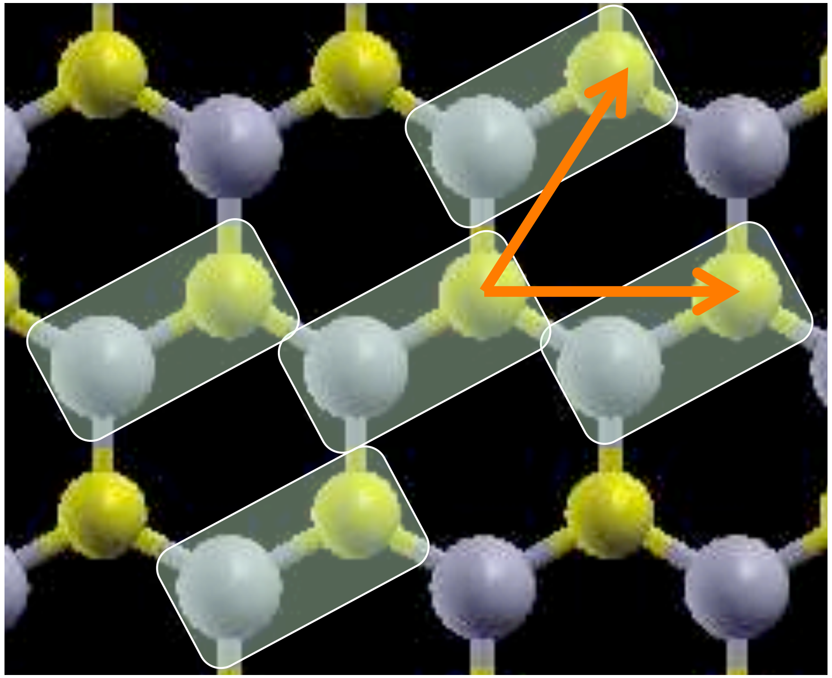
Bipartite lattice: 2 **interpenetrating** triangular sublattices



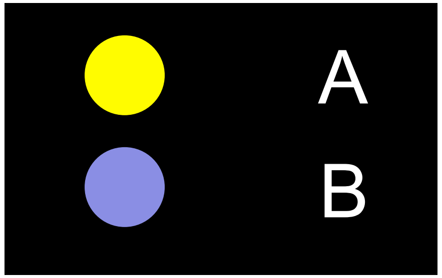
Graphene: 2 atoms per unit cell, 1 orbital per atom



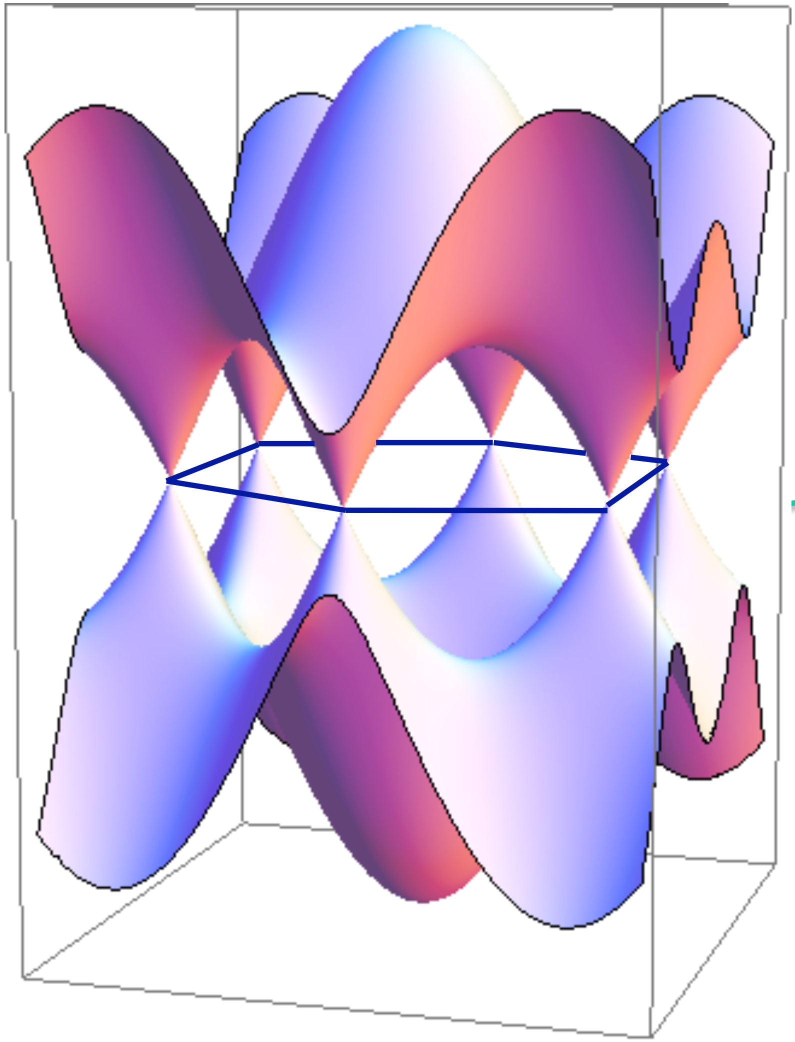
1 Pi orbital per atom
1 electron per Pi orbital

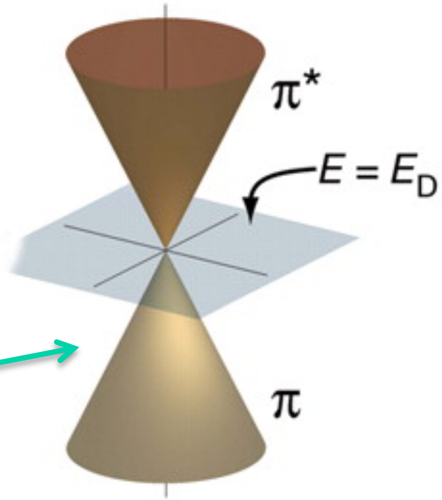


$$\mathcal{H}(\vec{k}) = \begin{array}{cc} \mathrm{A} & \mathrm{B} \\ \left(\begin{array}{cc} 0 & h(\vec{k}) \\ h^*(\vec{k}) & 0 \end{array} \right) \end{array} \begin{array}{c} \mathrm{A} \\ \mathrm{B} \end{array}$$

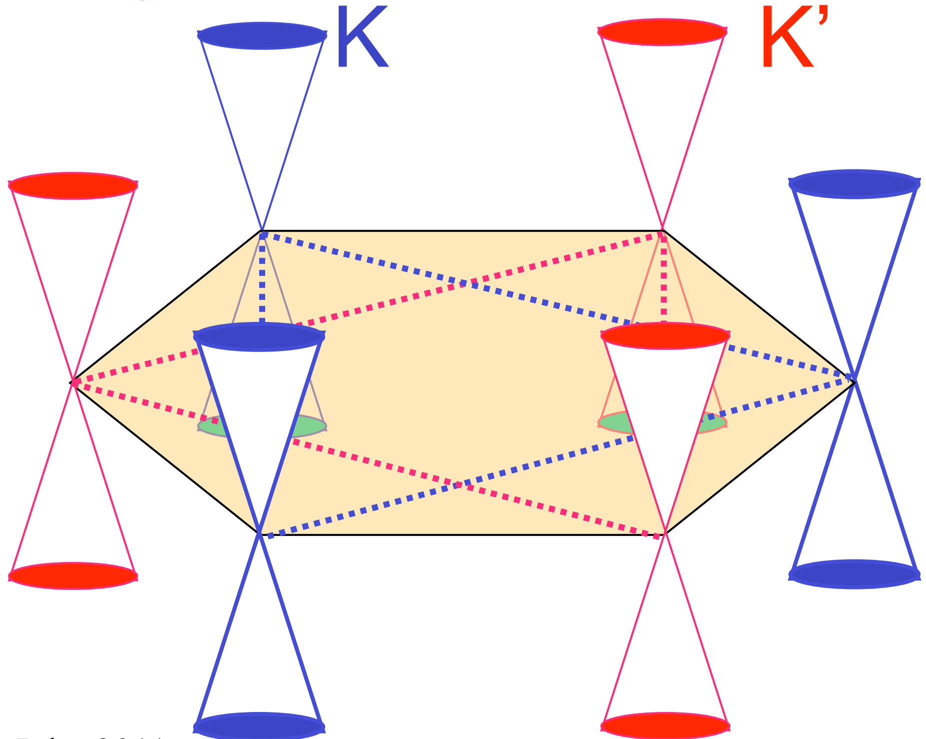


Graphene band structure: Dirac cones, valleys and all that





Dirac cones



Dirac electrons vs normal electrons: Landau Levels

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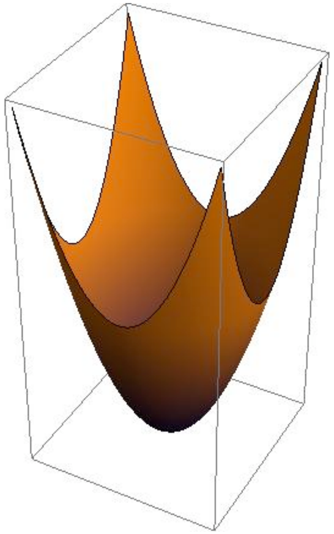

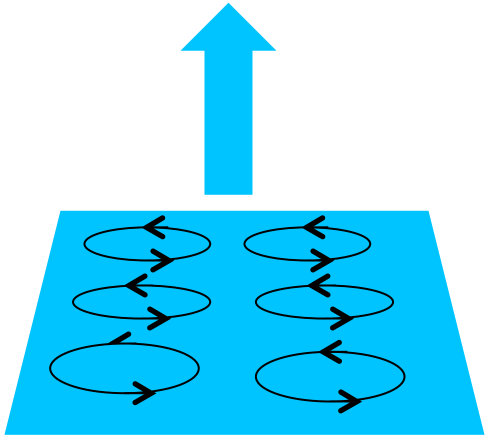

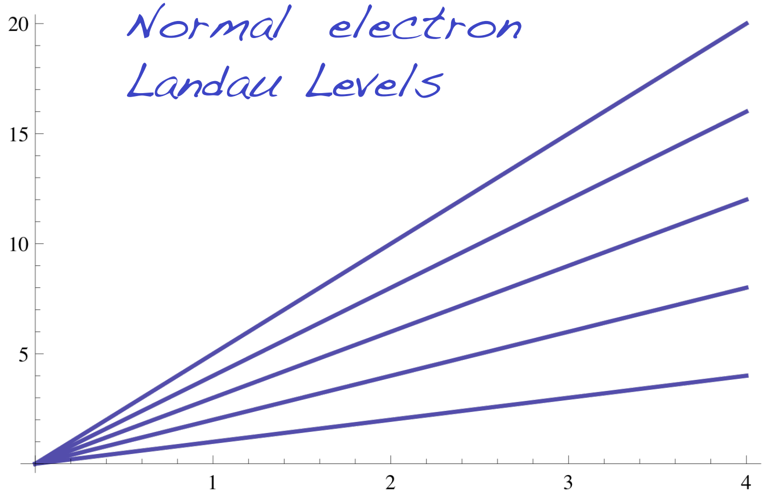

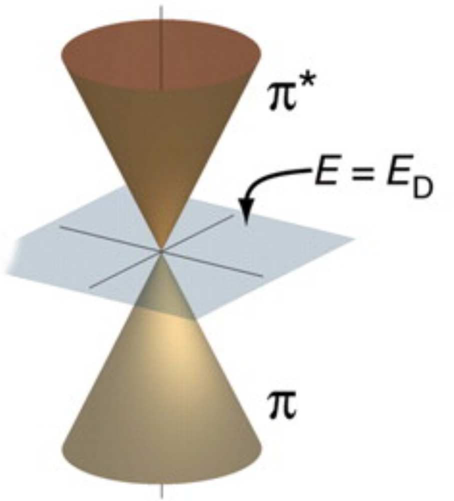

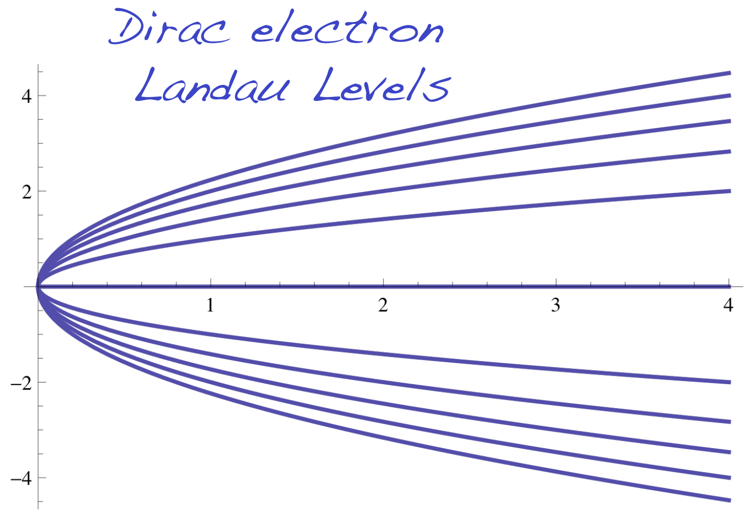

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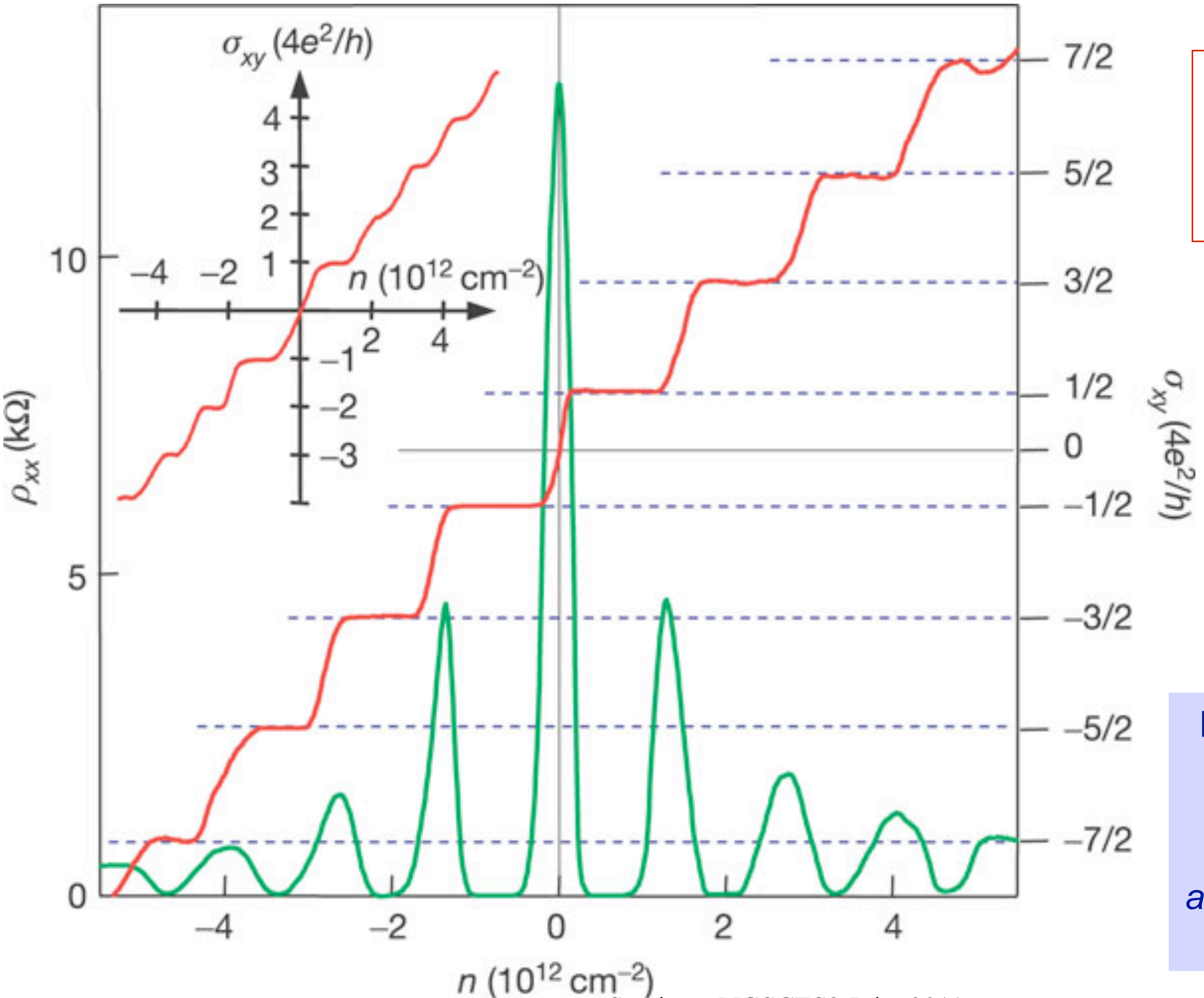


Integer Quantum Hall Effect

GOOD !

K .Novoselov *et al*, *Nature* **438**, 197 (2005)
Yuanbo Zhang *et al.*, *Nature* **438**, 201 (2005)

Conductivity

Drude-Sommerfield Formulas

$$\sigma = \frac{e^2 n \tau}{m}$$

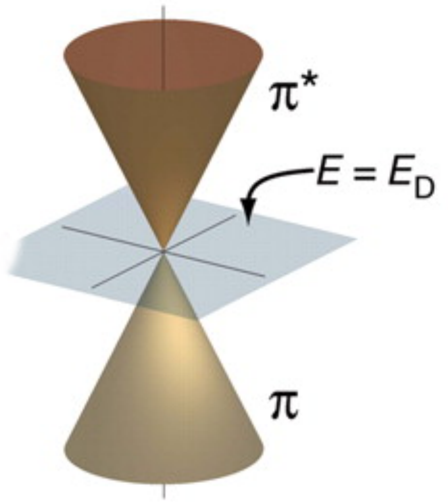
$$\sigma = \frac{1}{3} e^2 v_F^2 g(E_F) \tau$$

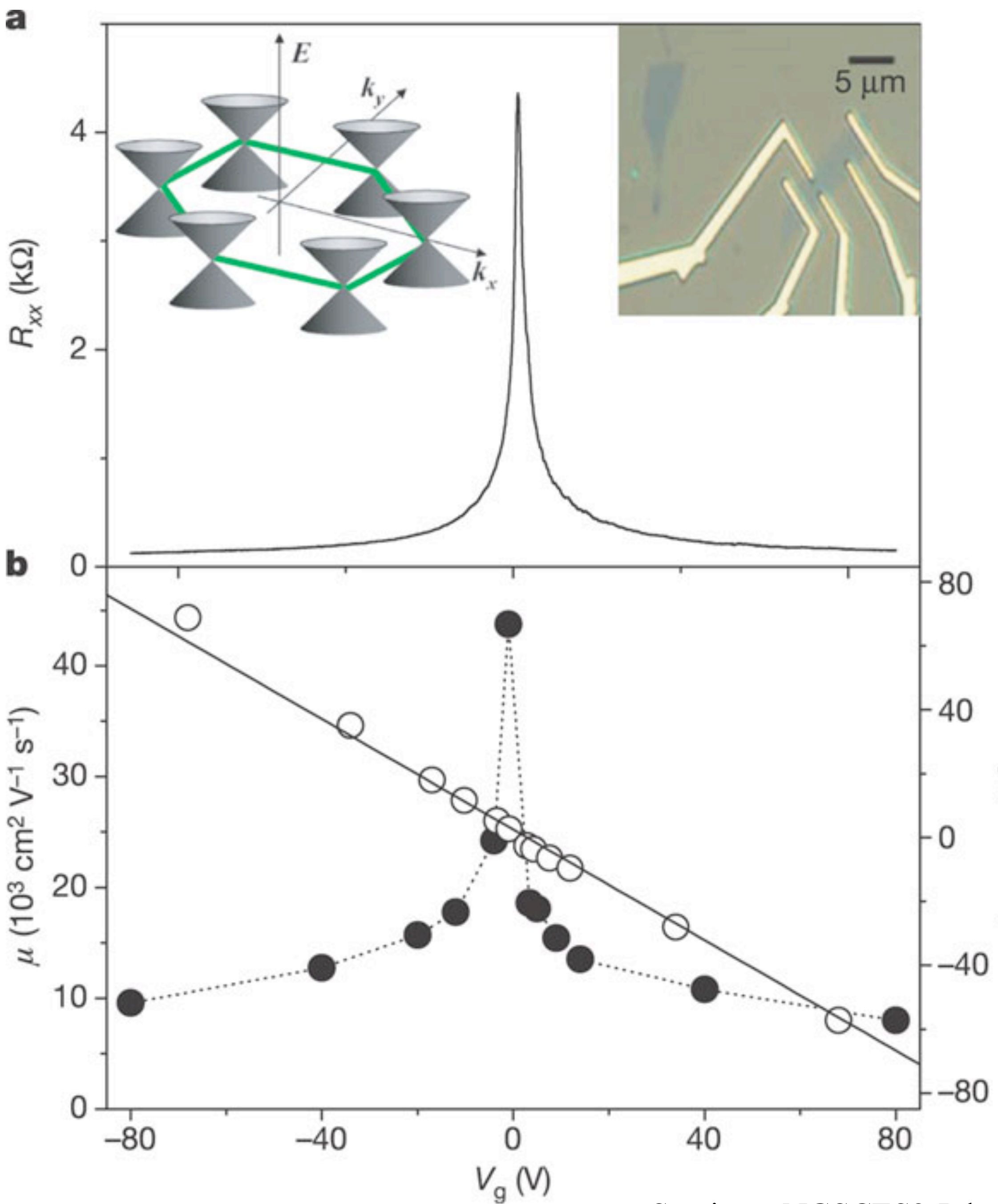
$$n = m = g(E_F) = 0$$

Quantum transport theories (different approaches)

$$\sigma \simeq \frac{1}{\pi} 4 \frac{e^2}{h}$$

Independent of scattering time !!!





Conducts even at zero Gate

Extrange

High Mobility

K .Novoselov *et al*, *Nature* **438**, 197 (2005)
Yuanbo Zhang *et al.*, *Nature* **438**, 201 (2005)

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-Electronic properties of graphene described by Dirac electrons
(theory works !!)
-Causes: Graphene not very much affected by adsorbates vs robustness
-New electronic properties (QHE, Klein tunneling, Dirac point conductance)
-New structural properties (2D)
-Potential applications in electronics

Graphene as a material for strong correlation?

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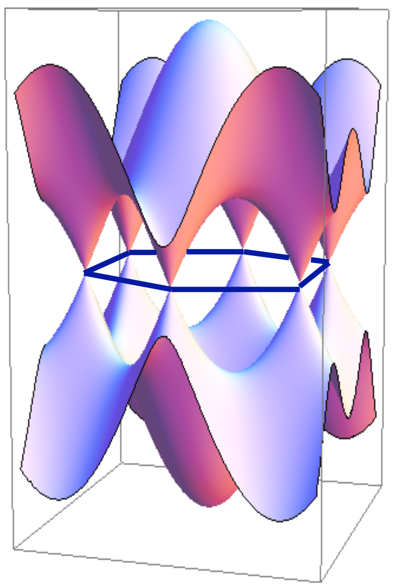
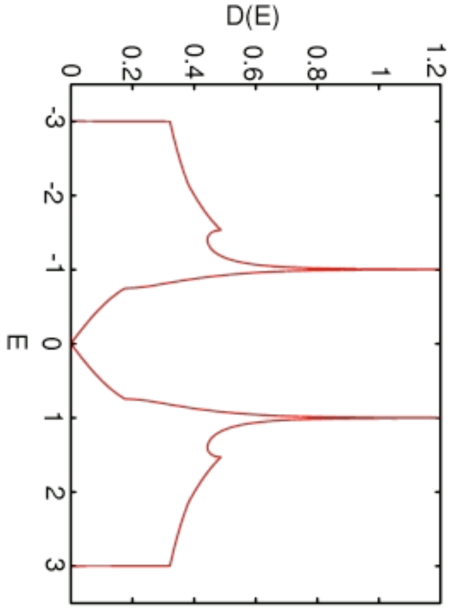




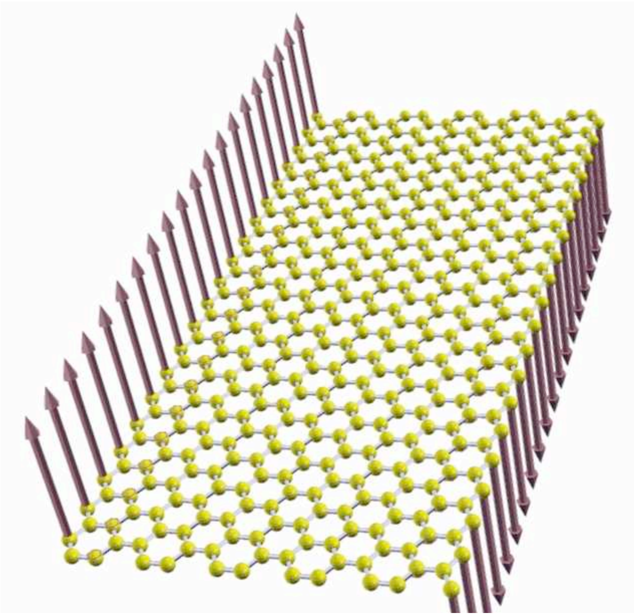
-Zero Gap Semiconductor
-Vanisihing DOS at Fermi Energy
-Very large Fermi velocity
-P orbitals

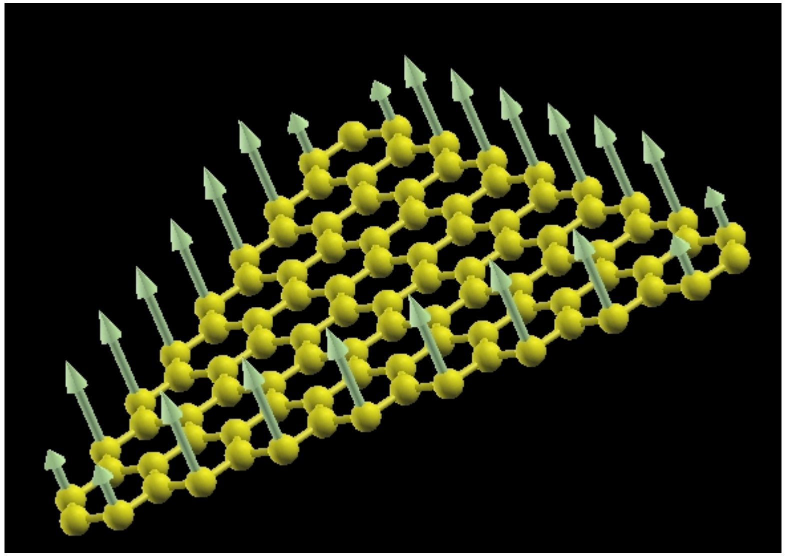
....
the wrong place to look for correlations?

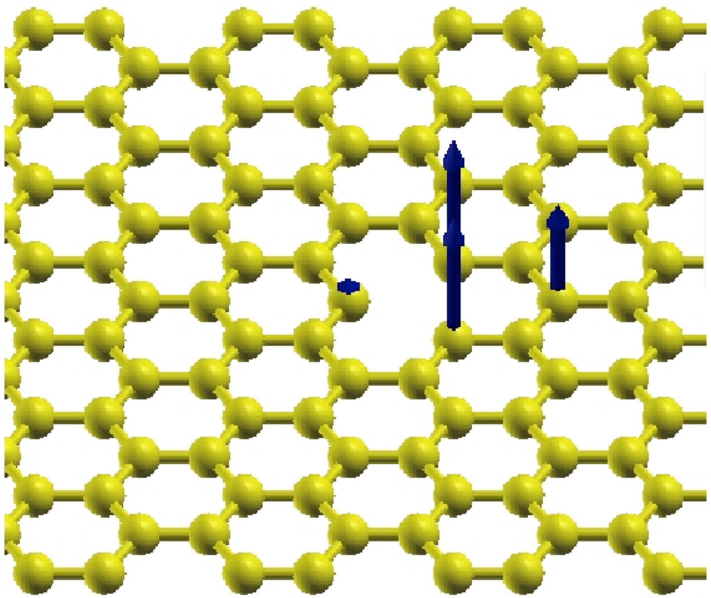
A route to magnetism in graphene

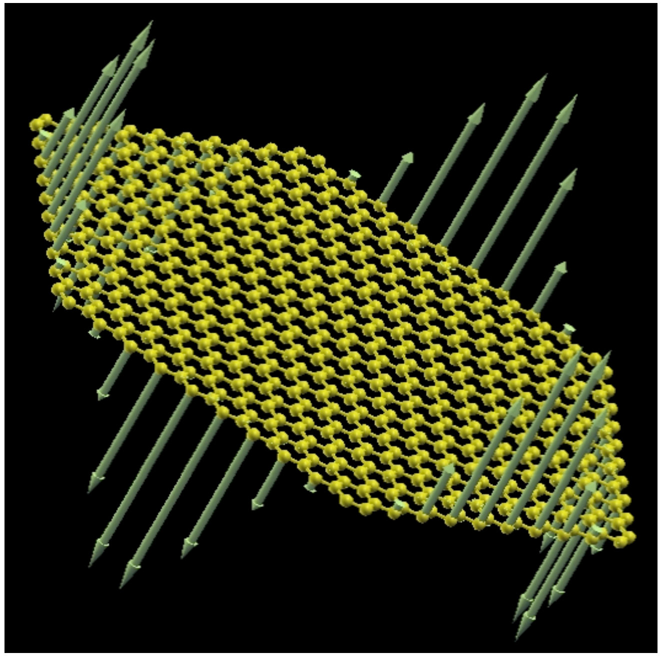
Santiago, NGSCES2 July 2011

Magnetism in the edges (ribbons, islands and vacancies)









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Properties

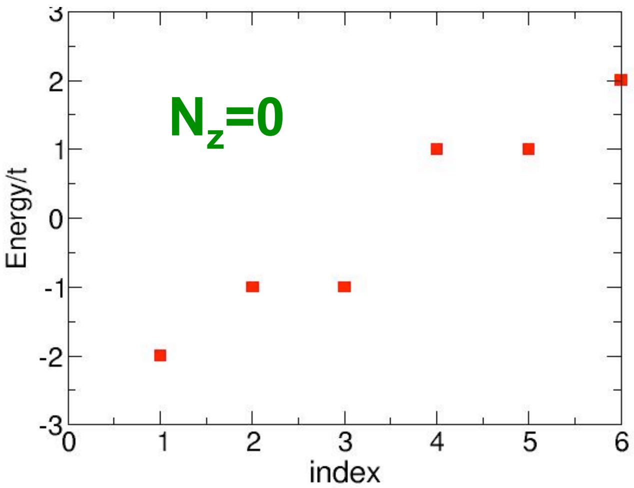
- Takes place at edges of properly passivated graphene
- Not related to dangling bonds
- Pi electron magnetism ("Dirac electrons")
- Robust prediction (model independent)
- Large spin stiffness and splitting: Thermally robust
- Local moments associated to superatomic states
- Non-local effects
- It affects transport: spin electronics

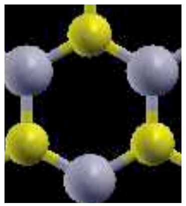
NEW KIND OF MAGNETISM

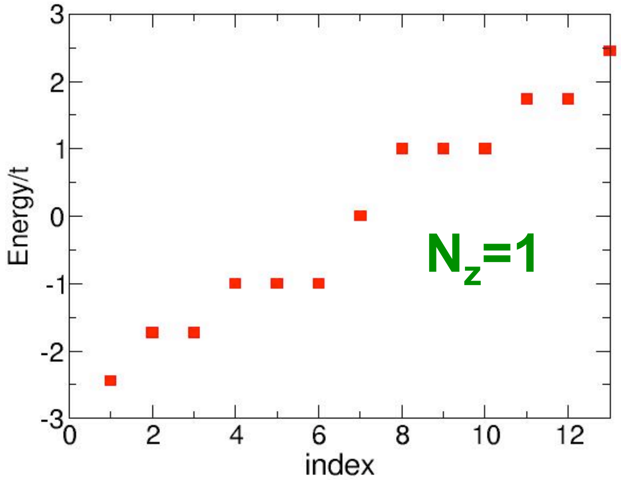
THEOREM 1 (U=0)

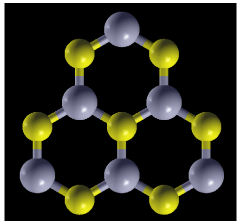
- Number of E=0 states in 1st neighbour TB model in bipartite lattice: $N_z=|N_A-N_B|$

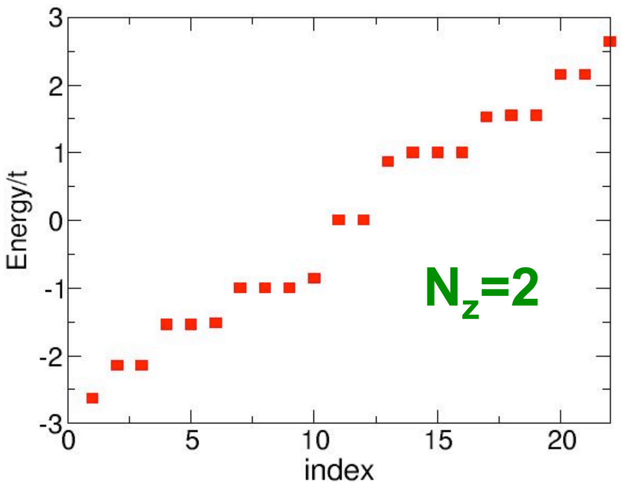
M. Inui, S. A. Trugman, and E. Abrahams, PRB**49**, 3190 (94)

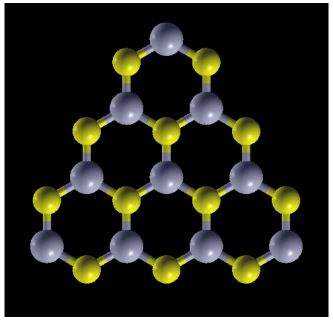












2 theorems for the Hubbard model bipartite lattices

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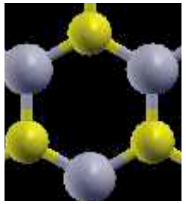
THEOREM 2 (U>0) (Lieb Theorem)

- Spin S of the ***exact ground state*** is given by $2S= N_z=|N_A-N_B|$

E. Lieb, Physical Review Letters, (1989)

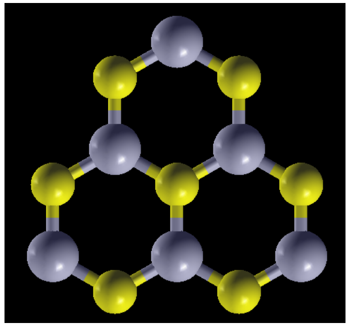
$|N_A-N_B|=0$



$S=0$

Trivial

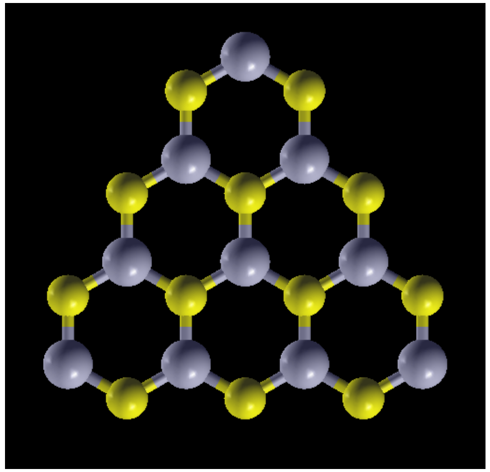
$|N_A-N_B|=1$



$S=1/2$

Trivial

$|N_A-N_B|=2$



$S=1$

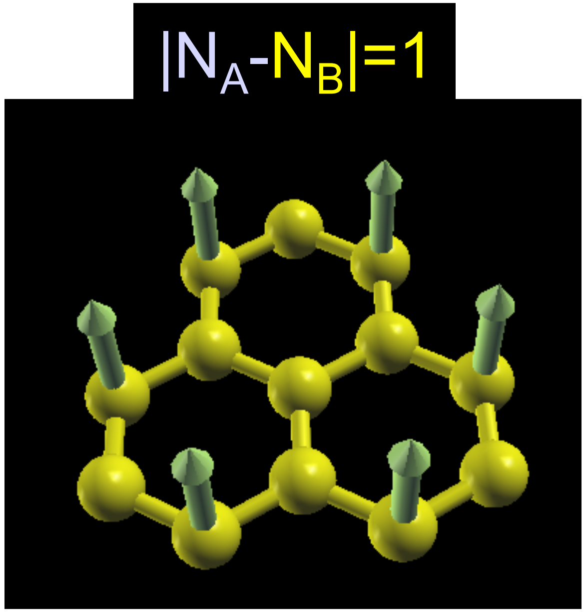
Non Trivial!!

Some technical remarks

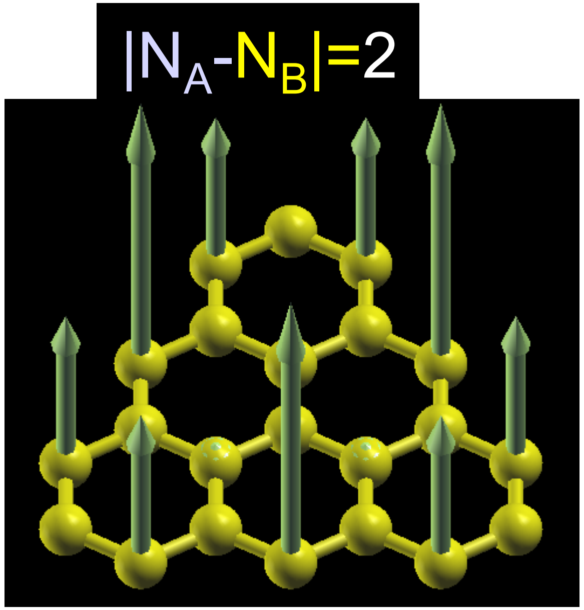
$$\mathcal{H} = \sum_{\vec{r},\vec{r}',\sigma} t_{\vec{r},\vec{r}'} c^{\dagger}_{\vec{r}\sigma} c_{\vec{r}'\sigma} + U \sum_{\vec{r}} n_{\vec{r},\uparrow} \langle n_{\vec{r},\downarrow} \rangle + n_{\vec{r},\downarrow} \langle n_{\vec{r},\uparrow} \rangle$$

Mean fielf approx.

Edge atoms are assumed to be passivated with H



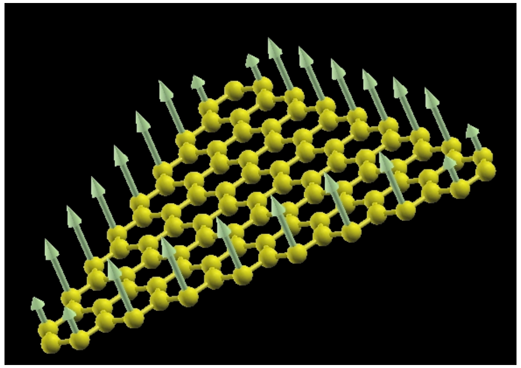
S=1/2



S=1

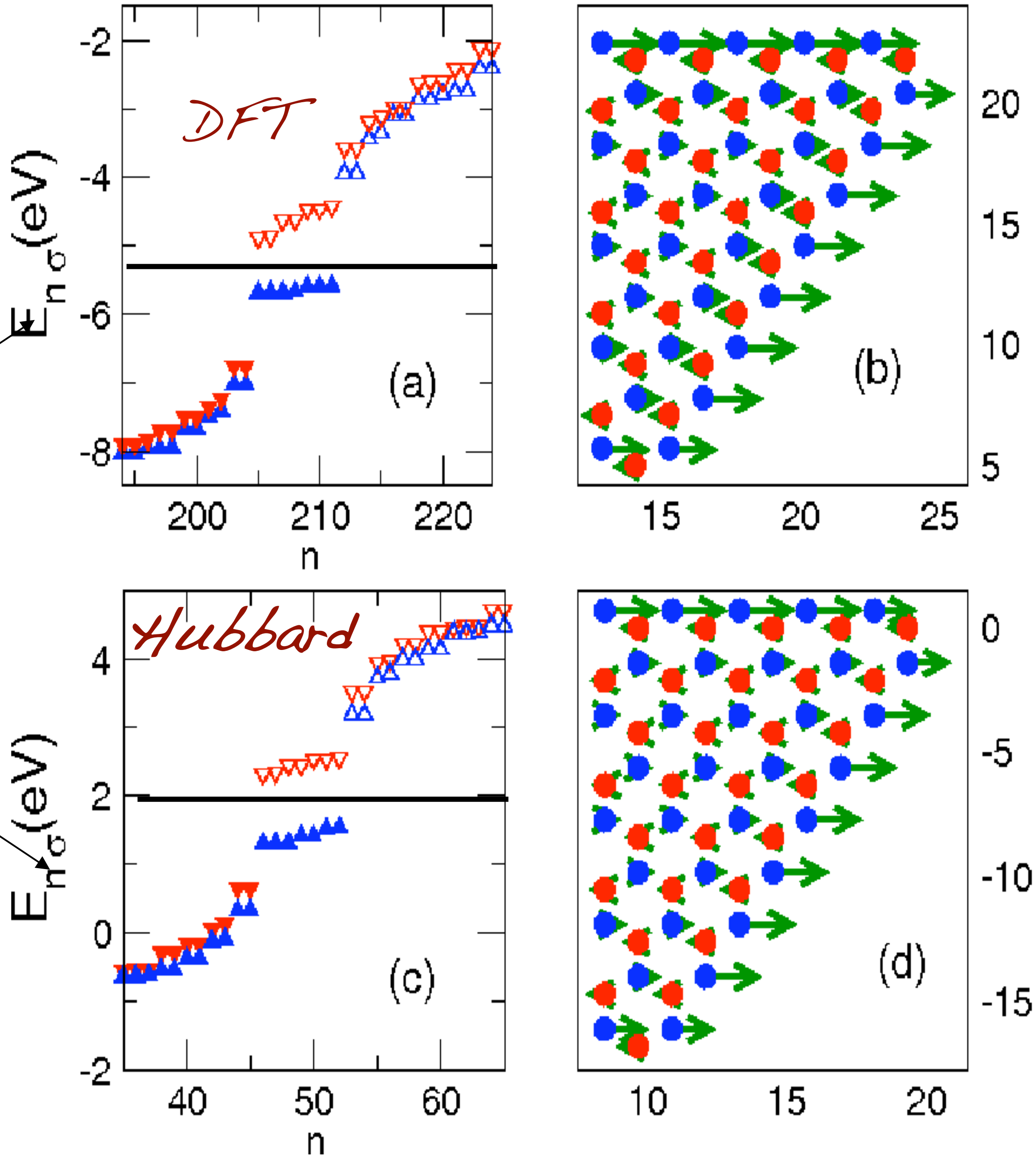
Zero energy states are sublattice polarized (in majority sublattice)

Mean field Hubbard model vs DFT



S=7/2

Mid-gap states spin Split and *dispersed*



Men field Hubbard model
(*U*=3.85 eV, t=2.7eV)

J. Fernández-Rossier, J. J. Palacios
PRL **99**, 177204 (07)

Zigzag ribbons: single particle band structure

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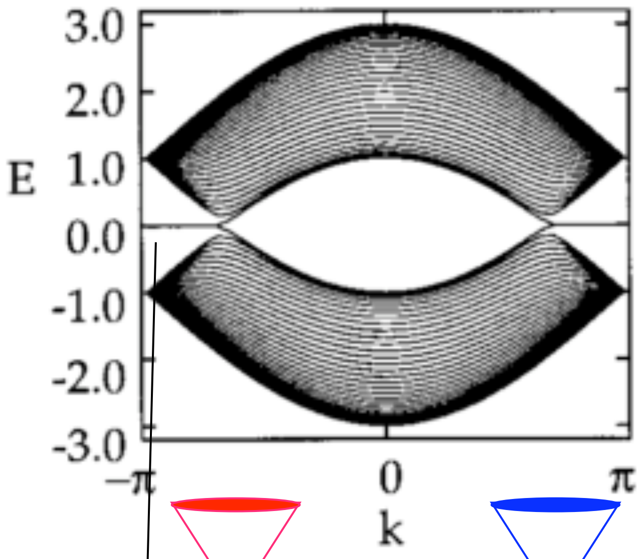
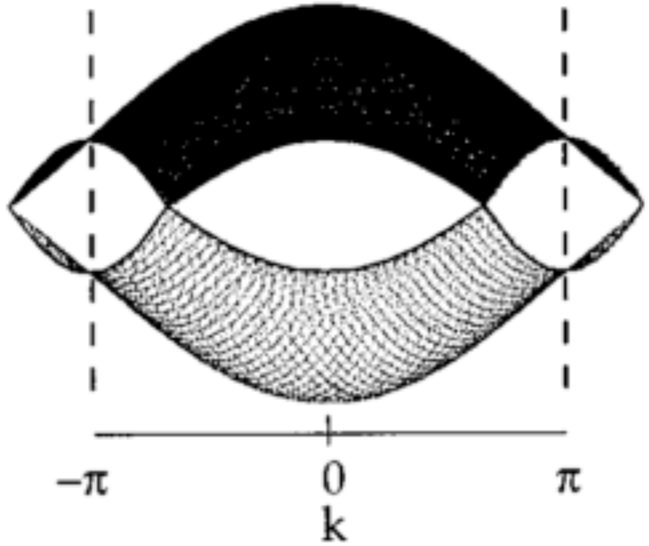
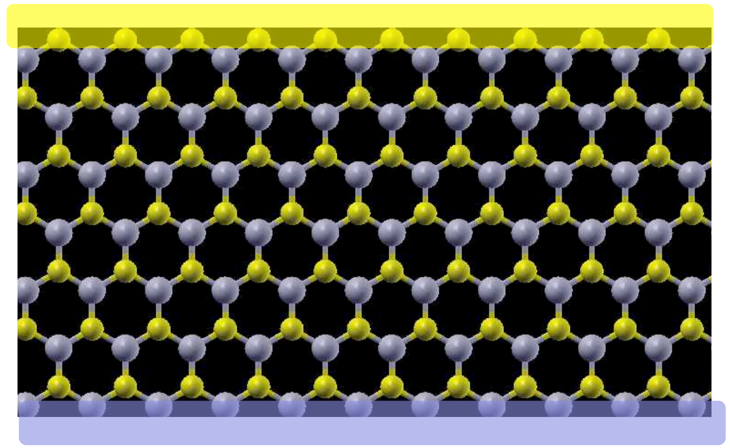
1D bands

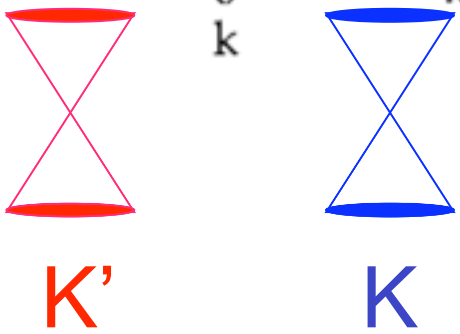


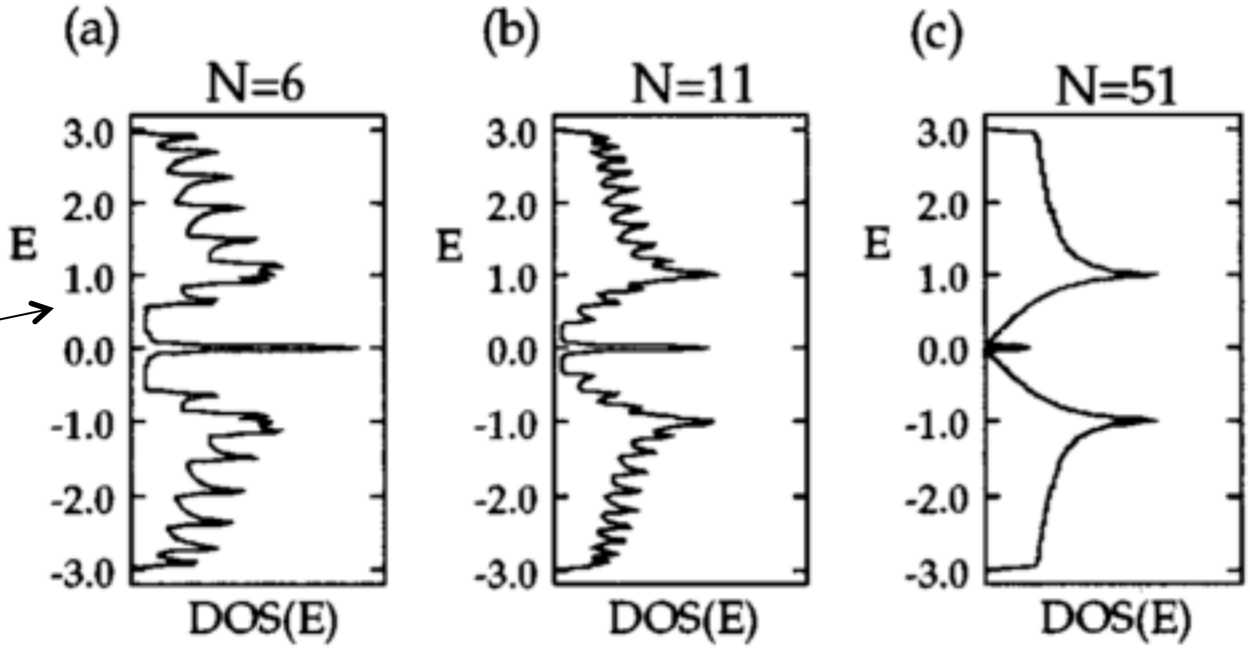
Folding 2D bands



Zigzag







Edge states
Flat band
High DOS

Nakada et al, PRB **54** (1996)

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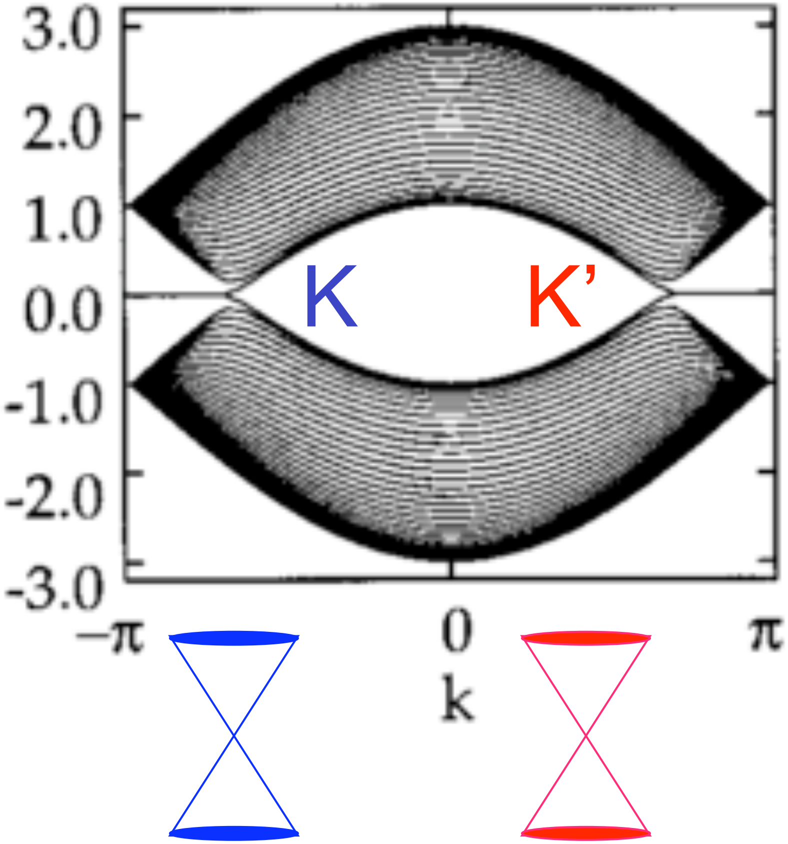
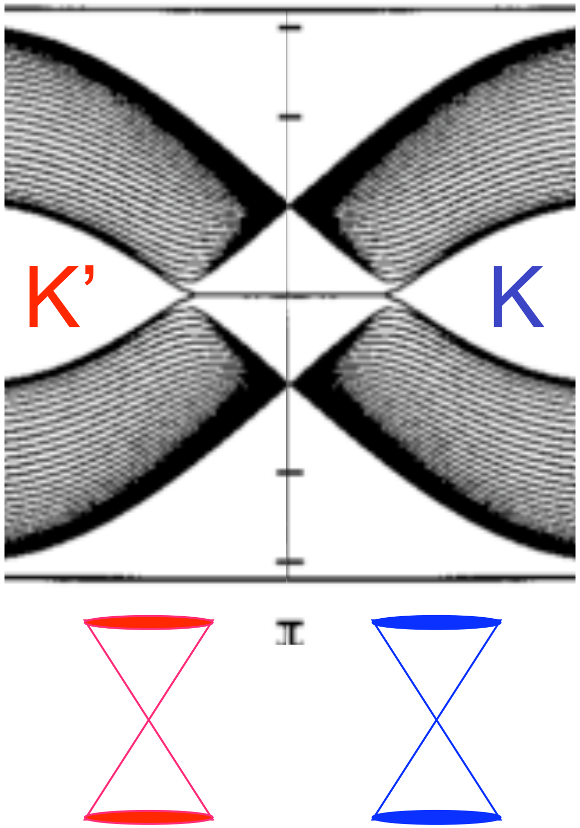
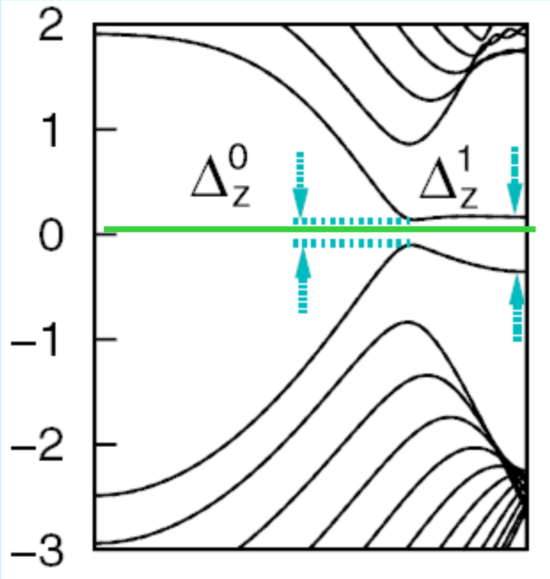




The effect of interaction: Mean field Hubbard vs DFT

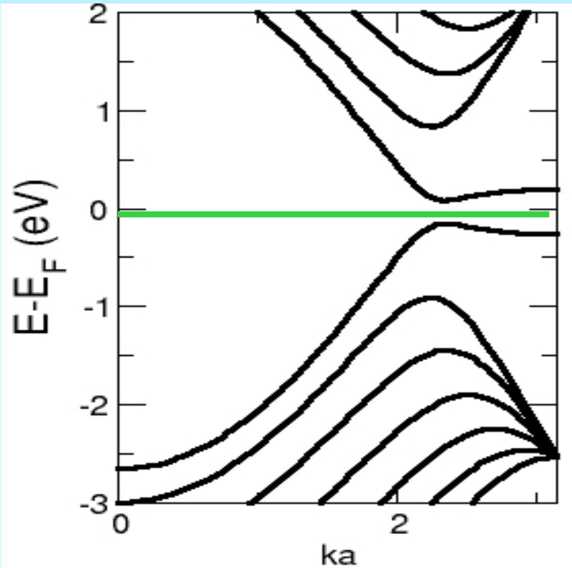
DFT

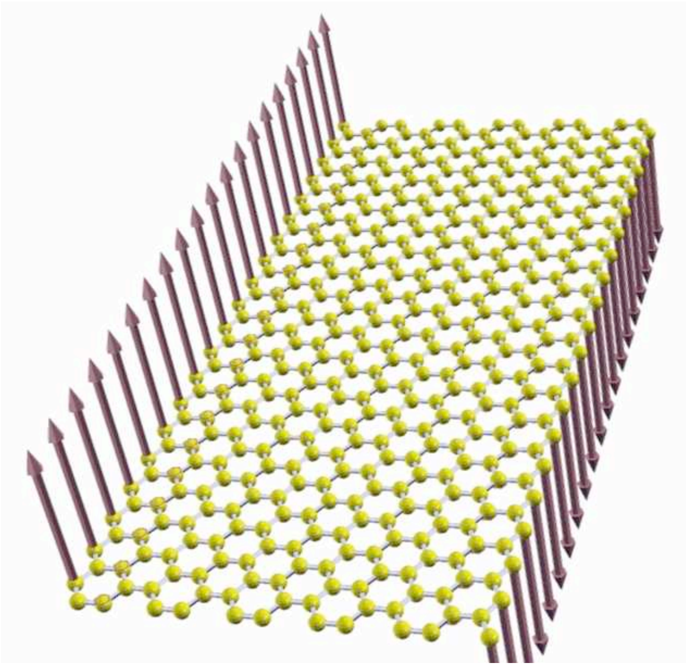
Son et al.,
PRL 2006
Nature 2006



Hubbard

JFR, PRB 77, 075430 (08)

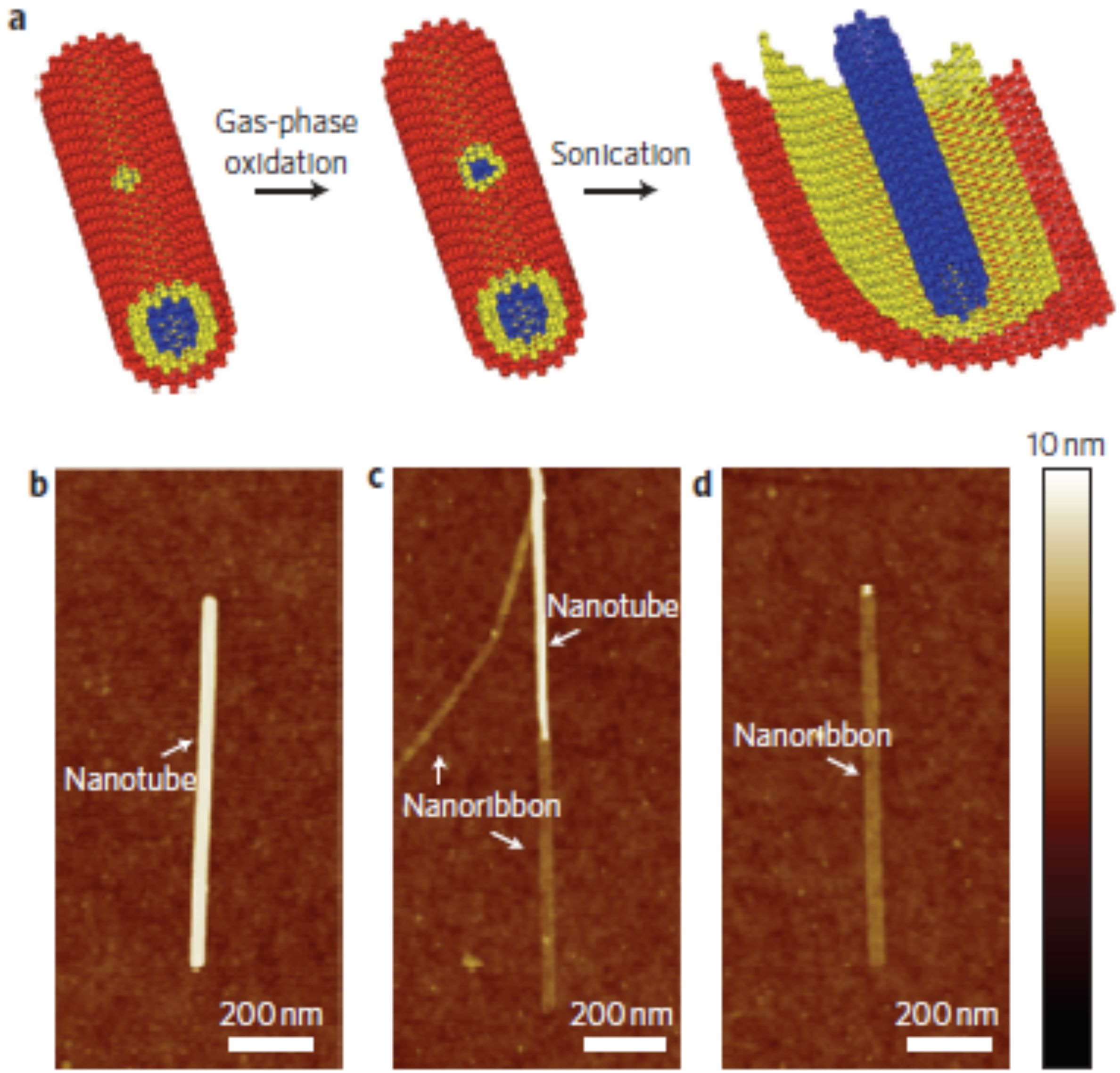




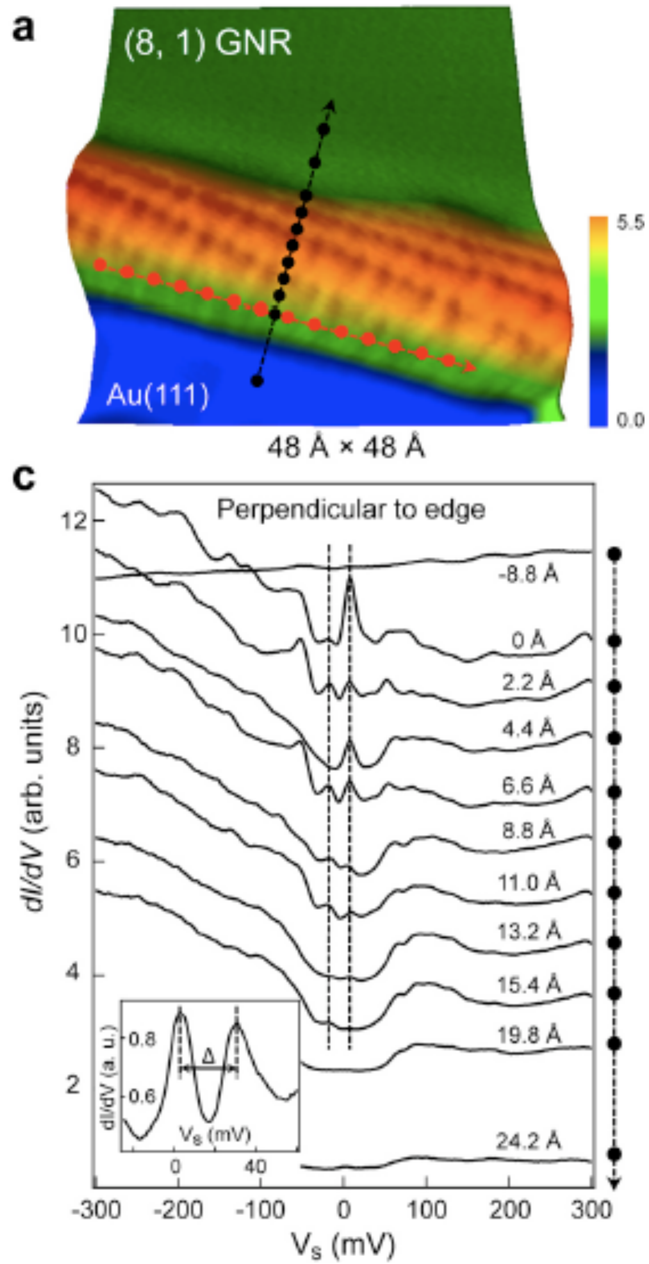
- Ferromagnetic order in the edges
- Antiferromagnetic inter-edge coupling
- Insulator

Experimental confirmation?

Smooth Graphene ribbons



Hong Jie Dai (2009-10)



Crommie (2011)

Graphene triangulene

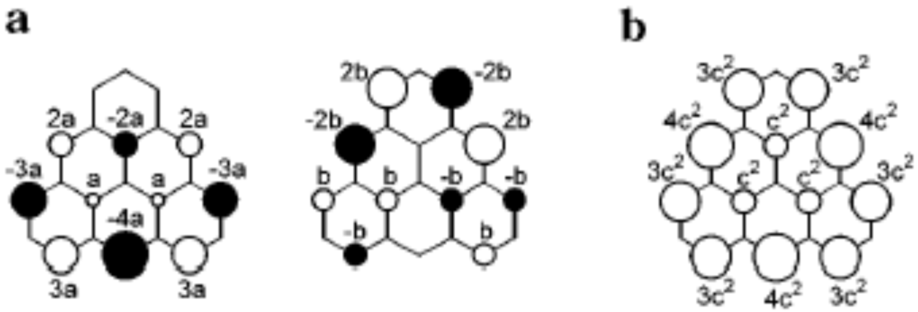


Figure 1. (a) A pair of degenerate π-NBMOs of triangulene **1** calculate by Hückel MO theory, showing the nondisjoint nature.[7] The coefficient are $a = 1/\sqrt{66}$ and $b = 1/\sqrt{22}$. (b) Spin density distribution of the tripl state of **1**. The coefficient is $c^2 = 2/33$.

J. Inoue, JACS 2001

Breaking sublattice symmetry

3 Spin-like degrees of freedom

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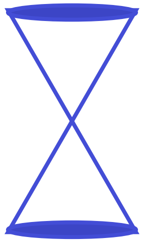
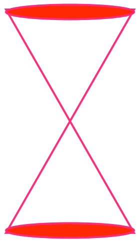
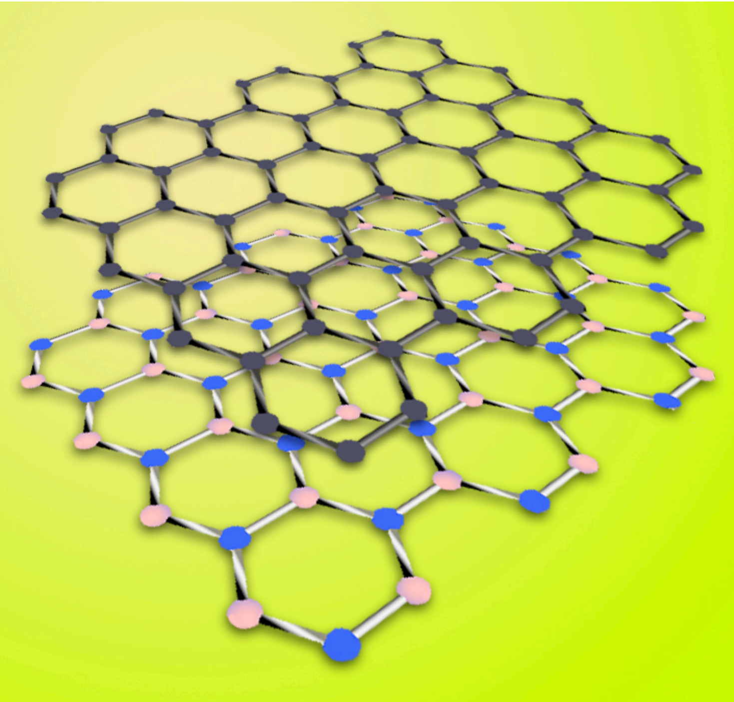
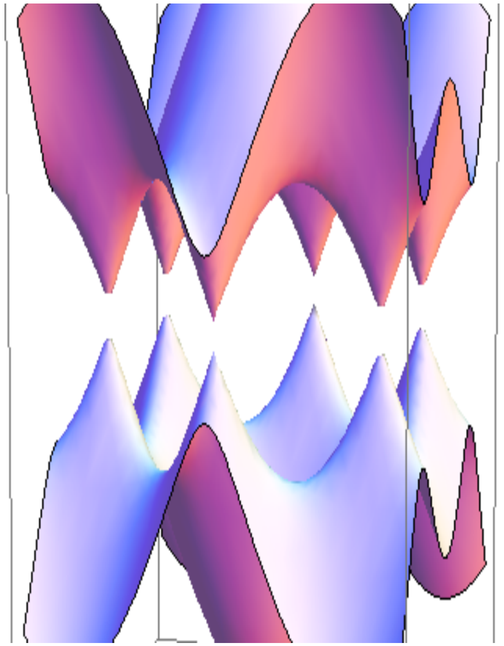
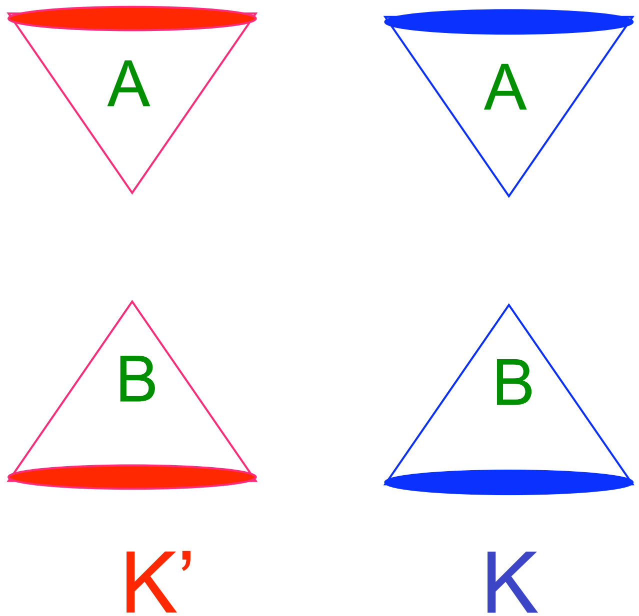
	Symbol	Value 1	Value 2	Hamiltonian
Spin	S_z	$\uparrow$	$\downarrow$	Good quantum number
Sublattice	σ_z	A	B	$\begin{pmatrix} 0 & h(\vec{k}) \\ h^*(\vec{k}) & 0 \end{pmatrix}$
Valley	τ_z	K 	K' 	Good quantum number

Experimental inspiration: Graphene on hexagonal BN



$$\mathcal{H}(\vec{k}) = \begin{array}{cc} \begin{array}{cc} A & B \end{array} & \\ \begin{pmatrix} \frac{\Delta}{2} & h(\vec{k}) \\ h^*(\vec{k}) & -\frac{\Delta}{2} \end{pmatrix} & \begin{array}{c} A \\ B \end{array} \end{array}$$





Effect of staggered potential on graphene ribbons

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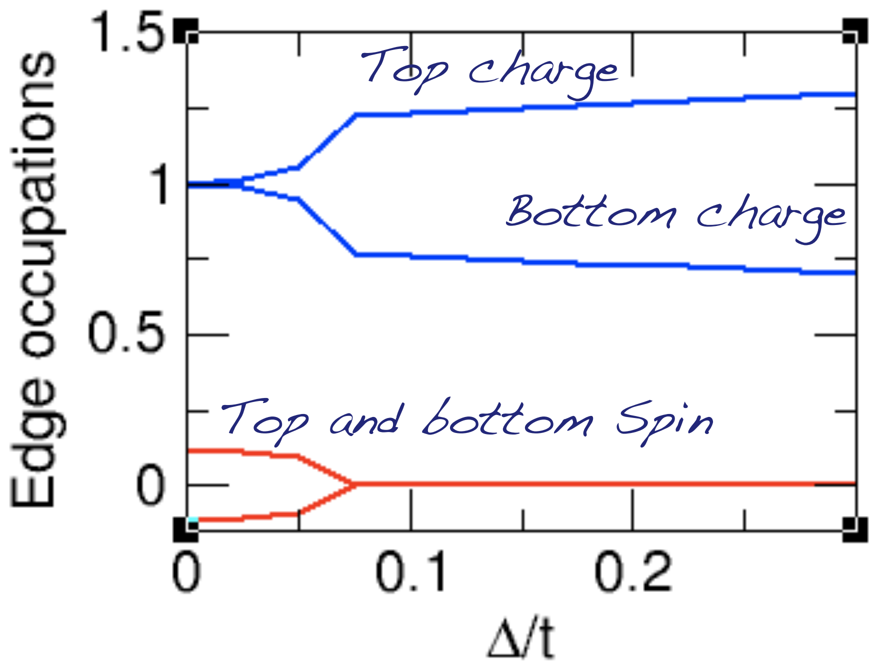

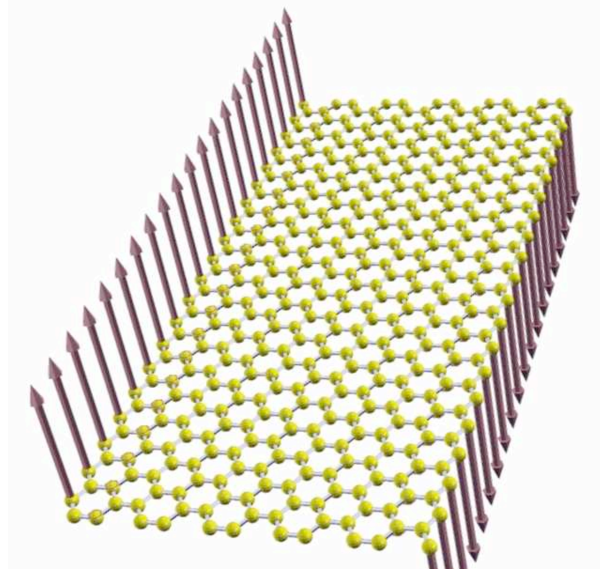

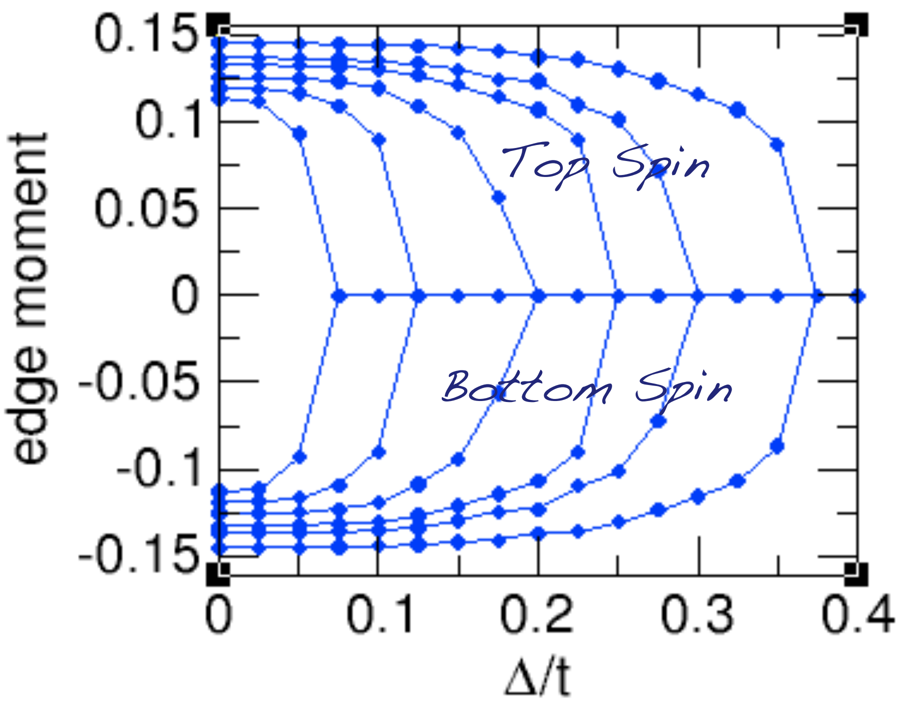

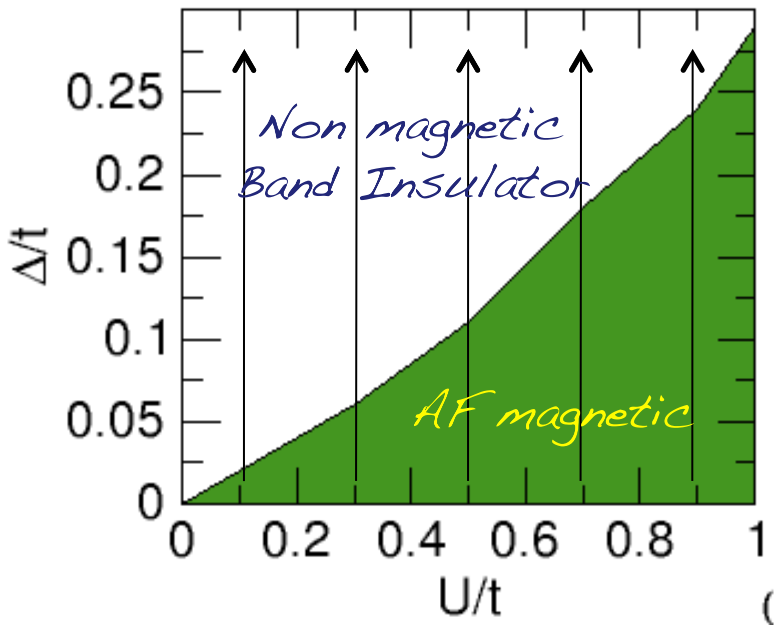

Effect of staggered potential on graphene ribbons

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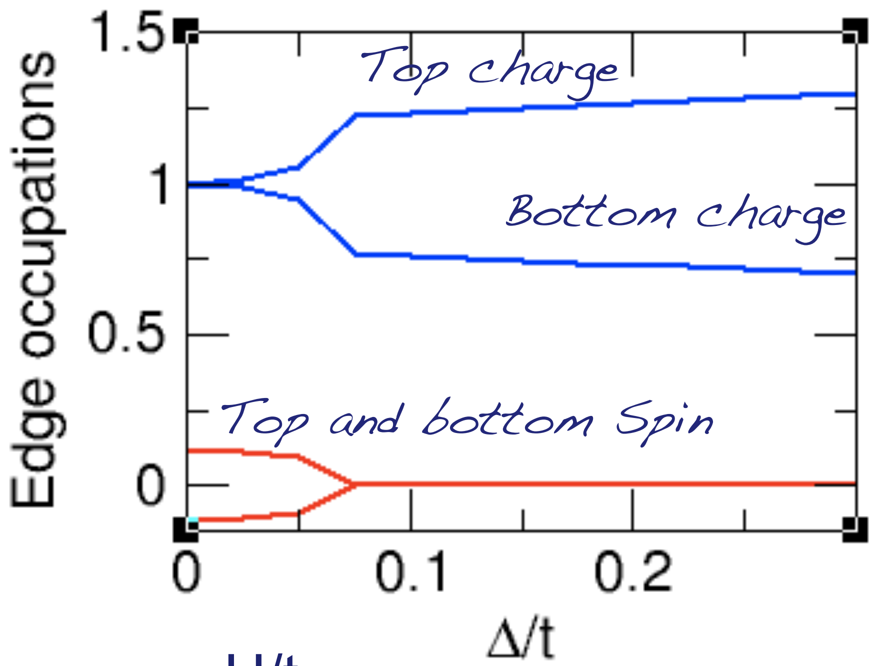

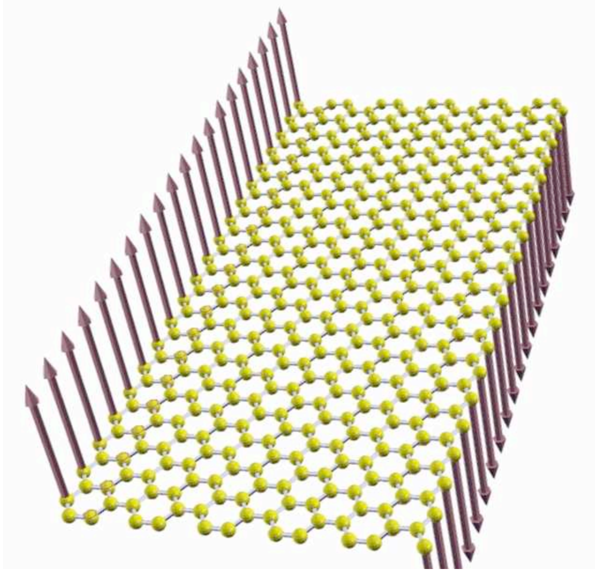

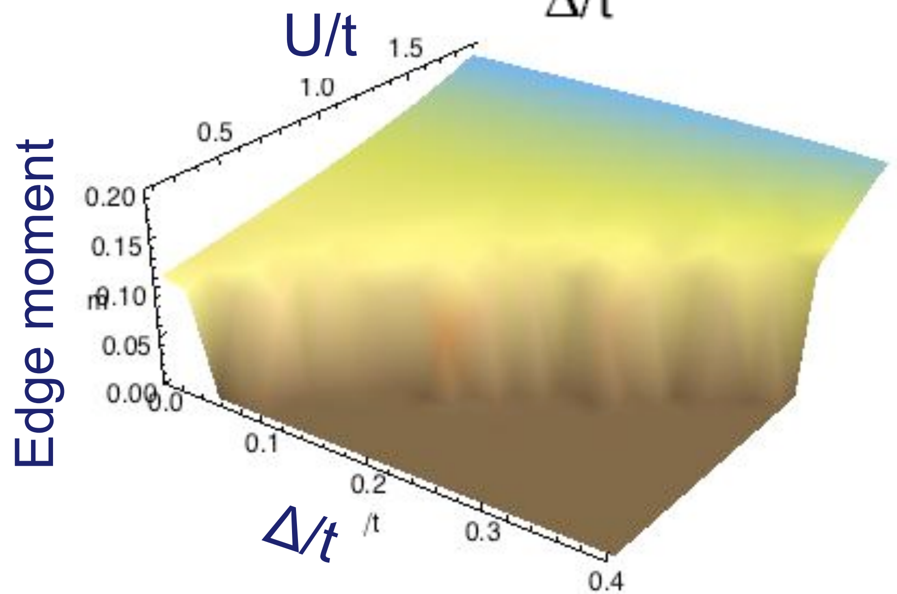

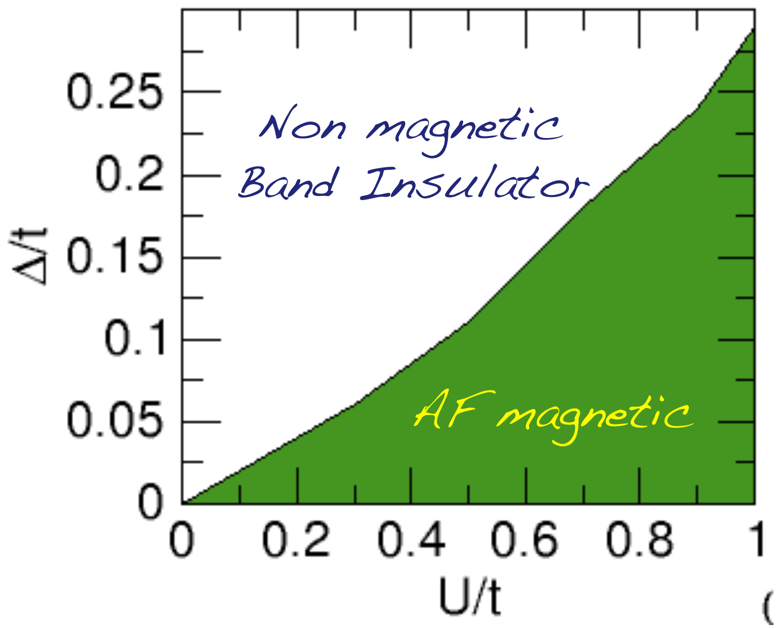

Effect of staggered potential

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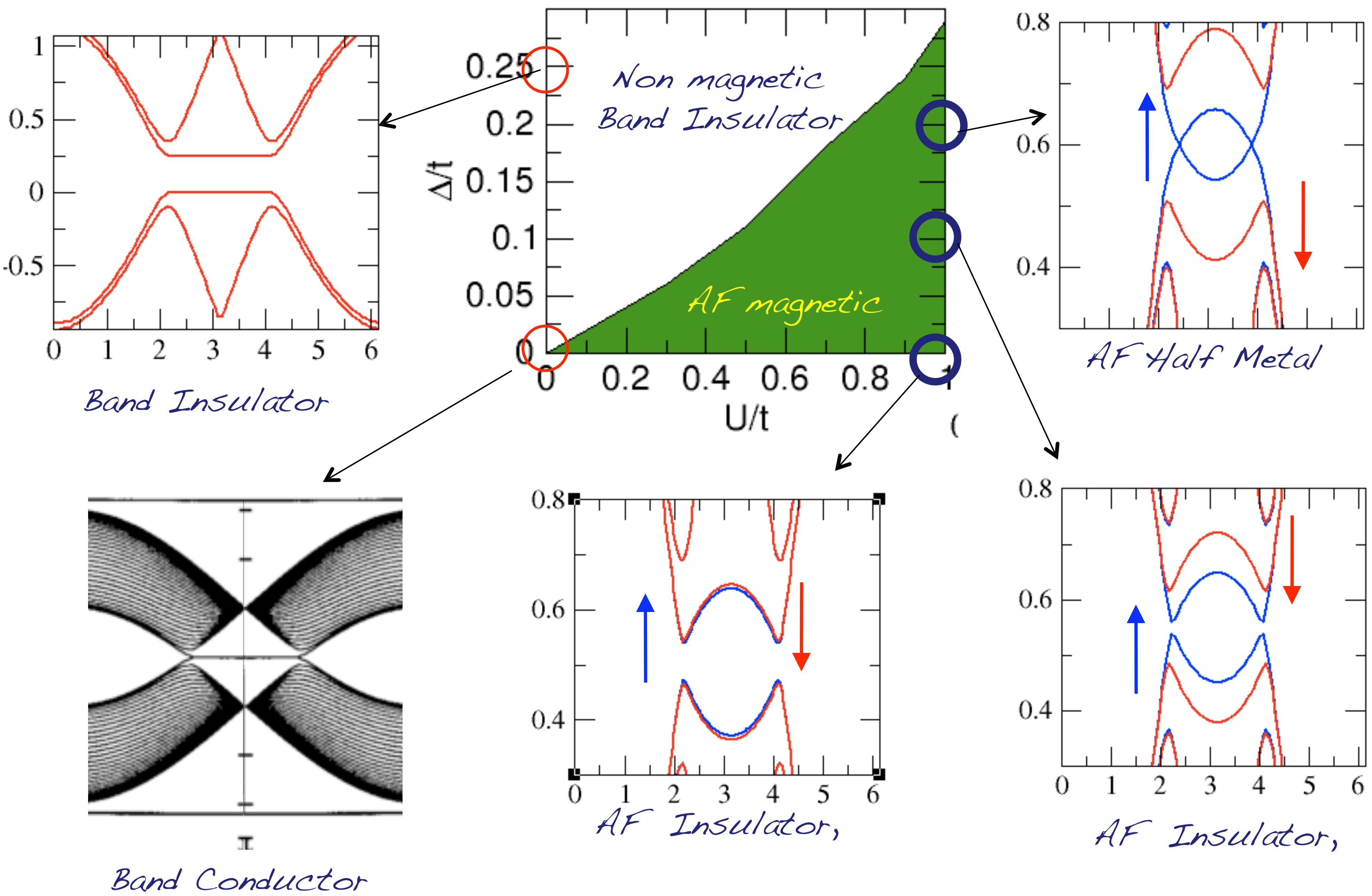

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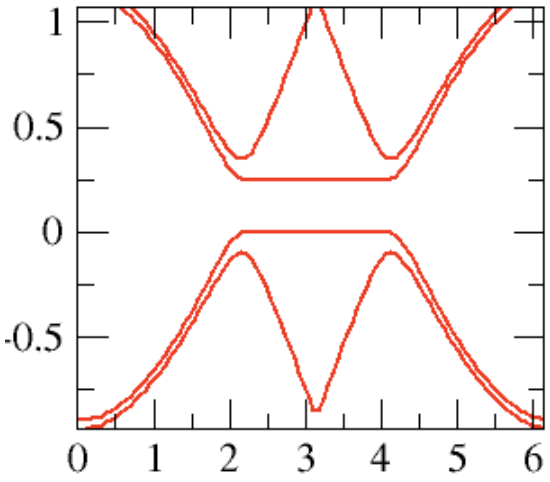
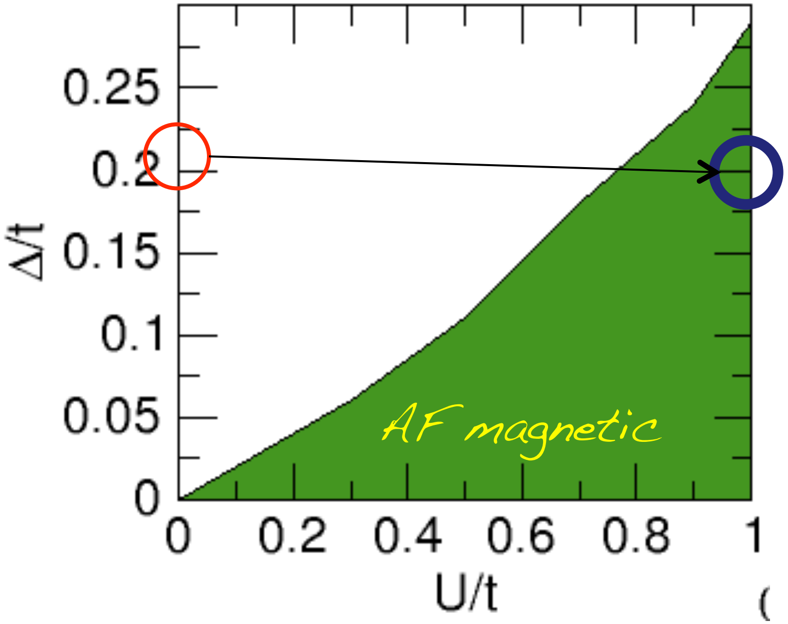
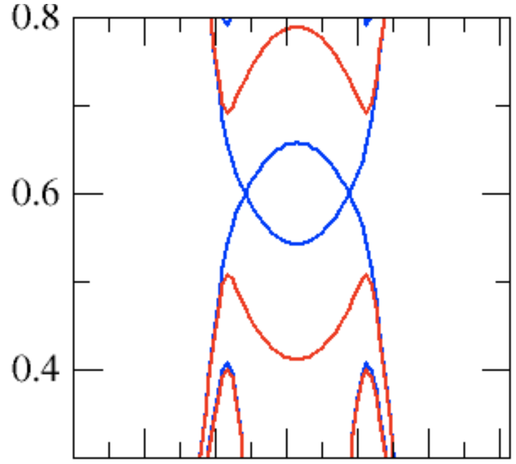


Band Insulator





AF Half Metal

Interaction turns the non-magnetic insulator
into a magnetic Half metal

Graphene as a topological insulator

C. L. Kane and E. J. Mele,
Quantum Spin Hall Effect in Graphene,
Phys. Rev. Lett. **95**, 226801 (2005)

C. L. Kane and E. J. Mele,
Z2 Topological Order and the Quantum Spin Hall Effect,
Phys. Rev. Lett. **95**, 146802 (2005)

$$\vec{L}\cdot\vec{S} = L^z S^z + \frac{1}{2}\left(L^- S^+ + L^+ S^-\right)$$

$$L^- S^+$$

$$|l=1, m=0, \sigma=\uparrow\rangle \rightarrow |l=1, m=-1, \sigma=\downarrow\rangle$$

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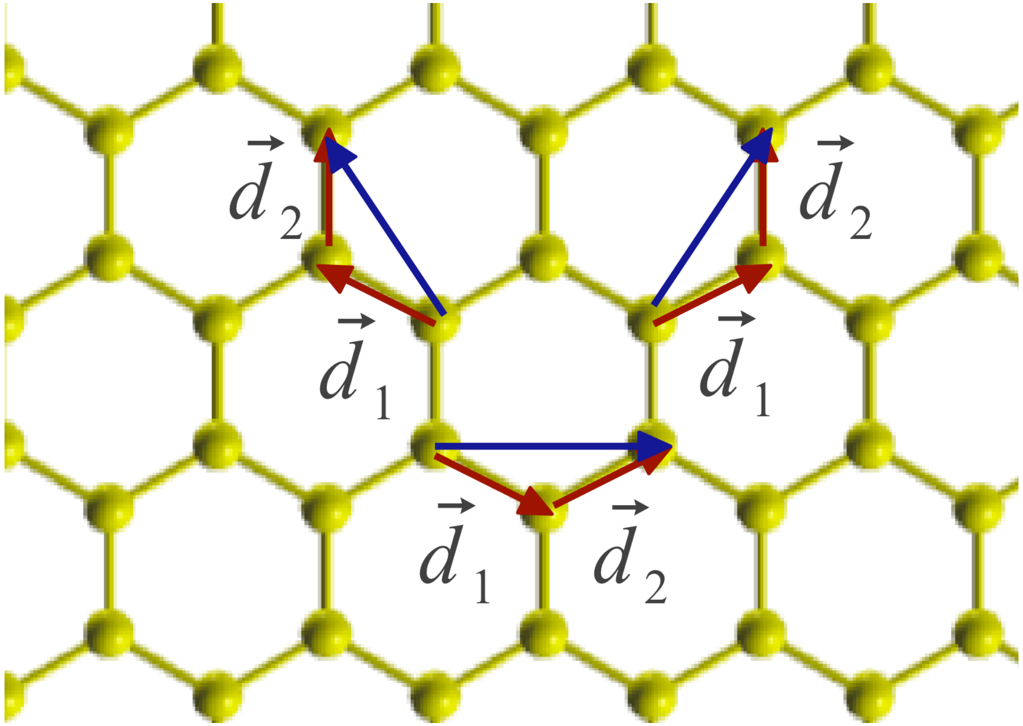

Spin dependent second neighbour hopping

$$\mathcal{H}_{SO} = it_{\mathrm{KM}}\vec{S}\cdot\left(\vec{d}_1 \times \vec{d}_2\right)$$

$$\mathcal{H}(\vec{k}) = \begin{pmatrix} \sigma h_{so}(\vec{k}) & h(\vec{k}) \\ h^*(\vec{k}) & -\sigma h_{so}(\vec{k}) \end{pmatrix}$$

Spin orbit coupling in 2D graphene opens up a gap

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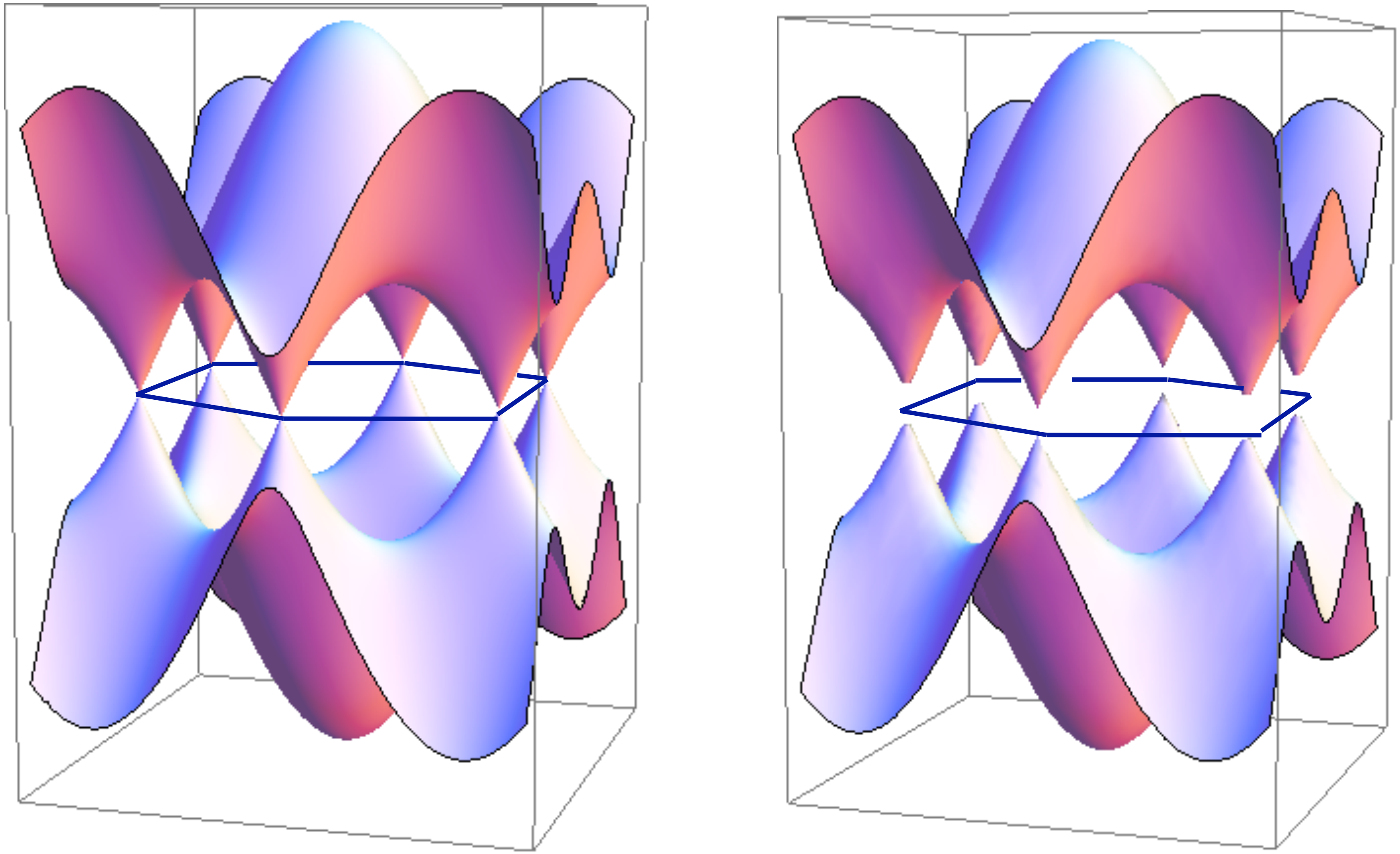
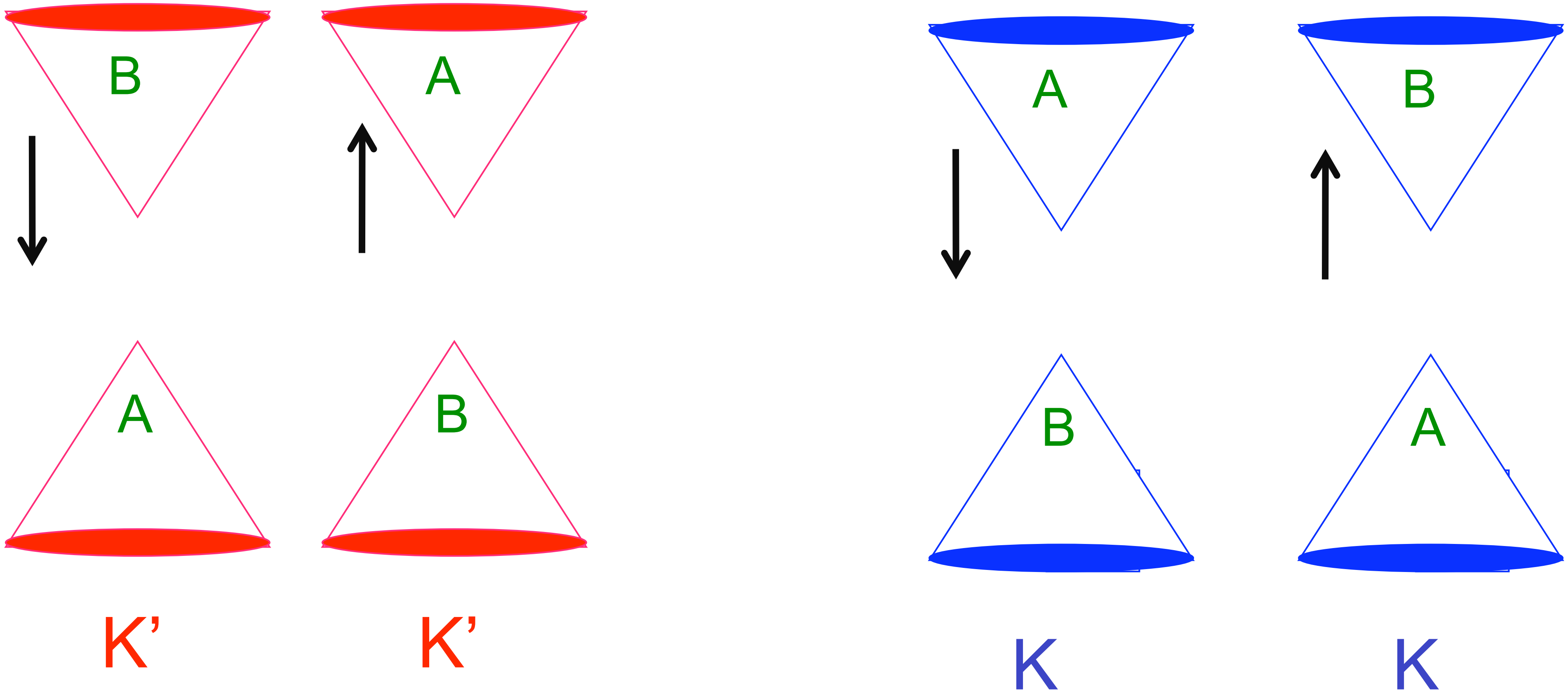


$$\mathcal{H}(\vec{k}) = \begin{pmatrix} 0 & h(\vec{k}) \\ h^*(\vec{k}) & 0 \end{pmatrix} \qquad \mathcal{H}(\vec{k}) = \begin{pmatrix} \sigma h_{so}(\vec{k}) & h(\vec{k}) \\ h^*(\vec{k}) & -\sigma h_{so}(\vec{k}) \end{pmatrix}$$

"Sign" of the gap is valley dependent

$$\mathcal{H}_{SO} = \Delta_{SO}\sigma_z\tau_z S_z$$



$$h_{SO}(K) = -h_{SO}(K') \equiv \Delta_{SO}$$

$$\mathcal{H}_{S_z}(K) = \begin{pmatrix} +S_z\Delta_{SO} & 0 \\ 0 & -S_z\Delta_{SO} \end{pmatrix} \quad \mathcal{H}_{S_z}(K') = \begin{pmatrix} -S_z\Delta_{SO} & 0 \\ 0 & +S_z\Delta_{SO} \end{pmatrix}$$

Edge states: the effect of spin orbit

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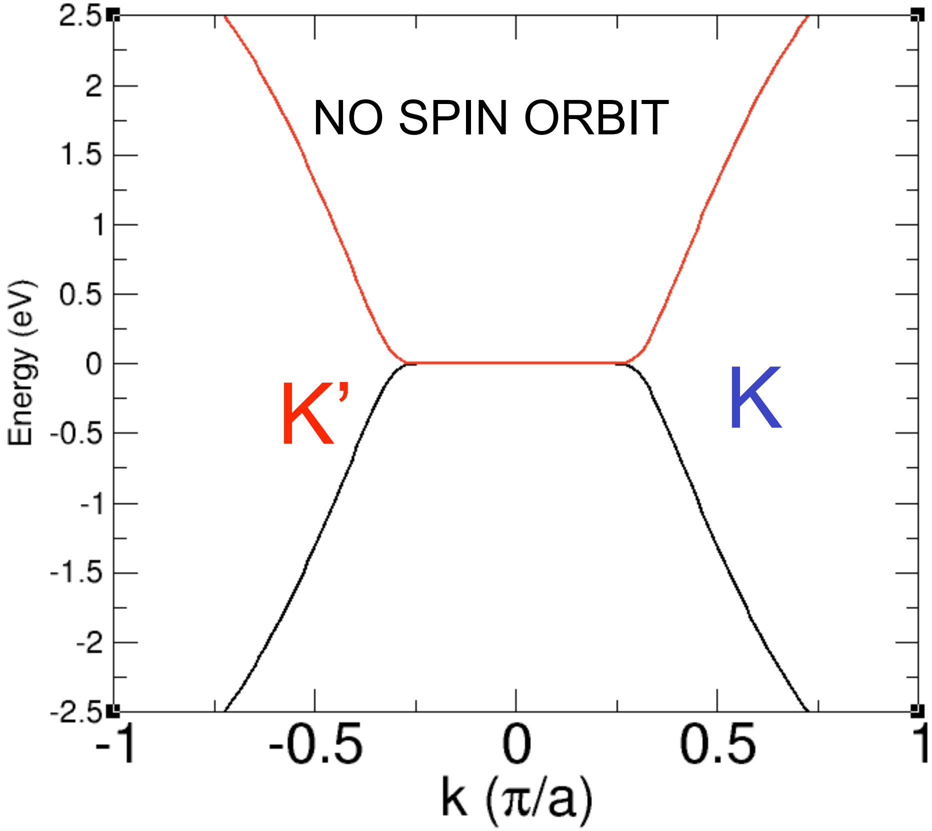

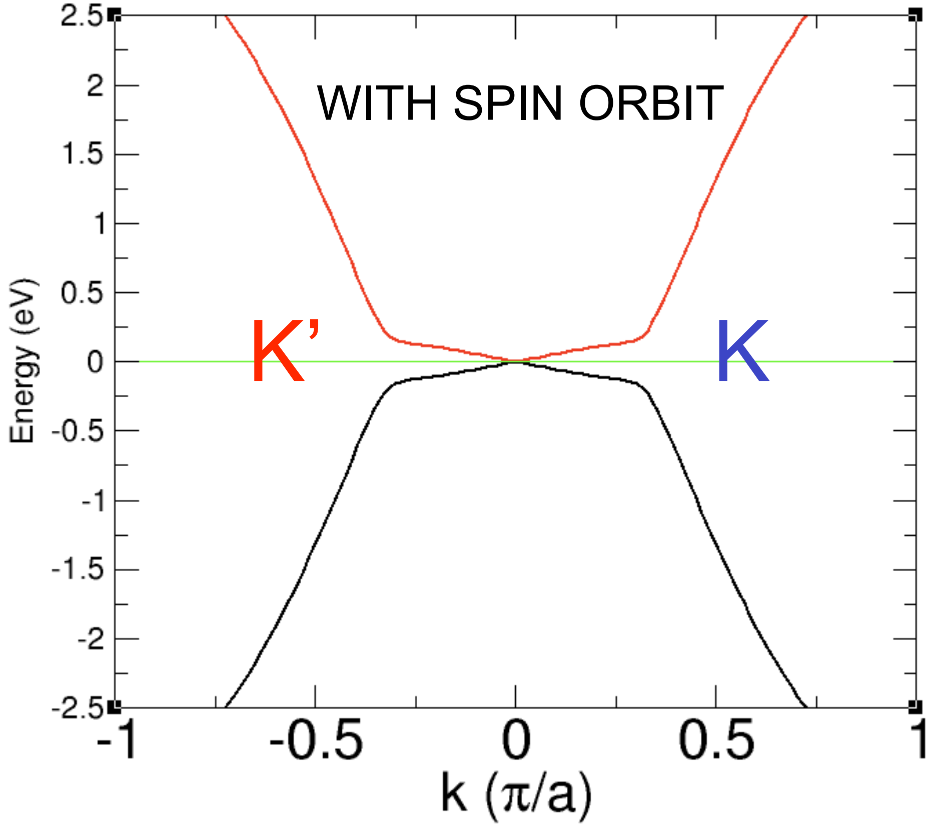

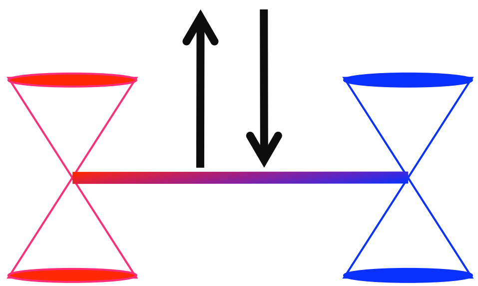

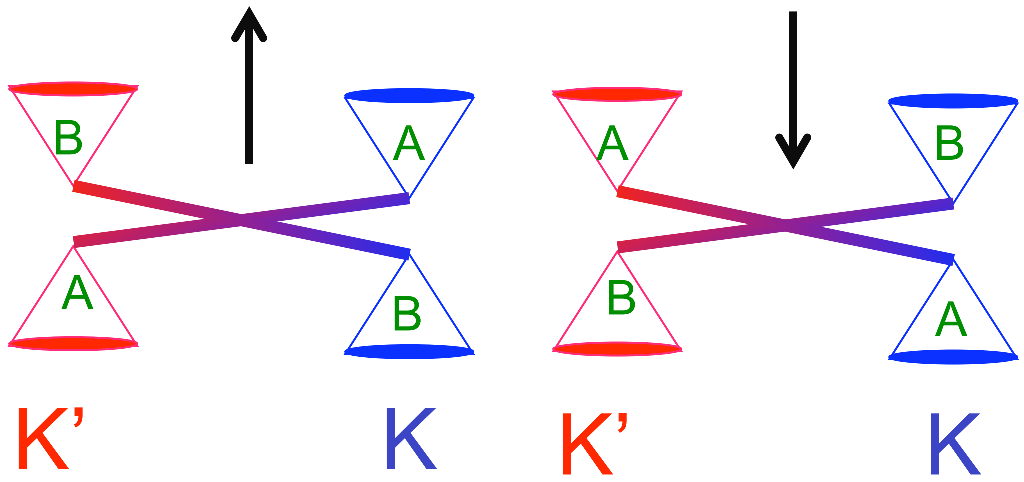

Spin filtered states

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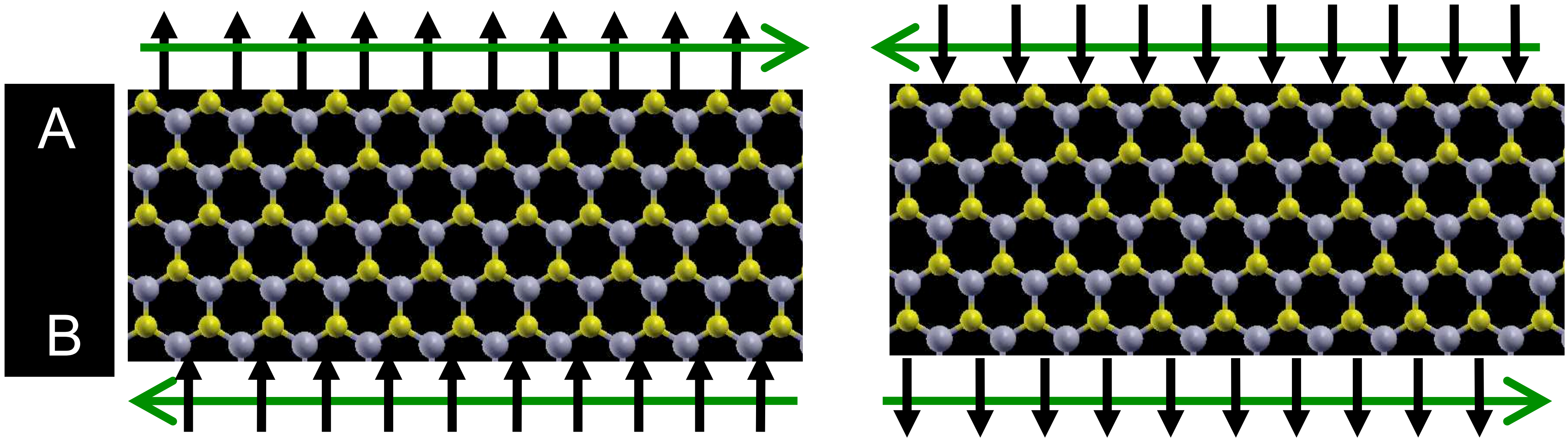
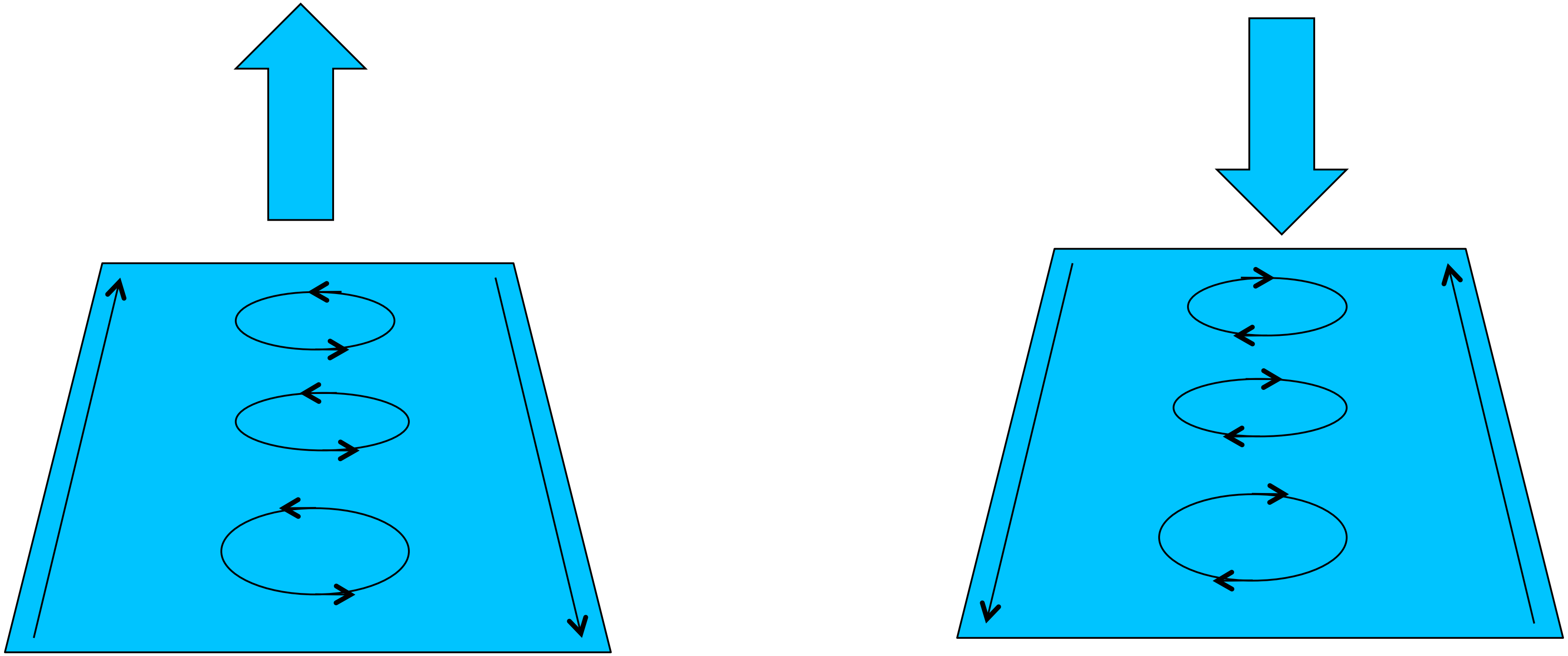
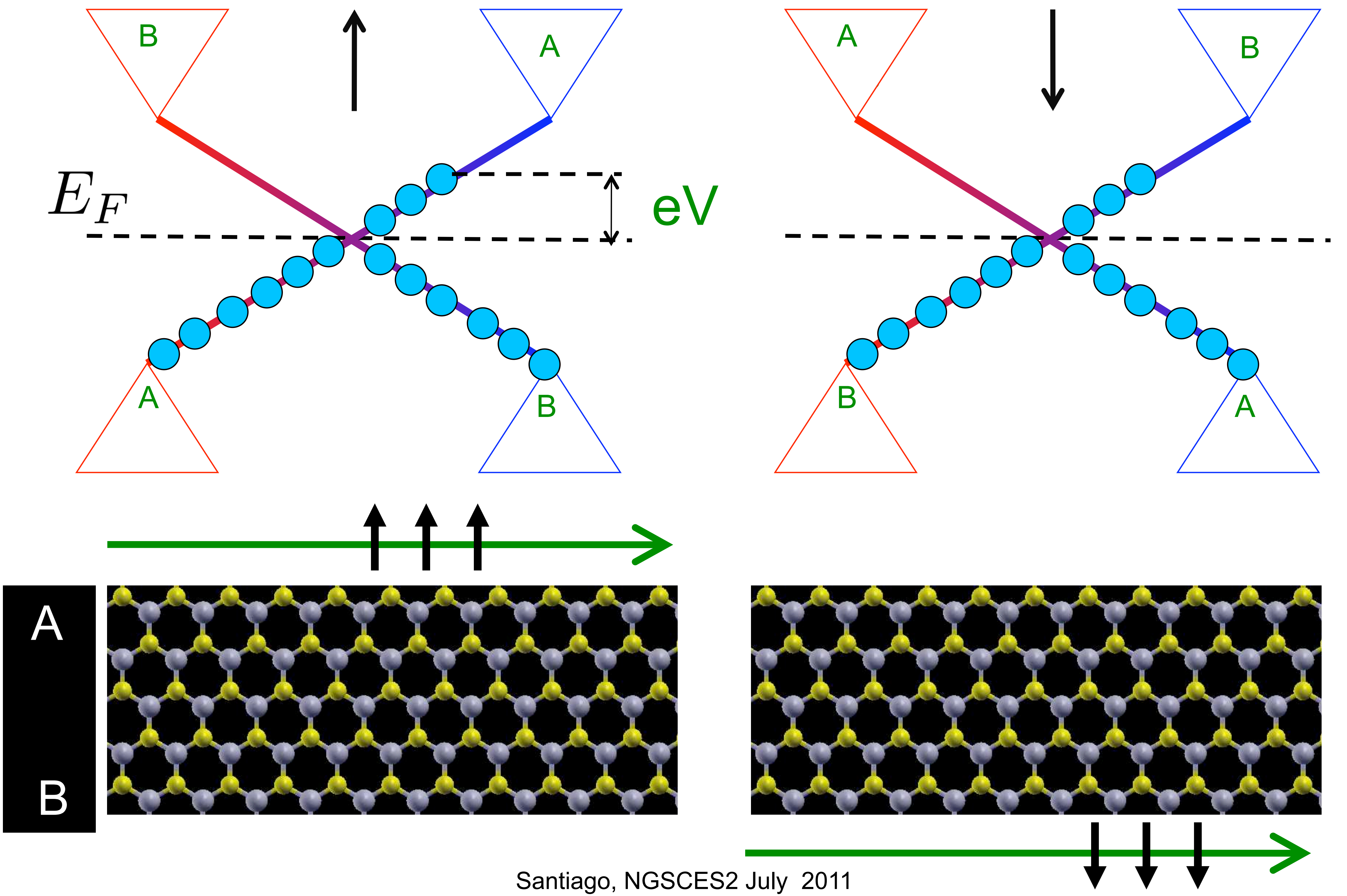


No inter-edge back scattering: quantization of condutcance

Spin Hall effect = 2 copies of Quantum Hall effect



Current flows implies spin accumulation



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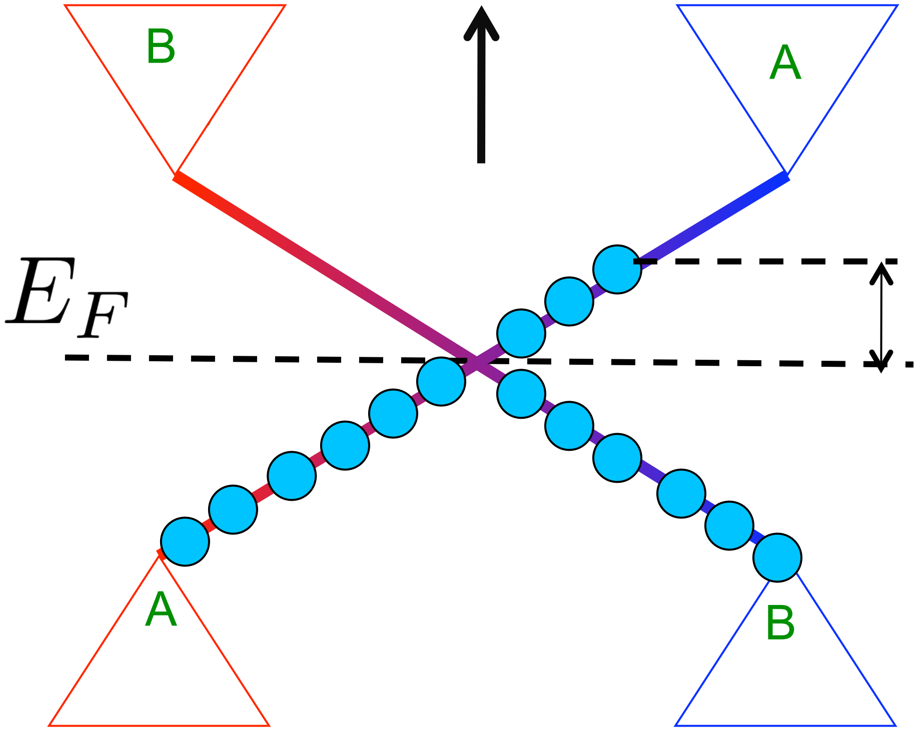


$$eV = \frac{eI}{G} \qquad G = \frac{e^2}{h}$$

$$\delta n = \int_{E_F}^{E_F + eV} \rho(E) dE$$

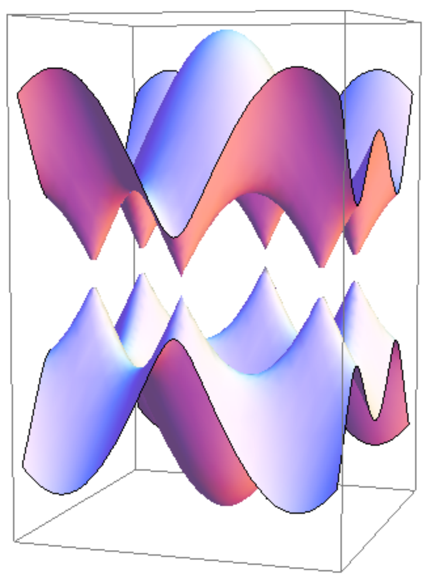
$$\delta n = \delta n_\uparrow^{\mathrm{A}} = \delta n_\downarrow^{\mathrm{B}}$$

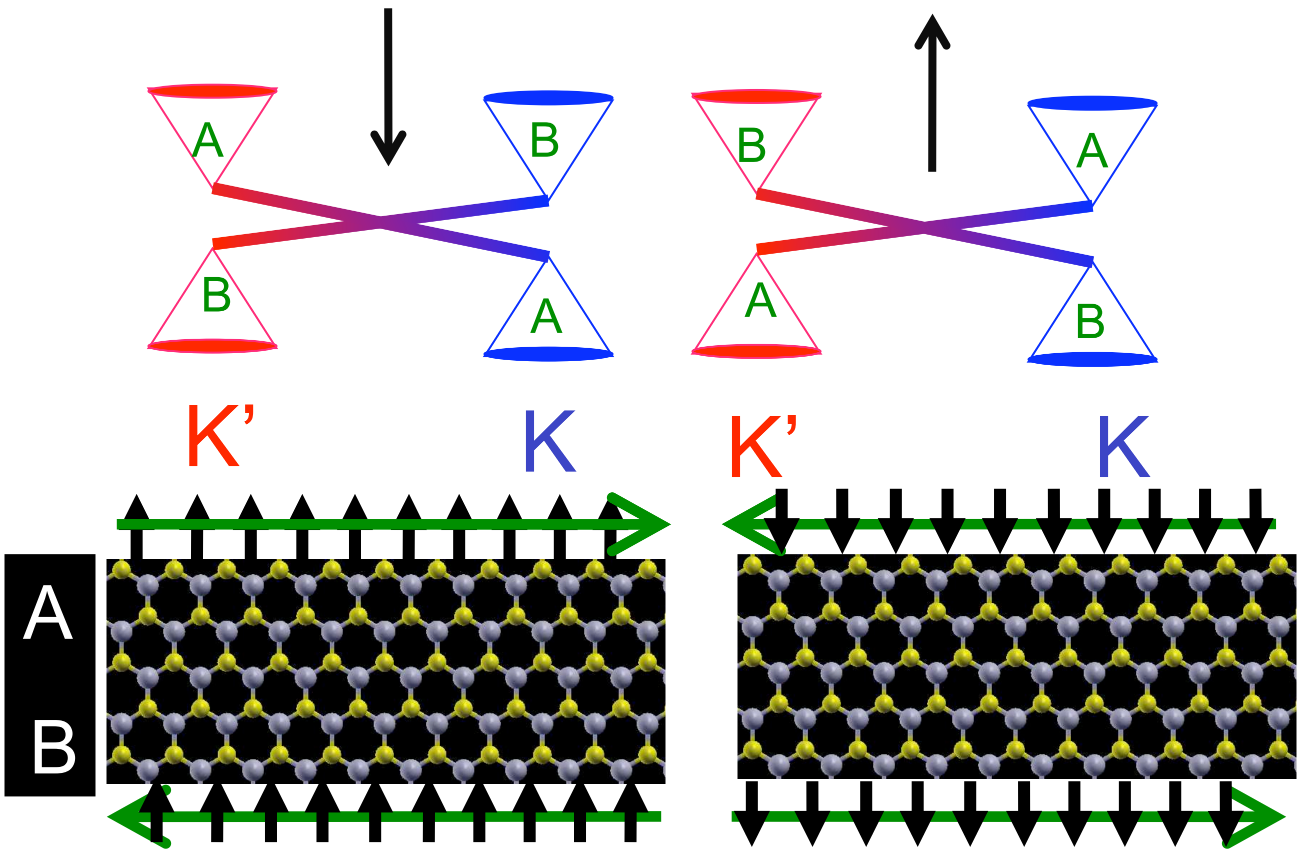
$$m = \frac{\delta n_\uparrow^{\mathrm{A}}}{2} = -\frac{\delta n_\downarrow^{\mathrm{B}}}{2}$$

$$\boxed{I_{\mathrm{edge}} = 4\pi \frac{e v_F}{a} m}$$

Soriano, JFR, PRB 2010

-Gap in bulk due to Spin orbit
-Spin filtered edge states with quantized conductance
--2 Copies of a Quantum Hall state
--Current implies spin accumulation (Spin Hall)





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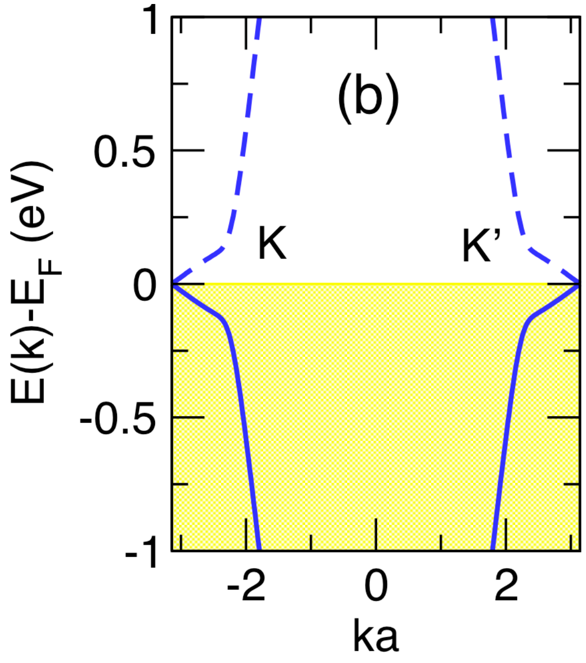
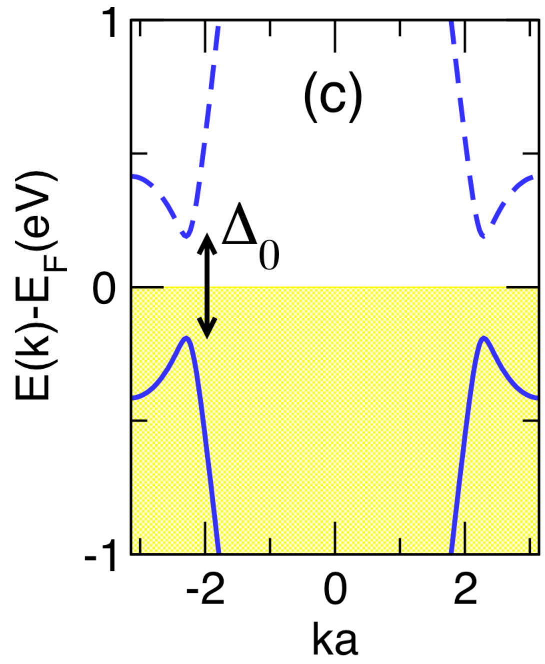




SO "on", Coulomb "off"
- -Conducting
- -Non magnetic edges
- -Spin currents in equilibrium

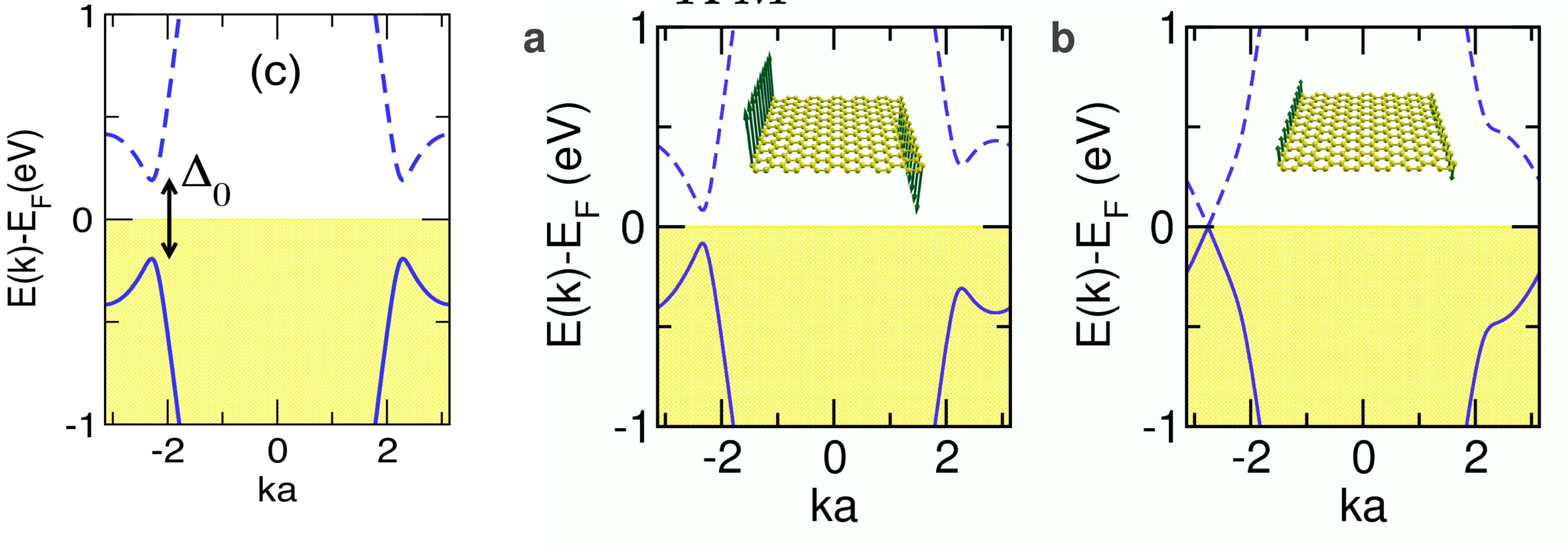
SO "off", Coulomb "on"
- -Non Conducting
- -Magnetic edges(AF)

Graphene ribbons: SO+ ee

D. Soriano, J. Fernández-Rossier,
Phys. Rev. B **82**, 161302 (2010)

Combined action of SO and Coulomb

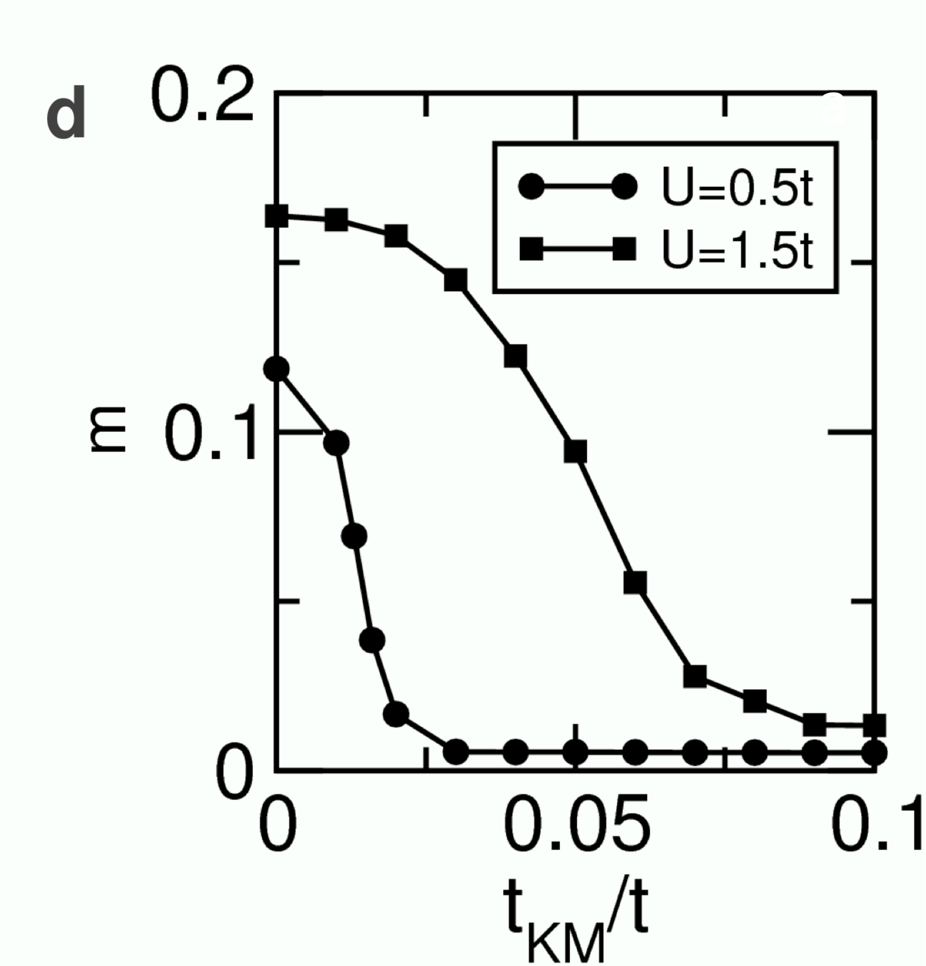
$t_{KM} = 0$ $\quad t_{KM} = 0.01t$ $\quad t_{KM} = 0.03t$

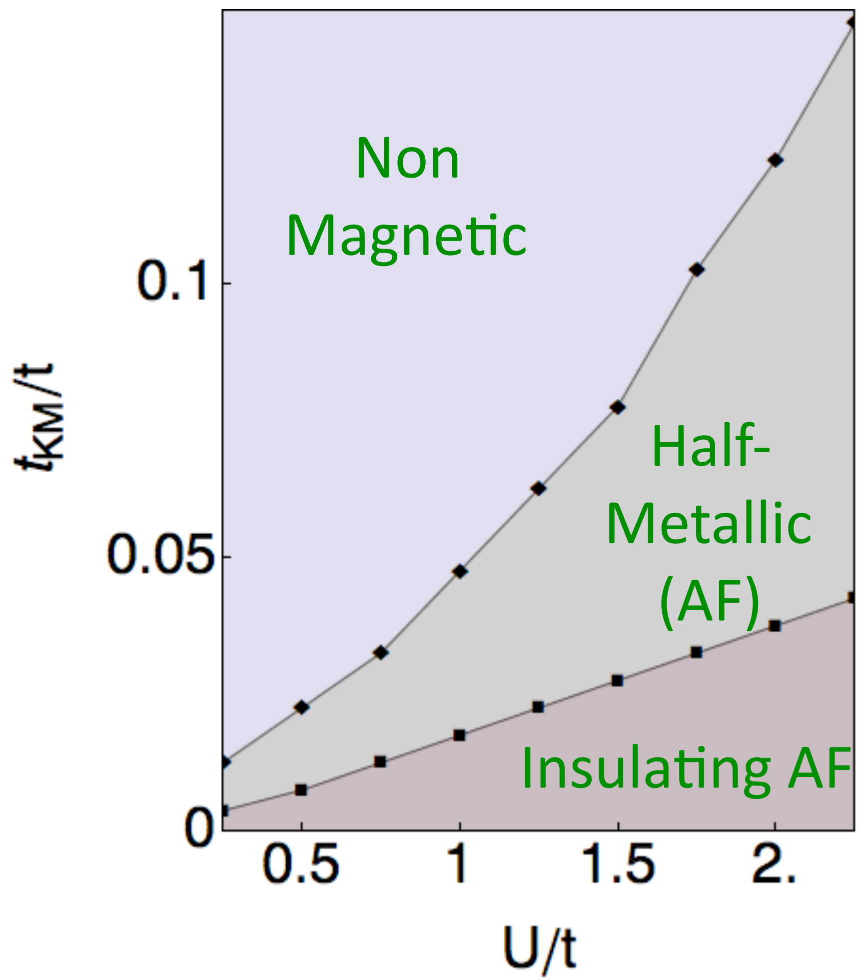


$$\mathcal{H} = \sum_{i,j,\sigma} t_{i,j}(\sigma) c^{\dagger}_{i,\sigma} c_{j,\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

$$t = U = 3eV \qquad i t_{KM} S_z \hat{z} \cdot \left(\vec{d}_1 \times \vec{d}_2\right)$$

SO depletes magnetization

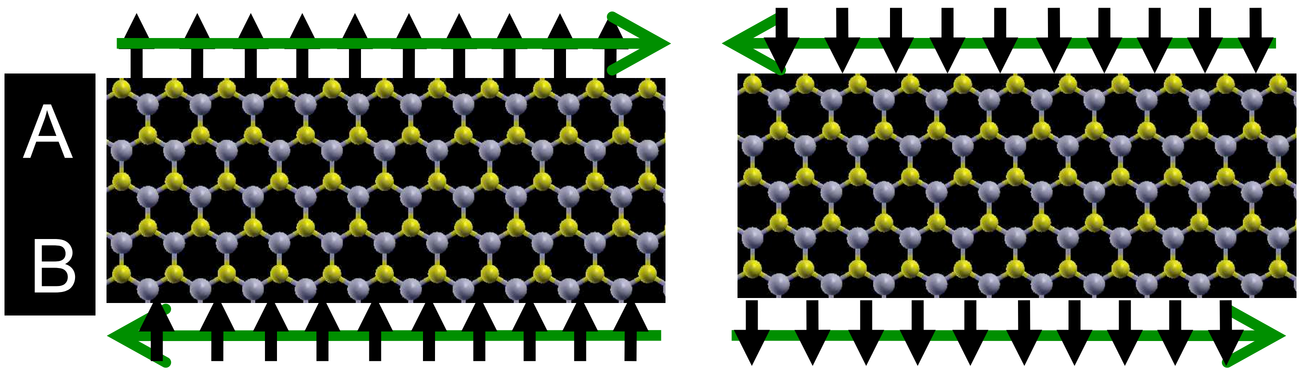




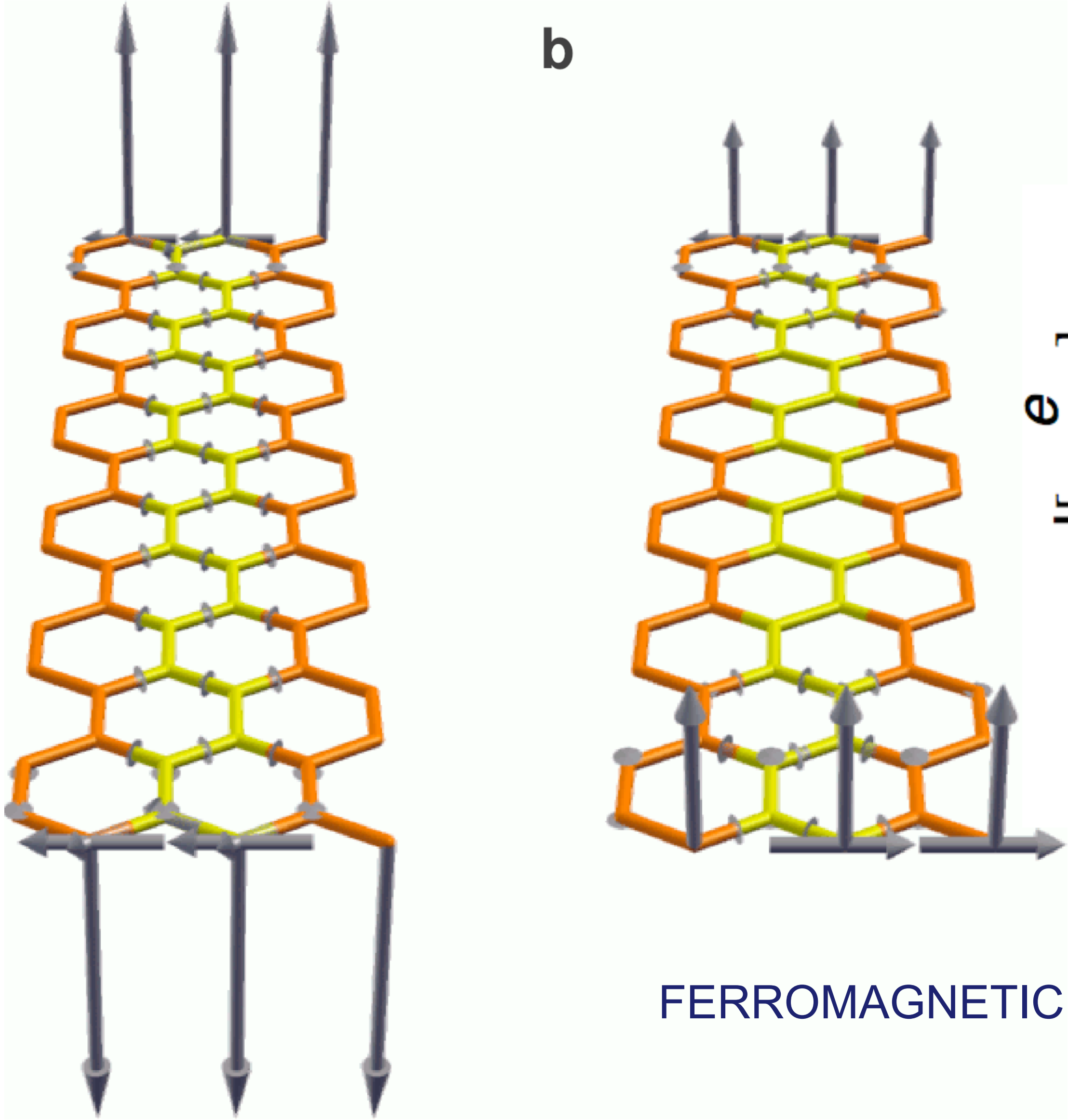
Magnetic order + spin currents= persistent charge currents?

$$\boxed{I_{\text{edge}} = 4\pi \frac{e v_F}{a} m}$$

Quantum Spin Hall effect

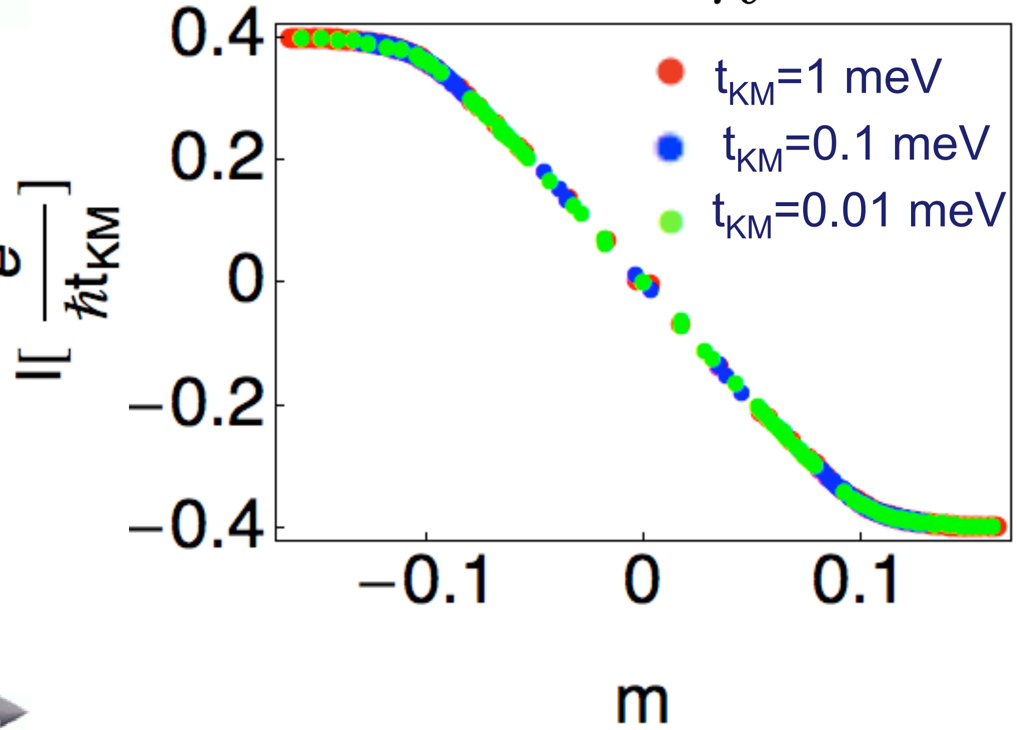


Persistent charge current



ANTIFERROMAGNETIC

$$|I_{\mathrm{edge}}| \simeq 0.4\frac{e}{\hbar}t_{KM}$$



Current in the edges is compensated by **counterflow** in bulk

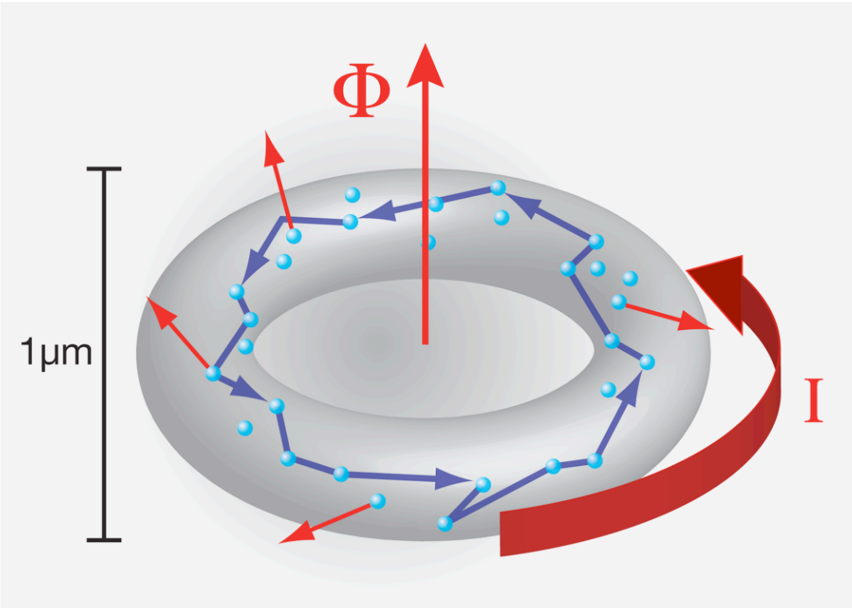
Estimate of the current

$$|I_{\rm edge}| \simeq 0.4\frac{e}{\hbar}t_{KM}$$

$$t_{KM} = 10\mu eV \longrightarrow |I_{\rm edge}| \simeq 0.4nA$$

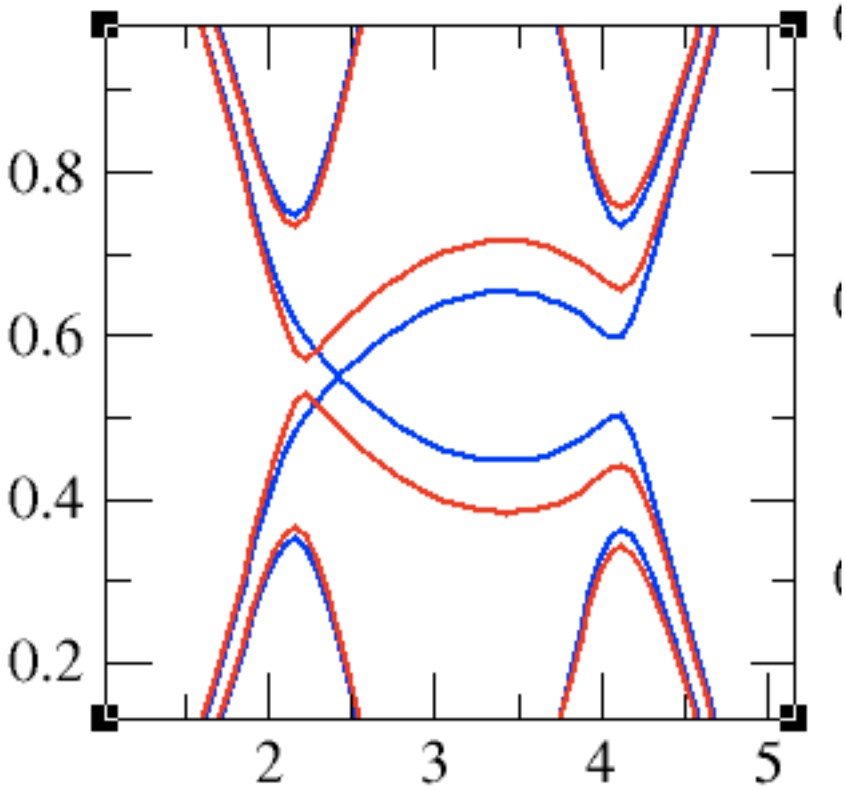
Realistic

Comparable to persistent currents in Mesoscopic gold rings



Persistent current in graphene:
- No external magnetic field
- Self sustained by spontaneous magnetic order
- Caused by Spin Orbit coupling

Graphene ribbons: SO+ ee + Stagg.



-Ferromagnetic Edges, AF coupled
-Half Metal in spin
-Half Metal in valley

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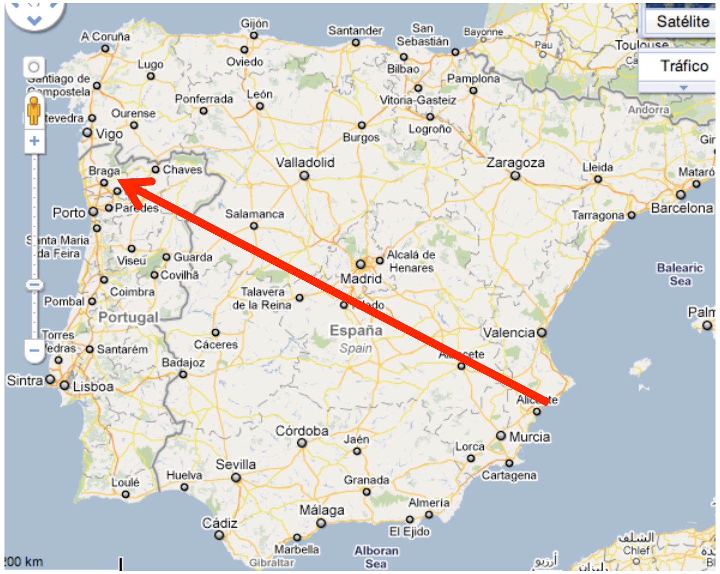
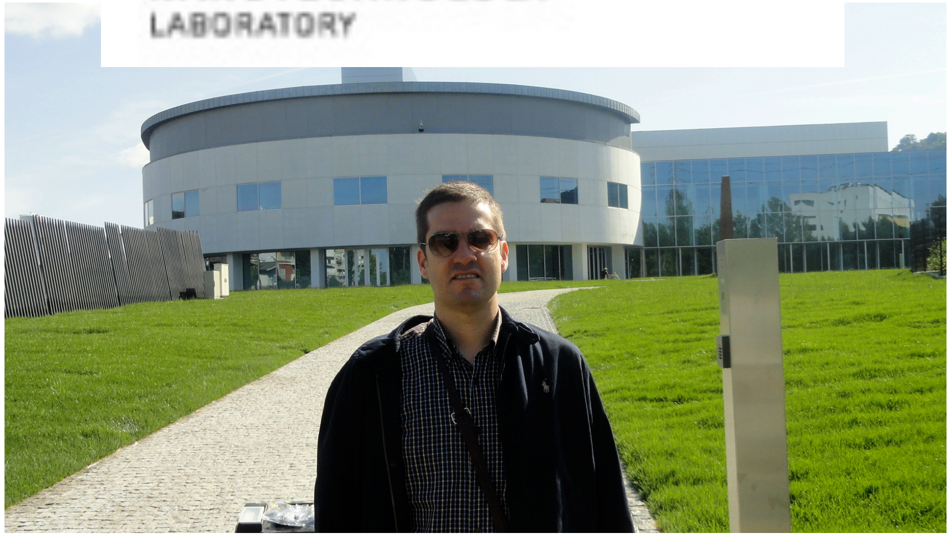
Moving to

INL
INTERNATIONAL IBERIAN
NANOTECHNOLOGY
LABORATORY



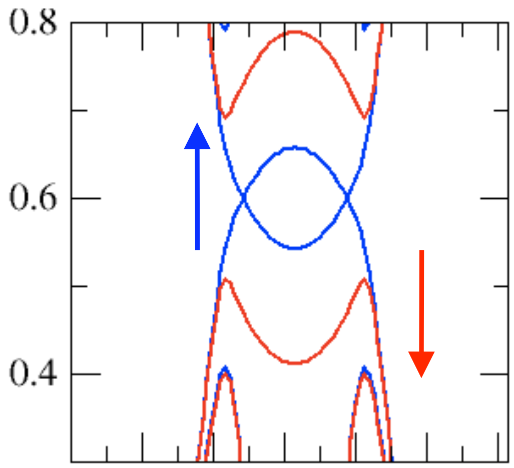


3 Postodc Openings for September 2011
Spintronics and Photonics in Semiconductors
(Graphene, Topological Insulators, Si, CdTe)
Up to 3 years
Very competitive salaries

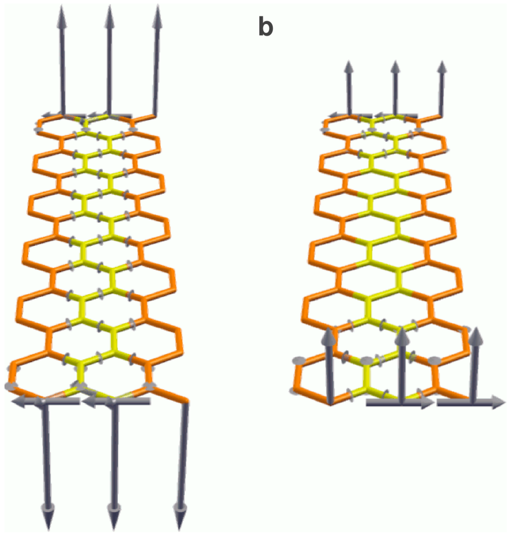
Joaquin.fernandez-rossier@inl.int

Final conclusions

The interplay between topological and conventional order can result in non-trivial electronic phases, even in chemically simple systems



AF Half Metal



Than you very much for your attention