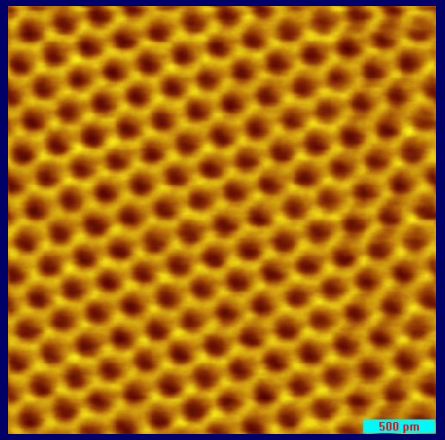
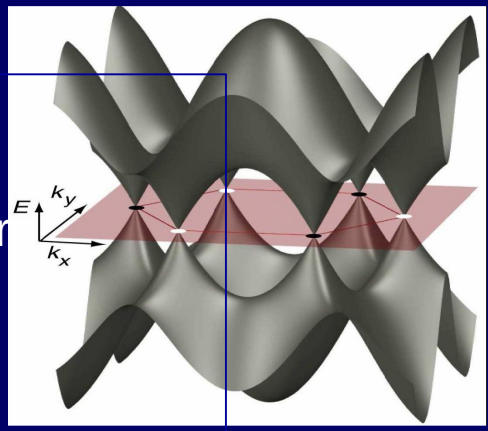
Electronic properties of Graphene and 2-D materials





- 2D materials – background
  - Carbon allotropes
  - Graphene Structure and Band structur
  - Electronic properties
- Electrons in a magnetic field
  - Onsager relation
  - Landau levels
  - Quantum Hall effect
- Engineering electronic properties
  - Kondo effect
  - Atomic collapse and artificial atom
  - Twisted graphene

Eva Y. Andrei

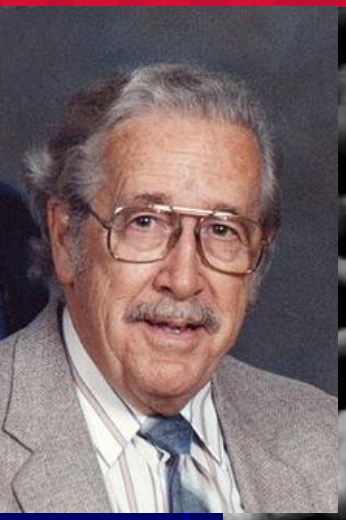
Rutgers University

Aug 27-29, 2018

Summer School on Collective Behaviour in Quantum Matter

ICTP

Graphene: a theorists invention



PHYSICAL REVIEW VOLUME 71, NUMBER 9 MAY 1, 1947

The Band Theory of Graphite

P. R. WALLACE*
National Research Council of Canada, Chalk River Laboratory, Chalk River, Ontario
(Received December 19, 1946)

The structure of the electronic energy bands and Brillouin zones for graphite is developed using the "tight binding" approximation. Graphite is found to be a semi-conductor with zero activation energy, i.e., there are no free electrons at zero temperature, but they are created at higher temperatures by excitation to a band contiguous to the highest one which is normally filled. The electrical conductivity is treated with assumptions about the mean free path. It is found to be about 100 times as great parallel to as across crystal planes. A large and anisotropic diamagnetic susceptibility is predicted for the conduction electrons; this is greatest for fields across the layers. The volume optical absorption is accounted for.

PHYSICAL REVIEW VOLUME 109, NUMBER 2 JANUARY 15, 1

Band Structure of Graphite*

J. C. SLONCZEWSKI† AND P. R. WEISS
Rutgers, The State Univ[illegible], New Brunswick, New Jersey

PHYSICAL REVIEW LETTERS
VOLUME 53 24 DECEMBER 1984 NUMBER 26

Condensed-Matter Simulation of a Three-Dimensional Anomaly

Gordon W. Semenoff
The Institute for Advanced Study, Princeton, New Jersey 08540, and Department of Physics,[a] University of British Columbia, Vancouver, British Columbia V6T 2A6, Canada
(Received 4 September 1984)

A condensed-matter analog of (2+1)-dimensional electrodynamics is constructed, and [illegible] of a recently discovered anomaly in such systems are discussed.

VOLUME 61, NUMBER 18 PHYSICAL REVIEW LE

Model for a Quantum Hall Effect without Landau Levels: Condensed-Matter Realization of the "Parity Anomaly"

F. D. M. Haldane
Department of Physics, University of California, San Diego, La Jolla, California 92093
(Received 16 September 1987)

A two-dimensional condensed-matter lattice model is presented which exhibits a nonzero quantization of the Hall conductance σ^{xy} in the *absence* of an external magnetic field. Massless fermions *without spectral doubling* occur at critical values of the model parameters, and exhibit the so-called "parity anomaly" of (2+1)-dimensional field theories.

No long range order in 2-Dimensions

David Mermin

Herbert Wagner

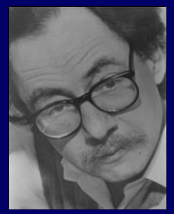
.. *long-range fluctuations*
can be created with little energy cost and
since they increase the entropy they are favored.

It is pointed out that a rigorous inequality first proved by Bogoliubov may be used to rule out the existence of quasi-averages (or long-range order) in Bose and Fermi systems for one and two dimensions and $T \neq 0$.

Commun. math. Phys. 31, 259—264 (1973)

There are no Goldstone Bosons in Two Dimensions*

Sidney Coleman**



VOLUME 17, NUMBER 22 PHYSICAL REVIEW LETTERS 28 NOVEMBER 1966

ABSENCE OF FERROMAGNETISM OR ANTIFERROMAGNETISM IN ONE- OR TWO-DIMENSIONAL ISOTROPIC HEISENBERG MODELS*

N. D. Mermin† and H. Wagner‡

Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, New York

(Received 17 October 1966)

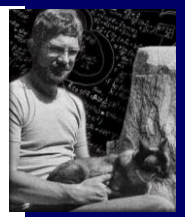
It is rigorously proved that at any nonzero temperature, a one- or two-dimensional isotropic spin-S Heisenberg model with finite-range exchange interaction can be neither ferromagnetic nor antiferromagnetic. The method of proof is capable of excluding a variety of types of ordering in one and two dimensions.

J. Phys. C: Solid State Phys., Vol. 6, 1973. Printed in Great Britain. © 1973

Ordering, metastability and phase transitions in two-dimensional systems

J M Kosterlitz and D J Thouless

Department of Mathematical Physics, University of Birmingham, Birmingham B15 2TT, UK



…continuous symmetries cannot be spontaneously broken at finite temperature in systems with sufficiently short-range interactions in dimensions D ≤ 2.

No long range order in 2D

… No Magnets

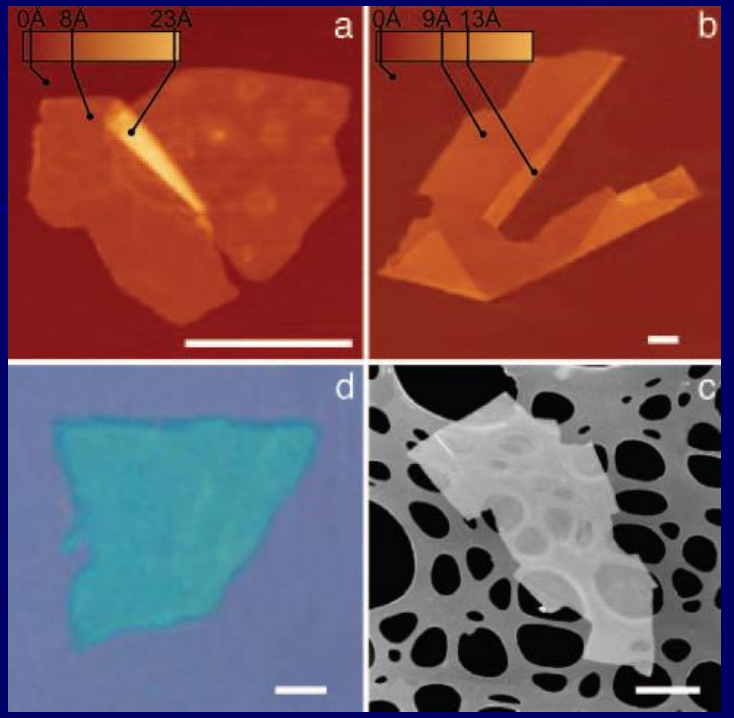
….No superfluids

…No superconductors

… No 2D crystals

E.Y. Andrei

First 2D materials



Graphene, hBN, MoS_2, $NbSe_2$, $Bi_2Sr_2CaCu_2O_x$,

PNAS

Two-dimensional atomic crystals

K. S. Novoselov*, D. Jiang*, F. Schedin*, T. J. Booth*, V. V. Khotkevich*, S. V. Morozov†, and A. K. Geim*‡

*Centre for Mesoscience and Nanotechnology and School of Physics and Astronomy, University of Manchester, Manchester M13 9PL, United Kingdom; and †Institute for Microelectronics Technology, Chernogolovka 142432, Russia

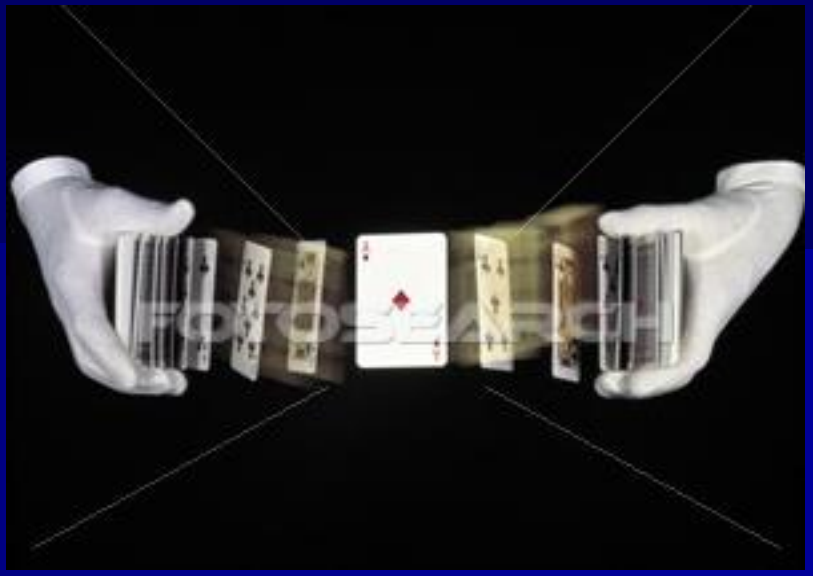
Edited by T. Maurice Rice, Swiss Federal Institute of Technology, Zurich, Switzerland, and approved June 7, 2005 (received for review April 6, 2005)

We report free-standing atomic crystals that are strictly 2D and can be viewed as individual atomic planes pulled out of bulk crystals or as unrolled single-wall nanotubes. By using micromechanical cleavage, we have prepared and studied a variety of 2D crystals including single layers of boron nitride, graphite, several dichalcogenides, and complex oxides. These atomically thin sheets (essentially gigantic 2D molecules unprotected from the immediate environment) are stable under ambient conditions, exhibit high crystal quality, and are continuous on a macroscopic scale.

wafer (Fig. 1*d*), because even a monolayer adds up sufficiently to the optical path of reflected light so that the interference color changes with respect to the one of an empty substrate (phase contrast). The whole procedure takes literally half an hour to implement and identify probable 2D crystallites. Their further analysis was done by atomic force microscopy (AFM), for which single-layer crystals were selected as those exhibiting an apparent (12) thickness of approximately the interlayer distance in the corresponding 3D crystals.

Can We Cheat Nature?

ANY LAYERED MATERIAL



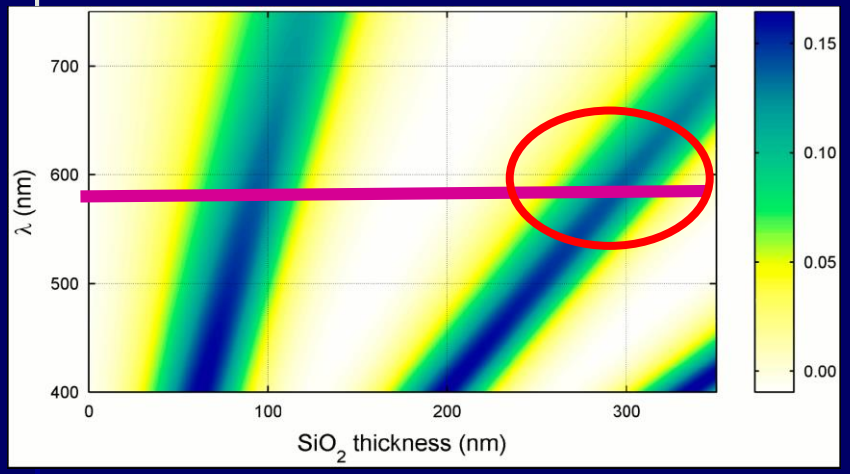
SLICE DOWN TO
ONE ATOMIC PLANE?

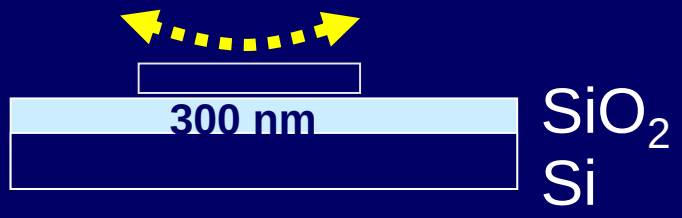
A. Geim

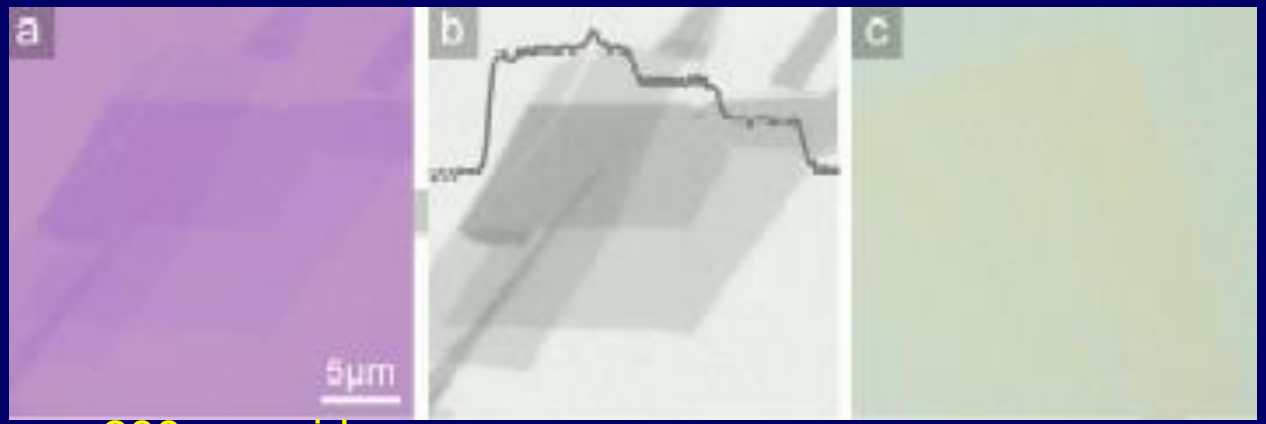
Making graphene

P. Blake et.al, 2007
D. S. L. Abergel 2007
S. Roddaro et. al Nano Letters 2007

Novoselev et al (2005)



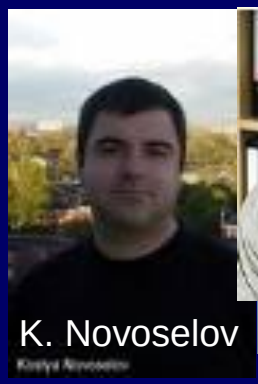




300nm oxide
White light

300nm oxide
560nm green light

200nm oxide
White light

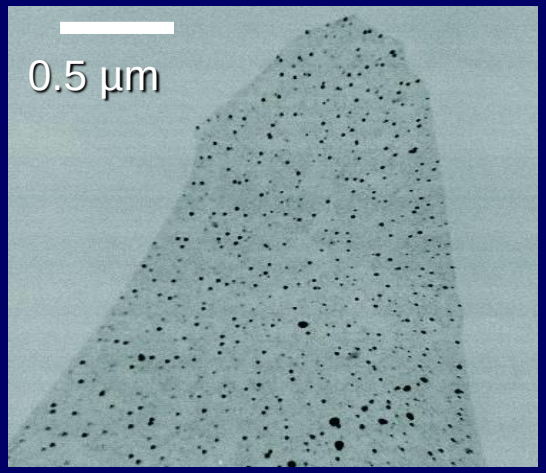

K. Novoselov


Andre Geim

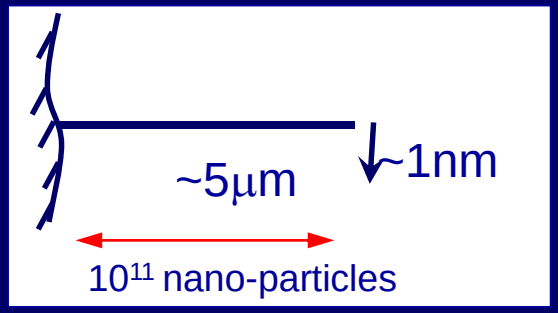
E.Y. Andrei

Properties: Mechanical

Unsupported graphene with Cu particles



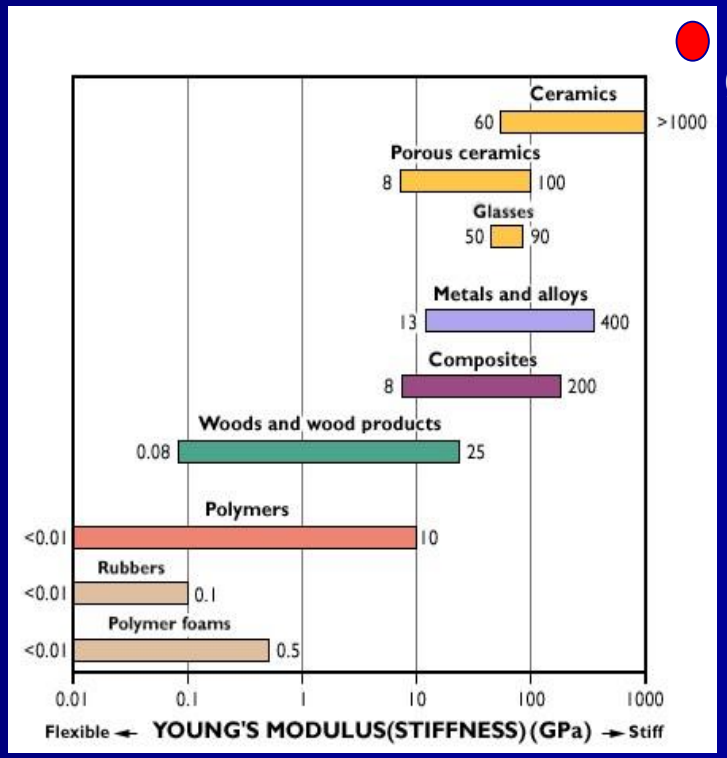
Young's modulus E ~ 2TPa
Stiffest materal



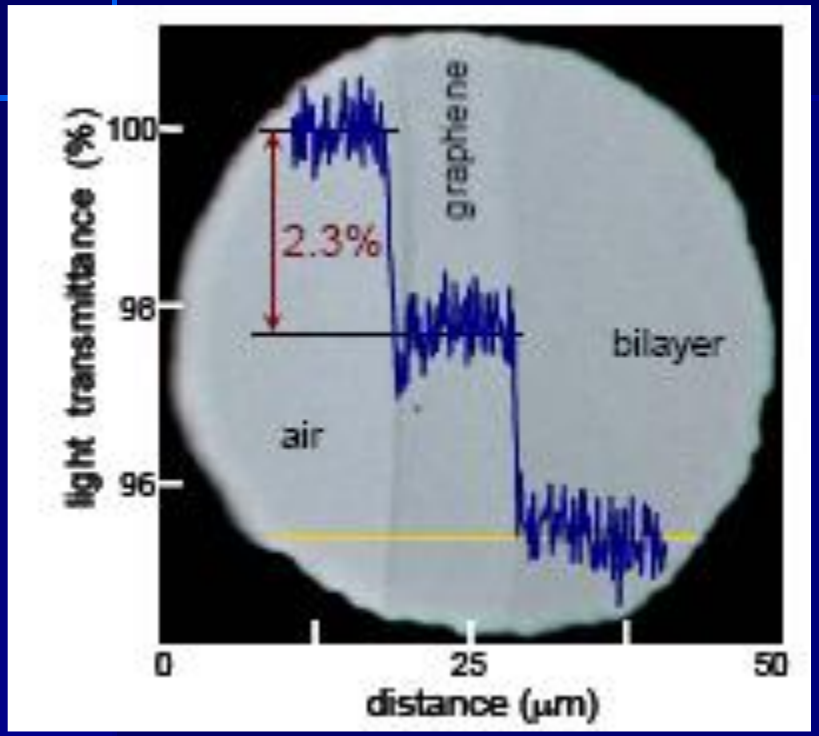
T. Booth et al,Nano Letters'08

- Young's modulus ~ 2 TPa

graphene



Properties: Optical

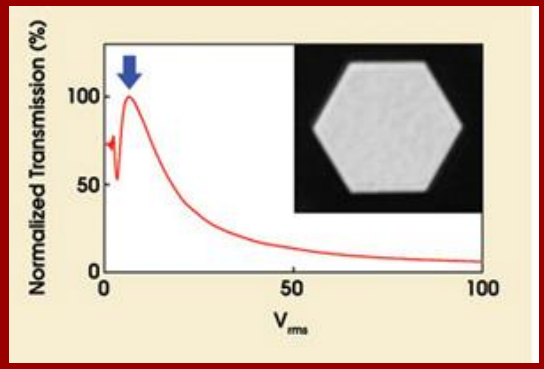


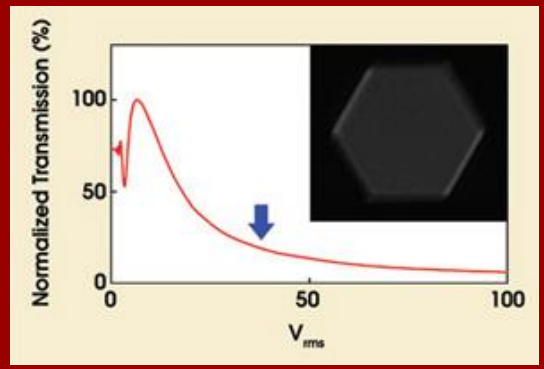
Transmittance at Dirac point:

$T=1-\alpha\pi=97.2\%$

R.R. Nair et al, Science (2008).

,

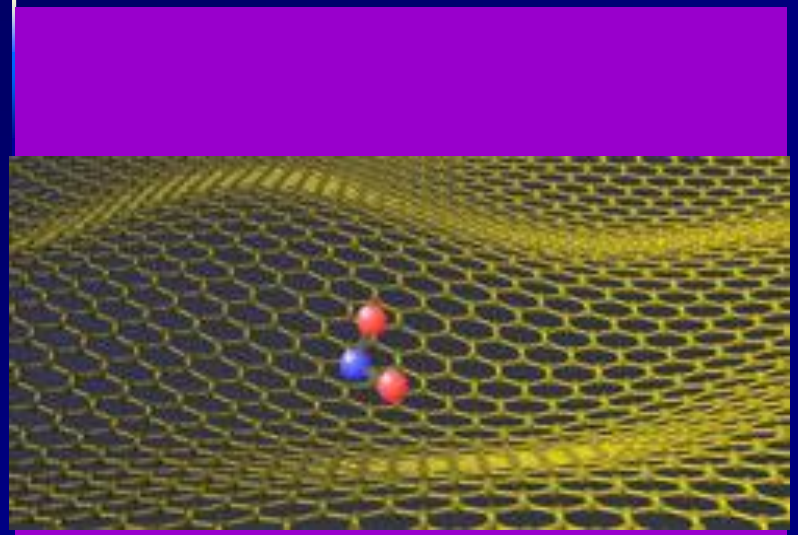


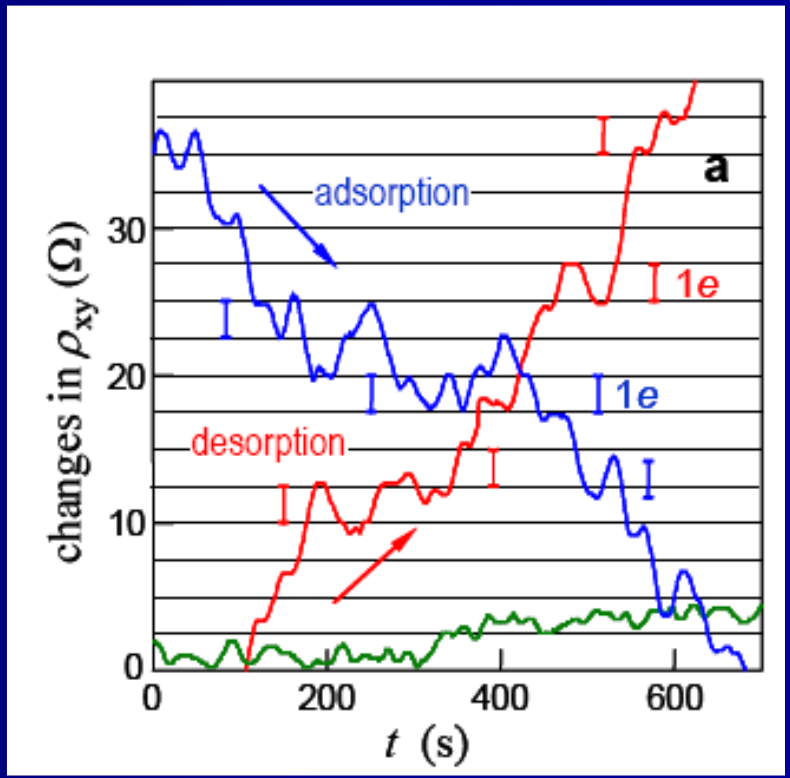


P. Blake *et al*, *Nano Letters*, '08

Properties: Chemical

Single molecule detection
NO_2, NH_3, CO

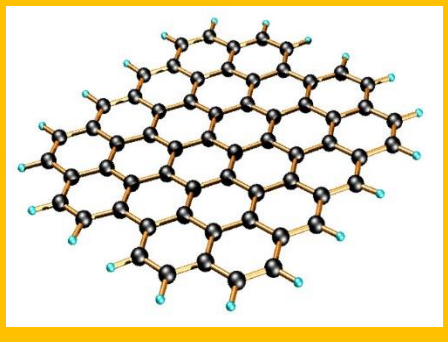




F Schedin *et al*,*Nature Materials* '07

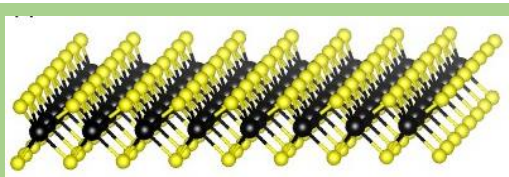
2D Building Blocks

Graphene family



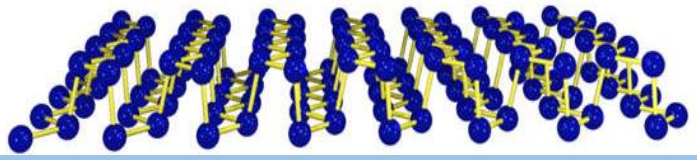
E.g.: Graphene, hBN, Silicene, Germanene, Stanene.

Transition Metal Dichalcogenides (TMDCs)



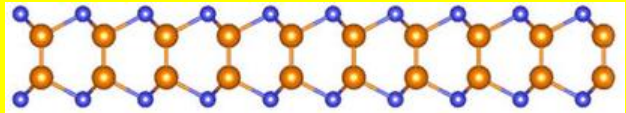
E.g.: MoS_2 ,WSe_2 , NbS_2, TaS_2

Phosphorene family



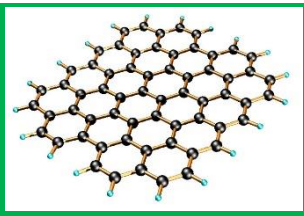
E.g.: Phosphorene, SnS, GeS, SnSe, GeSe

Group 13 Monochalcogenides



E.g.: GaS, InSe

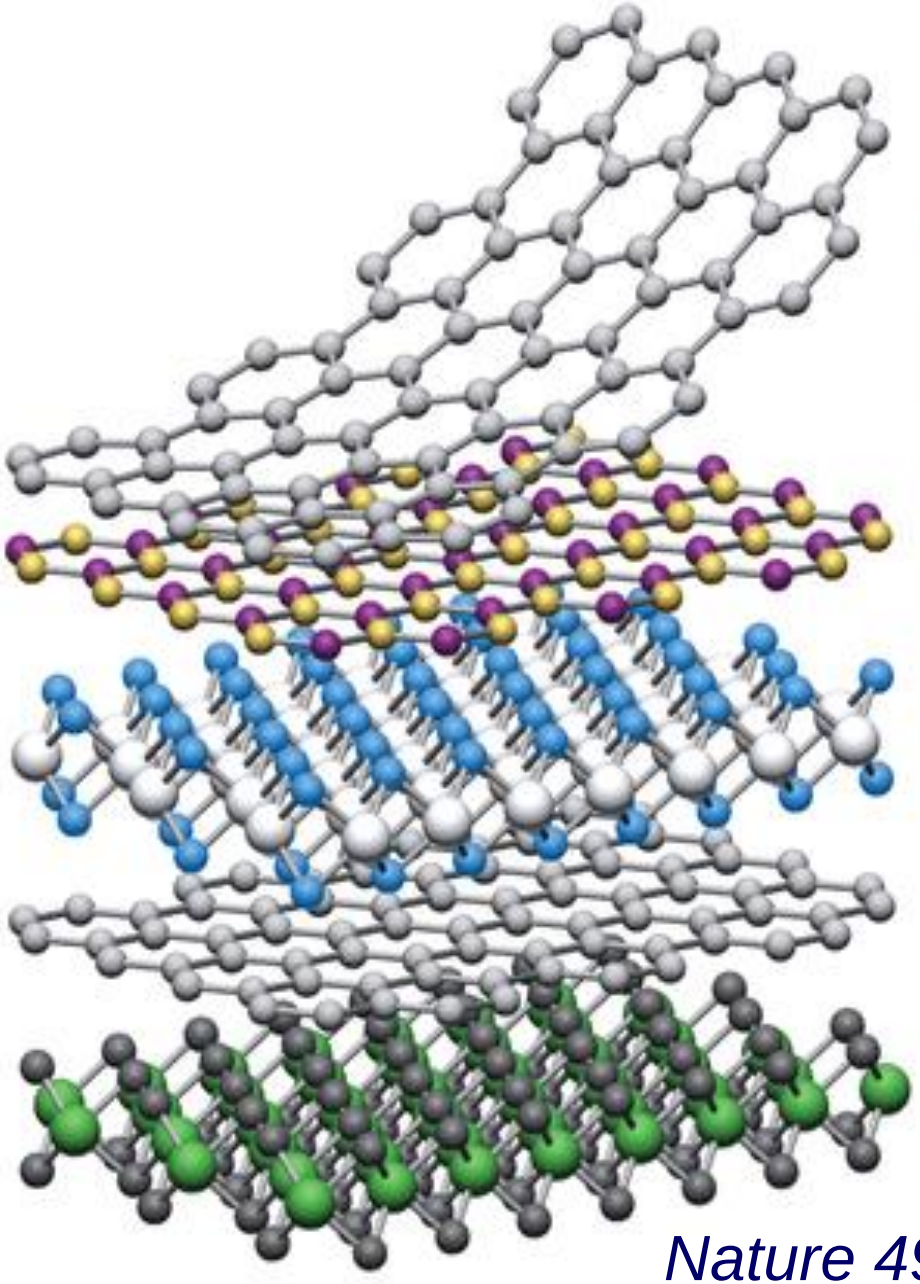
Group 2 Monochalcogenides

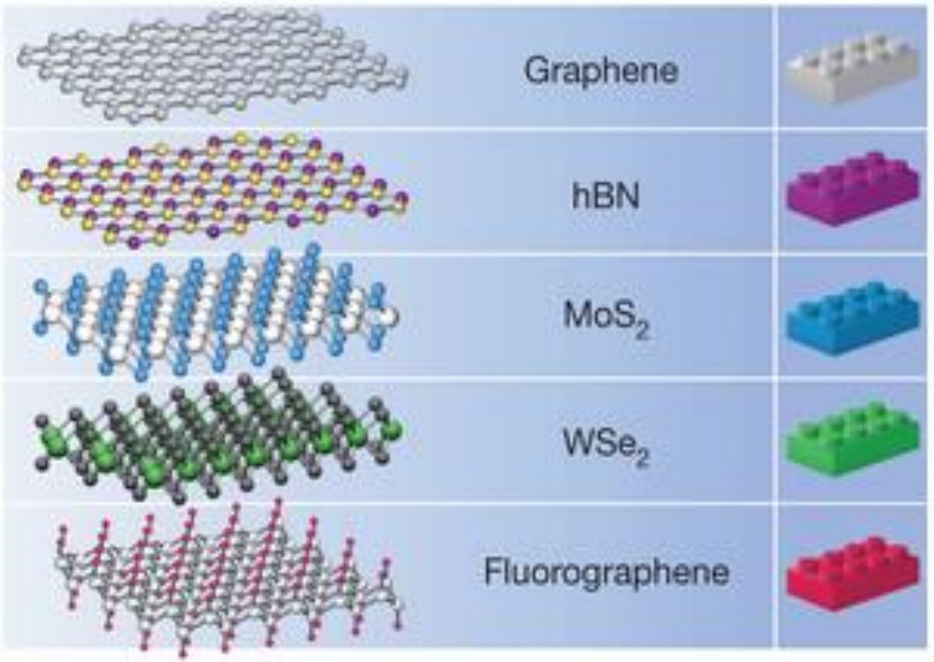


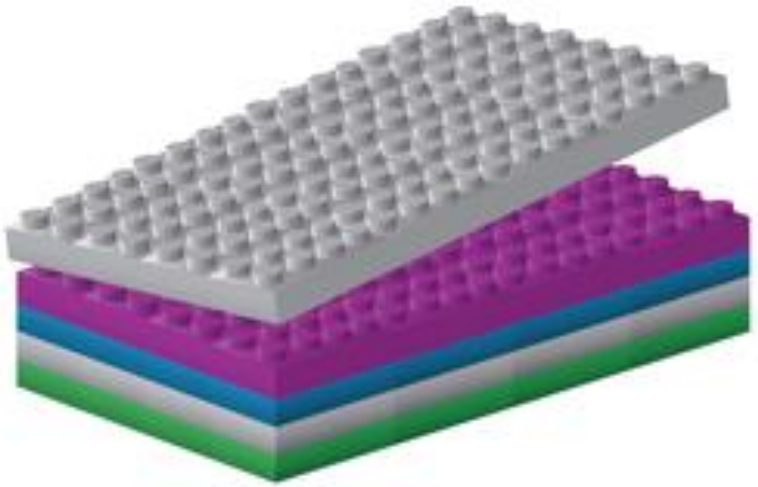
E.g.: BaS, CaS, MgS

- About 40 2D materials are currently known.
- About half of them have been isolated.
- Others shown to be stable using simulations.

Van der Waals heterostructures

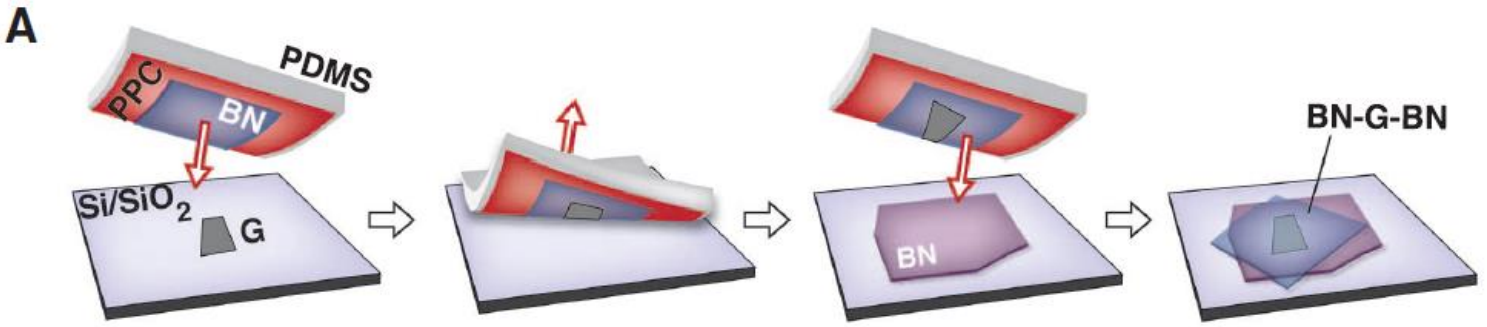


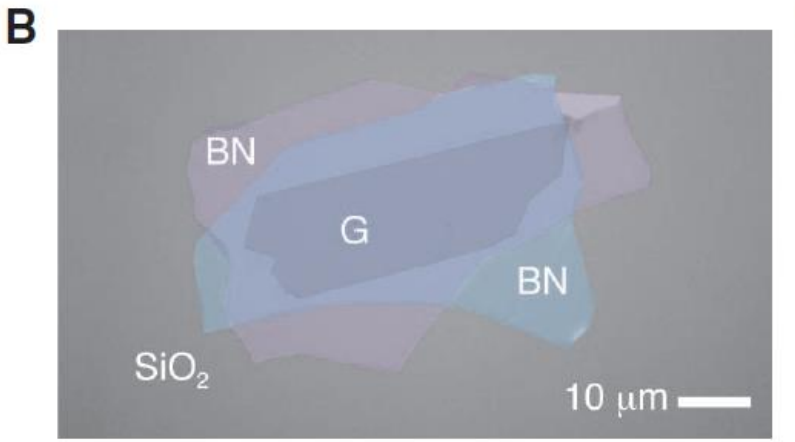


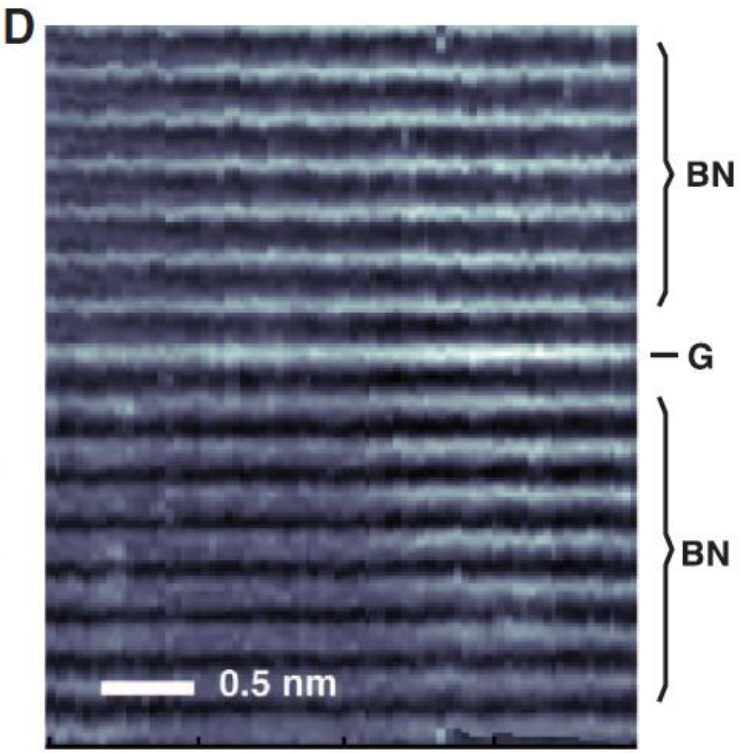


Nature 499, 419 (2013)

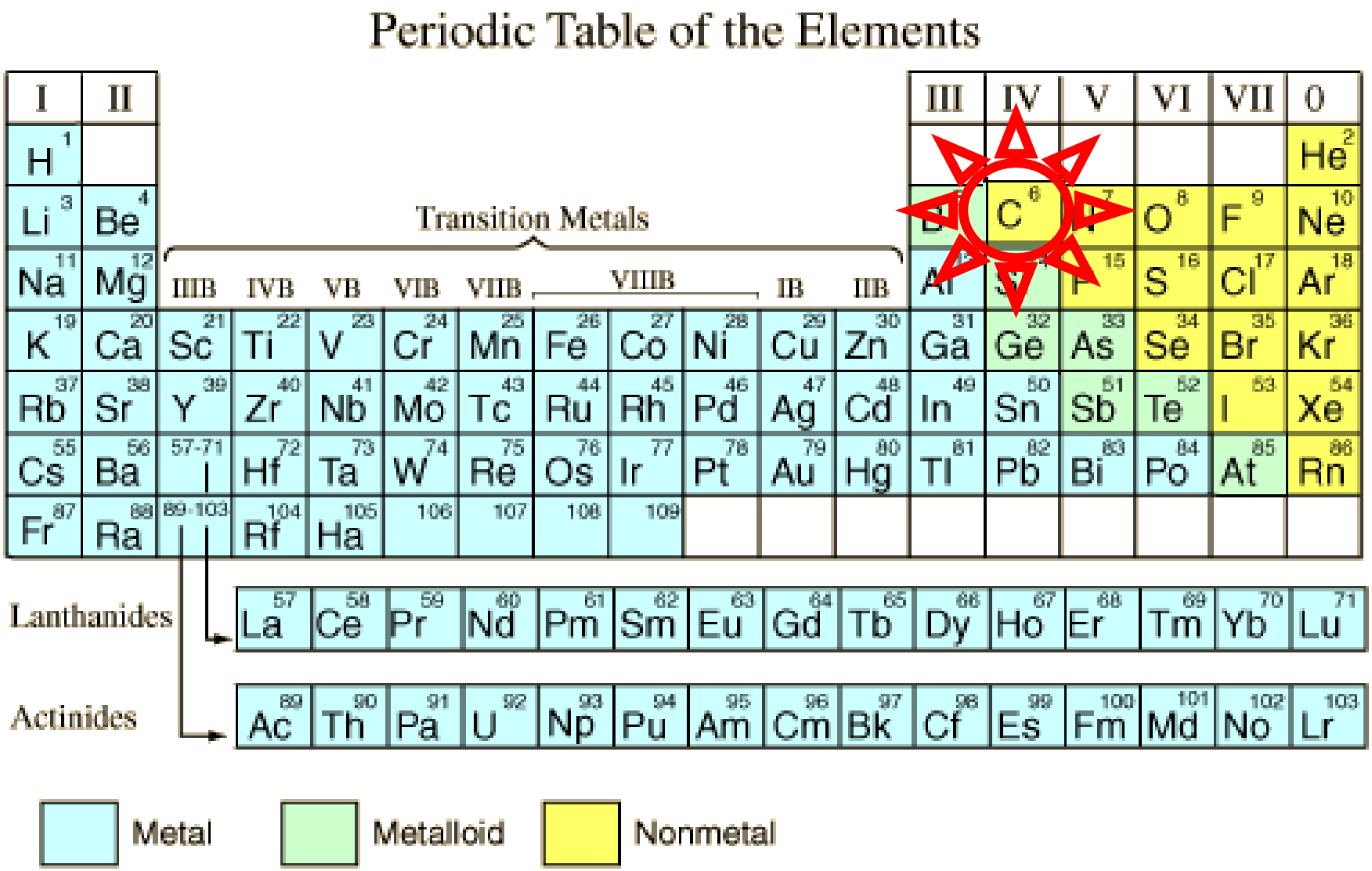
Stacking 2D Layers



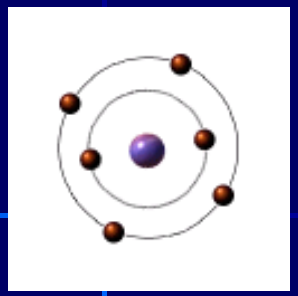




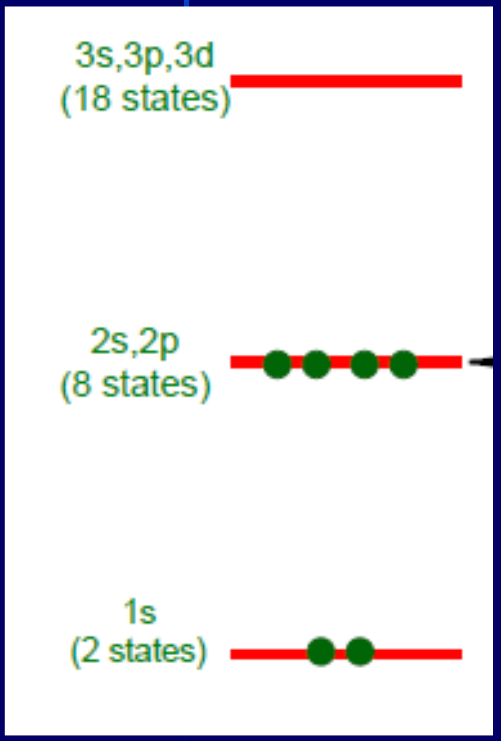
The most important element in nature



Carbon chemical bonds



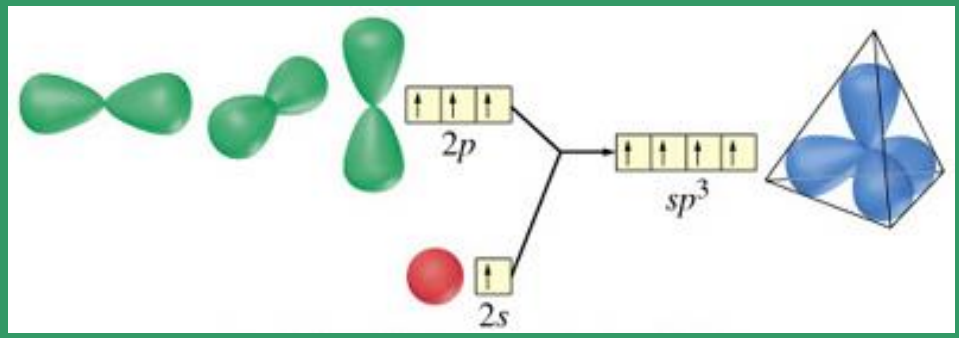
Carbon: Z=6
4 valence electrons $2s^2 2p^2$

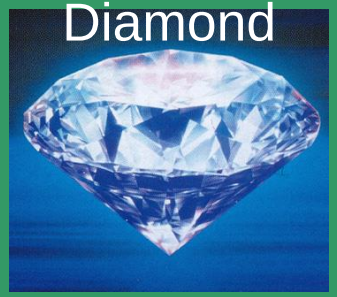


sp^3

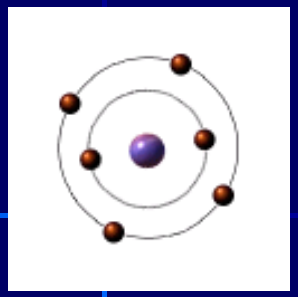
$2S + 2p_x + 2p_y + 2p_z$ hybridize

4 sp^3 orbitals: tetrahedron





Carbon chemical bonds



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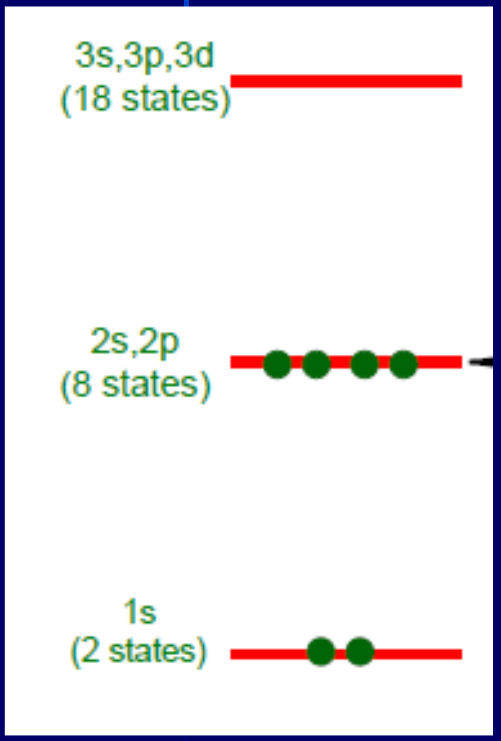
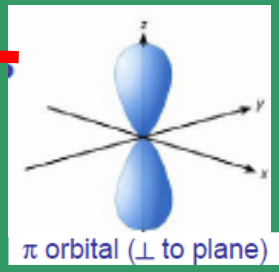


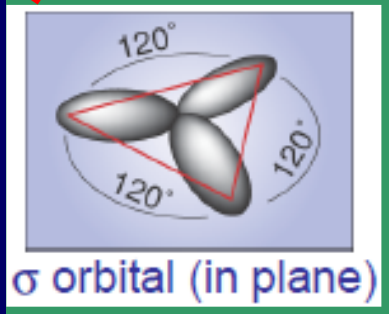
sp^2

$2S + 2p_x + 2p_y$ hybridize

3 planar σ orbitals: tetragon
1 Out of plane $2p_z$ [“π” orbital]

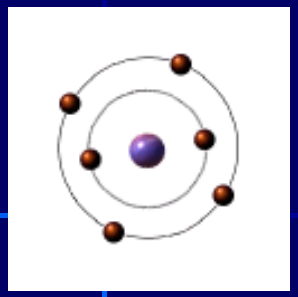


π electrons allow conduction

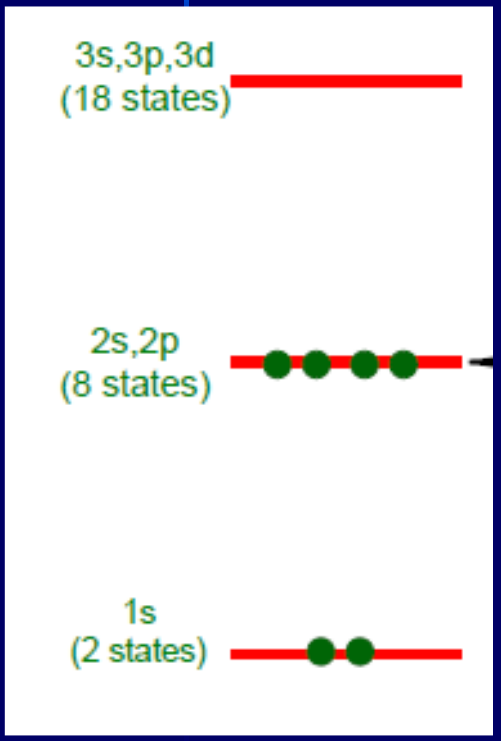


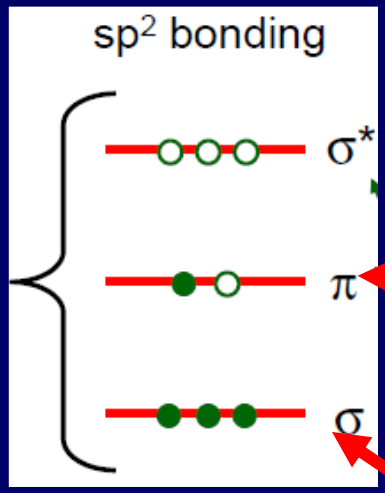
σ bonds: 2D and exceptional rigidity

Carbon chemical bonds



Carbon: Z=6
4 valence electrons $2s^2 2p^2$

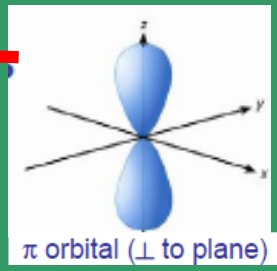


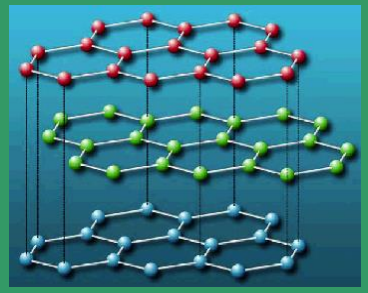


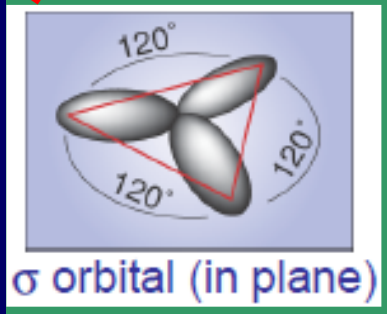
sp^2

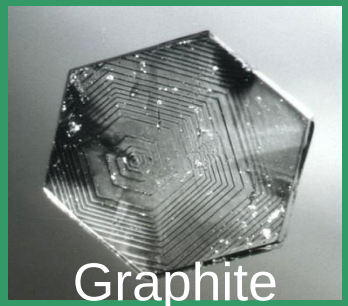
$2S + 2p_x + 2p_y$ hybridize

3 planar σ orbitals: tetragon
1 Out of plane $2p_z$ ["π" orbital]



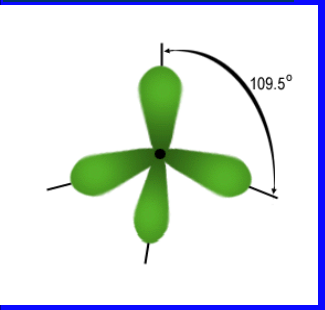


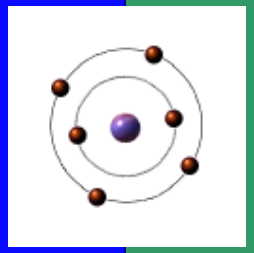


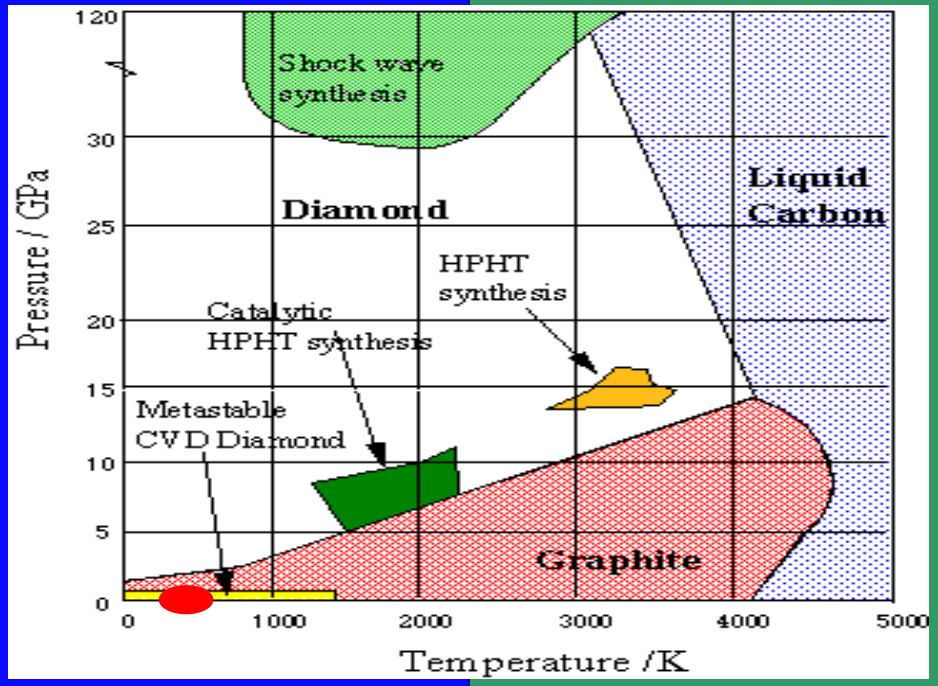


Carbon allotropes

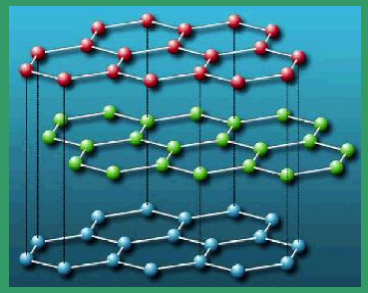
sp^3

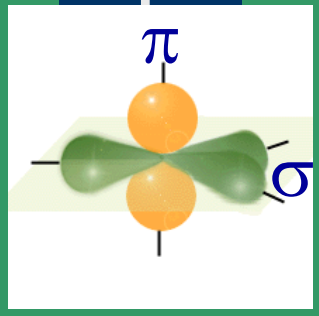


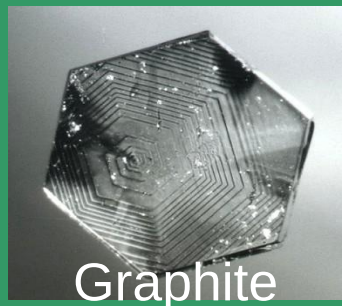




sp^2





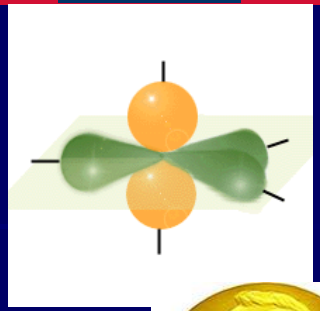


- Diamond is Metastable in ambient conditions!!

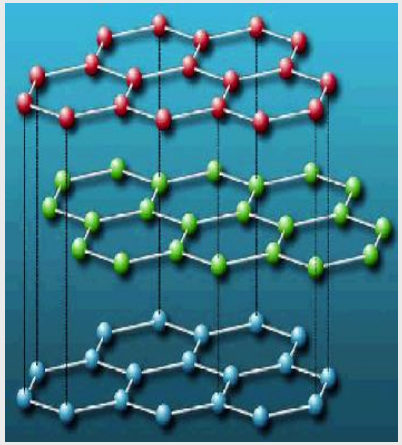
break

Carbon Allotropes

sp^2

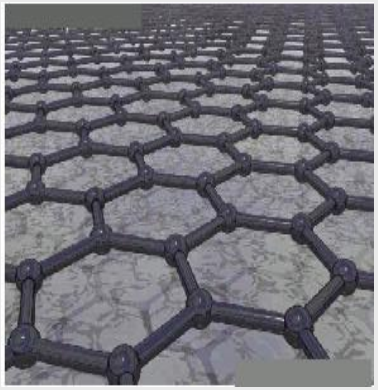


3D



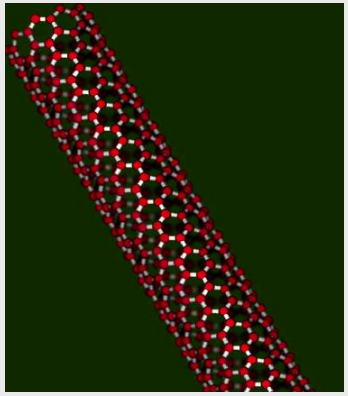
Graphite ~16 century

2D



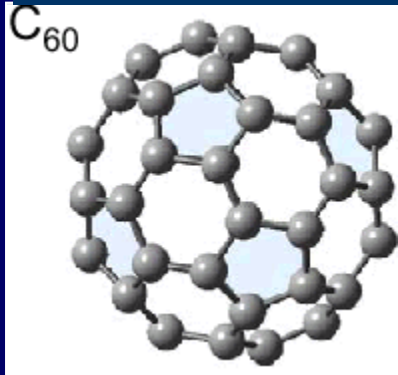
Graphene
Single -layer 2005

"1D"



Carbon nanotube
Multi-wall1991
Single wall 1993

"0D"



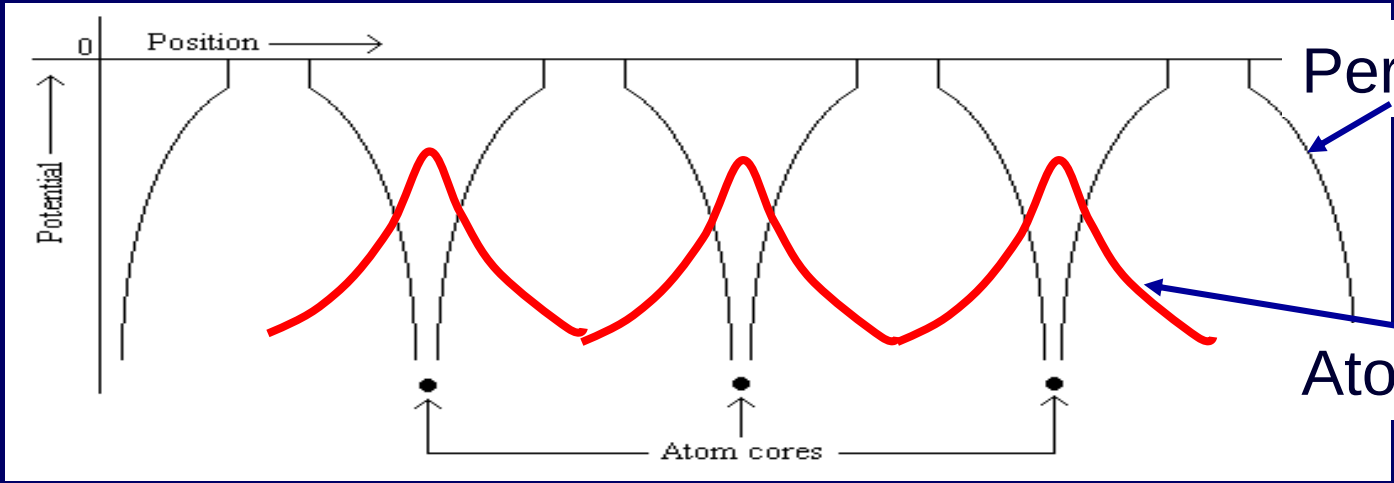
Buckyball
1985

E.Y. Andrei

Graphene

- 2D materials – background
  - Carbon allotropes
  - Graphene Structure and Band structure
  - Electronic properties
- Electrons in a magnetic field
  - Onsager relation
  - Landau levels
  - Quantum Hall effect
- Engineering electronic properties
  - Kondo effect
  - Atomic collapse and artificial atom
  - Twisted graphene

Tight binding model



Eigenstates of the isolated atom:

$$H_{at}\left|\varphi_{\alpha}\right\rangle = E_{\alpha}\left|\varphi_{\alpha}\right\rangle$$

- Overlaps between orbitals $\mapsto$ corrections to system Hamiltonian

$$H(r) = \sum_{R} H_{at}(r - R) + \Delta U(r$$

$$H\left|\psi_{k}\right\rangle = E_{k}\left|\psi_{k}\right\rangle$$

- Tight binding $\mapsto$ small overlaps $\mapsto$ small corrections ΔU

Tight binding model

Build Bloch waves out of atomic orbitals (Bravais lattice!)

$$\left|\psi_{k\alpha}(\boldsymbol{r})\right\rangle = \sum_{\boldsymbol{R}_j} e^{ik\cdot R_j} \left|\varphi_\alpha(\boldsymbol{r}-\boldsymbol{R}_j)\right\rangle$$

Lattice vector

Solutions have to satisfy:

1. Normalization $\left\langle\psi_k\middle|\psi_k\right\rangle = 1$
2. Eigenstate of the Hamiltonian $\left\langle\psi_k\middle|H\middle|\psi_k\right\rangle = E_k$
3. Algebra $\mapsto$Find Solutions in terms of:

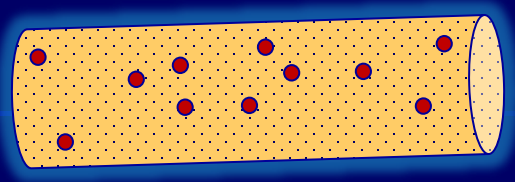
- Nearest neighbor transfer (hopping) integral $\left\langle\varphi_i\middle|H\middle|\varphi_j\right\rangle = t_{ij}$
- Nearest neighbour overlap integral $\left\langle\varphi_i\middle|\varphi_j\right\rangle = s_{ij}$

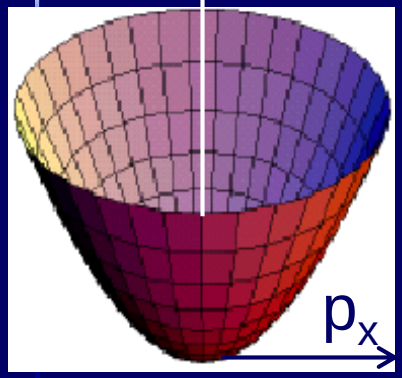
$$H = \sum_{<i,j>} t_{ij} c_i^\dagger c_j + h.c.$$

E.Y. Andrei

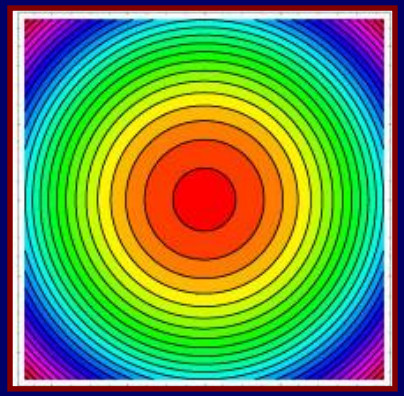
Band Structure

Simple metal



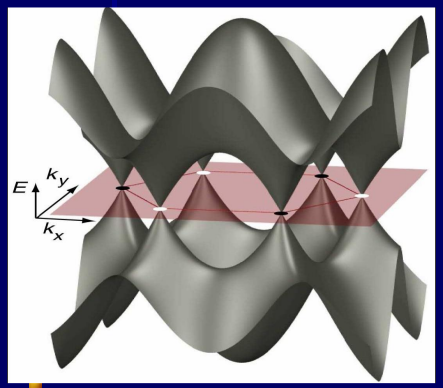


Bravais lattice
- **Parabolic dispersion**



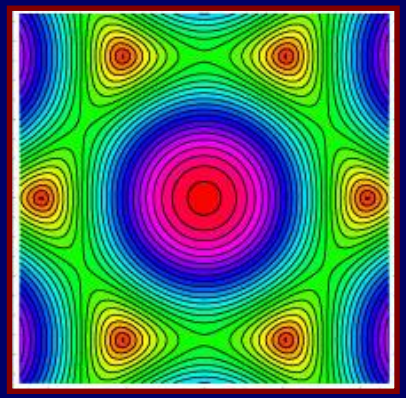
$$E = \frac{p^2}{2m^*}$$

How is graphene different?



honeycomb lattice Not Bravais
- **strong diffraction by lattice**

→ **unconventional dispersion**

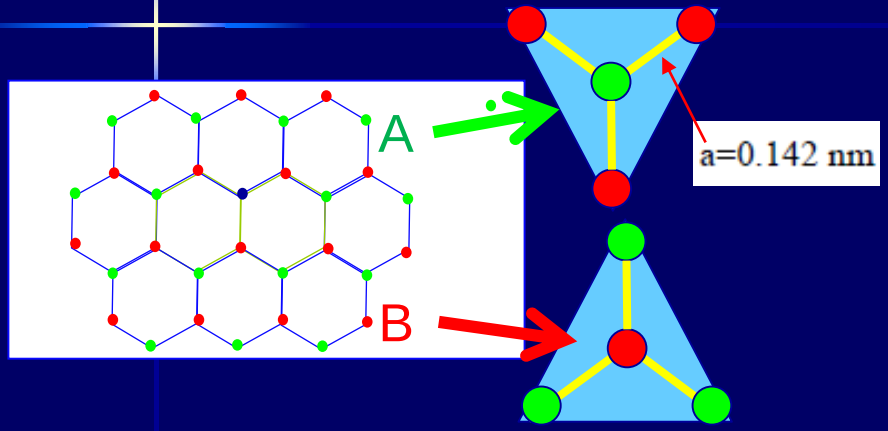


Wallace, 1947

E.Y. Andrei

Graphene honeycomb lattice

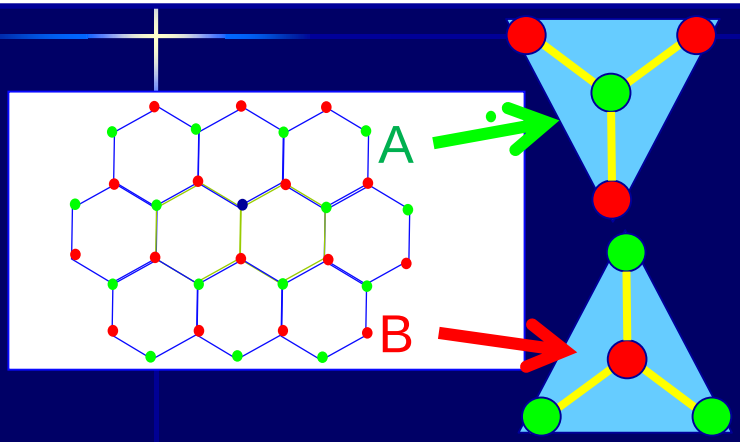
1. 2D
2. Honeycomb structure (non-Bravais)
3. 2 identical atoms/cell

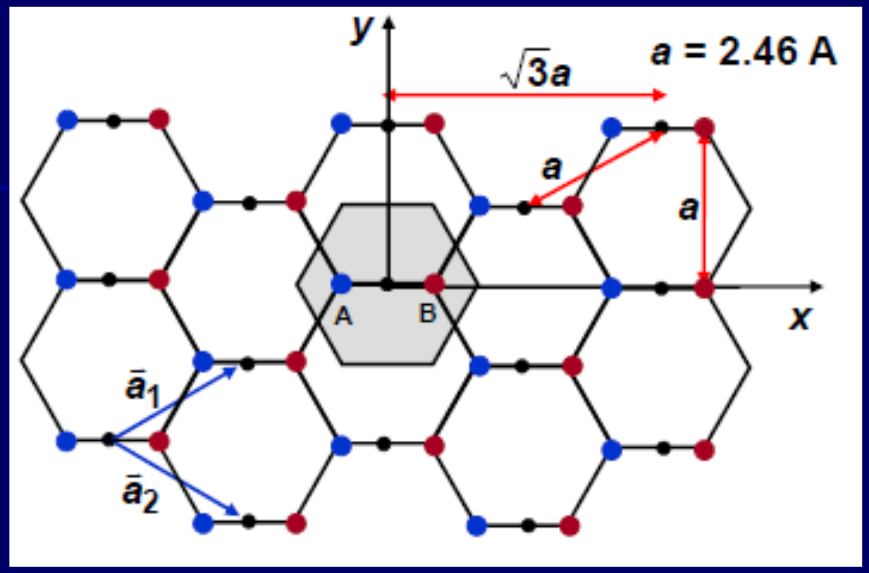


2 interpenetrating Bravais (triangular) lattices

Honeycomb lattice – two sets of Bloch functions

1. 2D
2. Honeycomb structure (non-Bravais)
3. 2 identical atoms/cell



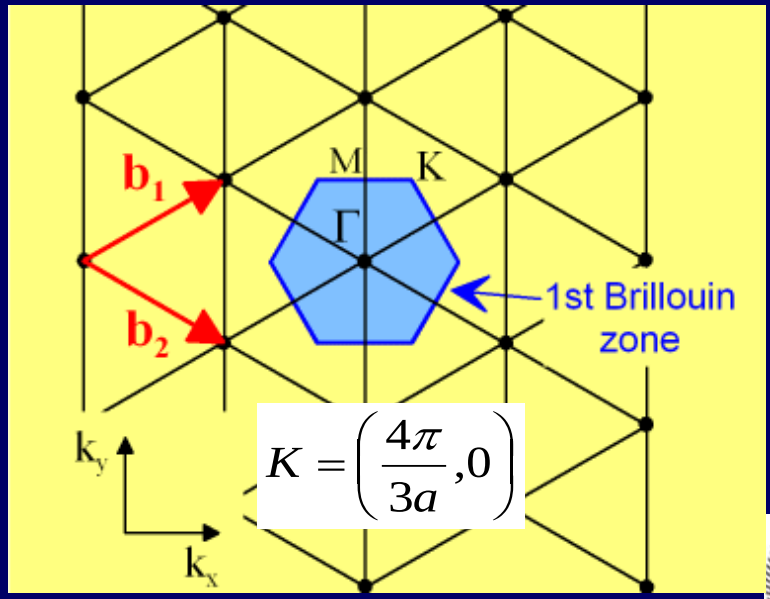


$$\Phi_A\left(\vec{k},\vec{r}\right)=\frac{1}{\sqrt{N}}\sum_{\vec{R}_A}^{N} e^{i\vec{k}.\vec{R}_A}\varphi_A\left(\vec{r}-\vec{R}_A\right)$$

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

sum over all type B atomic sites in N unit cells

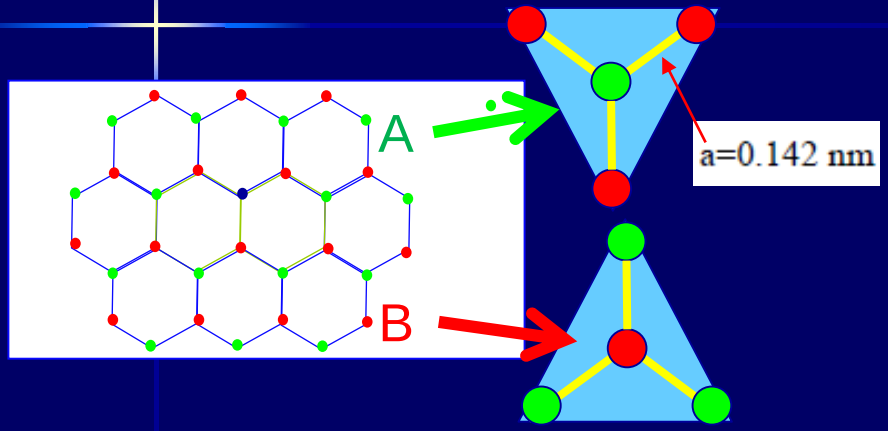
atomic wavefunction



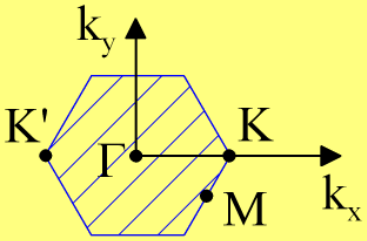
E.Y. Andrei

Honeycomb lattice – two sets of Bloch functions

1. 2D
2. Honeycomb structure (non-Bravais)
3. 2 identical atoms/cell



Brillouin zone



Two non-equivalent K-points

$$K = \frac{4\pi}{3a}(1,0)$$

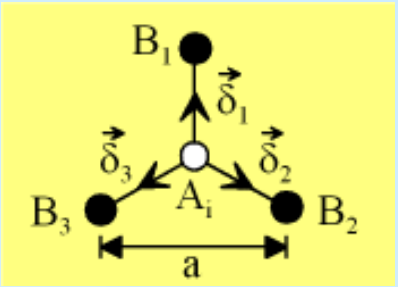
2 interpenetrating Bravais (triangular) lattices

$$\psi_{\vec{k}}(\vec{r}) = \alpha|\psi_A\rangle + \beta|\psi_B\rangle = \begin{pmatrix}\psi_\uparrow \\ \psi_\downarrow\end{pmatrix}$$

New degree of freedom –like spin up and spin down - but instead sublattice A or B ↦ pseudo-spin

Tight binding model of monolayer graphene : Energy solutions

$$H=\begin{pmatrix}\varepsilon_B & -tf\left(\vec{k}\right)\\ -tf^{*}\left(\vec{k}\right) & \varepsilon_B\end{pmatrix};\quad S=\begin{pmatrix}1 & sf\left(\vec{k}\right)\\ sf^{*}\left(\vec{k}\right) & 1\end{pmatrix}$$



$$\varepsilon_A\equiv\langle\varphi_A|H|\varphi_A\rangle;\varepsilon_B=\langle\varphi_B|H|\varphi_B\rangle$$

$$t\equiv\langle\varphi_A|H|\varphi_B\rangle$$

$$identical\ atoms:\varepsilon_0=\varepsilon_A=\varepsilon_B$$

$$f\left(\vec{k}\right)=\sum_{\vec{\delta}_j=1}^{3}e^{i\vec{k}.\vec{\delta}_j}=e^{ik_ya/\sqrt{3}}+2e^{-ik_ya/2\sqrt{3}}\cos\left(\frac{k_xa}{2}\right)$$

Edward McCann arXiv:1205.4849

Secular equation gives the eigenvalues:

$$\det\left(H-ES\right)=0$$

$$\det\begin{pmatrix}\varepsilon_0-E & -\left(t+Es\right)f\left(\vec{k}\right)\\ -\left(t+Es\right)f^{*}\left(\vec{k}\right) & \varepsilon_0-E\end{pmatrix}=0$$

$$\left(E-\varepsilon_0\right)^2-\left(t+Es\right)^2\left|f\left(\vec{k}\right)\right|^2=0$$

$$E=\frac{\varepsilon_0\pm t\left|f\left(\vec{k}\right)\right|}{1\mp s\left|f\left(\vec{k}\right)\right|}$$

Note:

If atoms on the two sublattices are different:

$$H=\begin{pmatrix}\varepsilon_A & -tf\left(\vec{k}\right)\\ -tf^{*}\left(\vec{k}\right) & \varepsilon_B\end{pmatrix}$$

Solutions more complicated

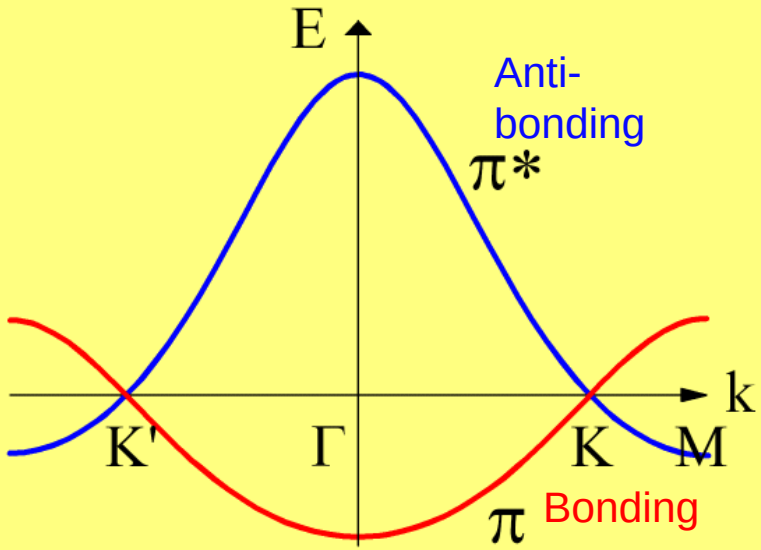
Graphene tight binding band structure

$$E = \frac{\varepsilon_0 \pm t\left|f\left(\vec{k}\right)\right|}{1 \mp s\left|f\left(\vec{k}\right)\right|}$$

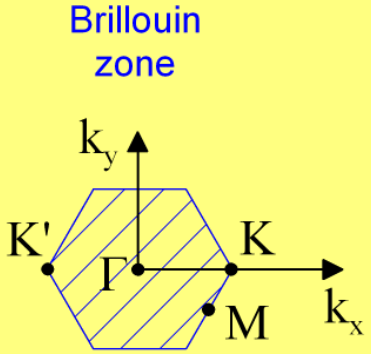
$$f\left(\vec{k}\right) = e^{ik_y a/\sqrt{3}} + 2e^{-ik_y a/2\sqrt{3}} \cos\left(\frac{k_x a}{2}\right)$$

Typical parameter values :

$$\varepsilon_0 = 0, t = 3.033eV, s = 0.129$$



Two bands: no energy gap at the K-points



Two non-equivalent
K-points

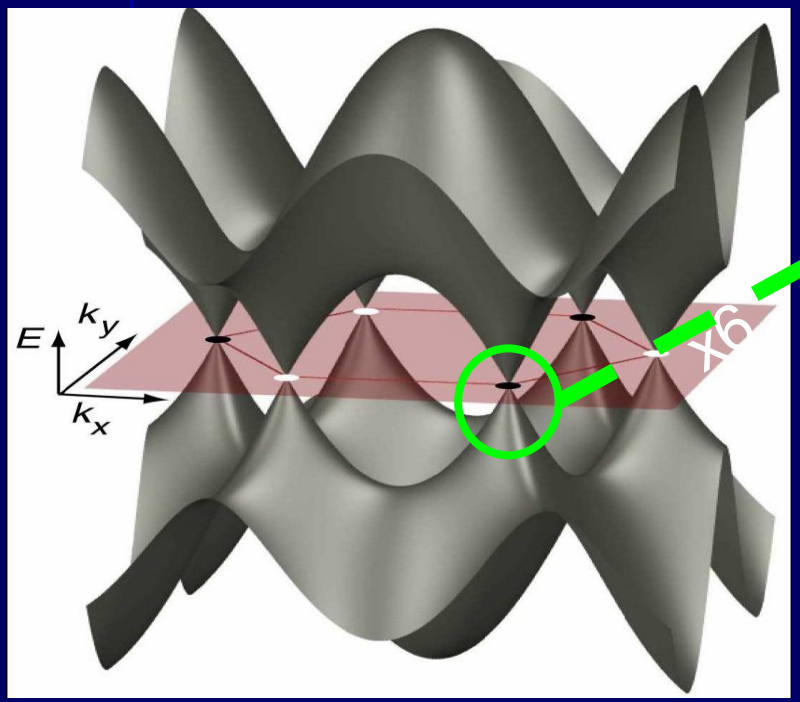
E.Y. Andrei

Band Structure

$$\psi_{\vec{k}}(\vec{r}) = c_A|\psi_A\rangle + c_B|\psi_B\rangle = \begin{pmatrix}\psi_\uparrow \\ \psi_\downarrow\end{pmatrix}$$

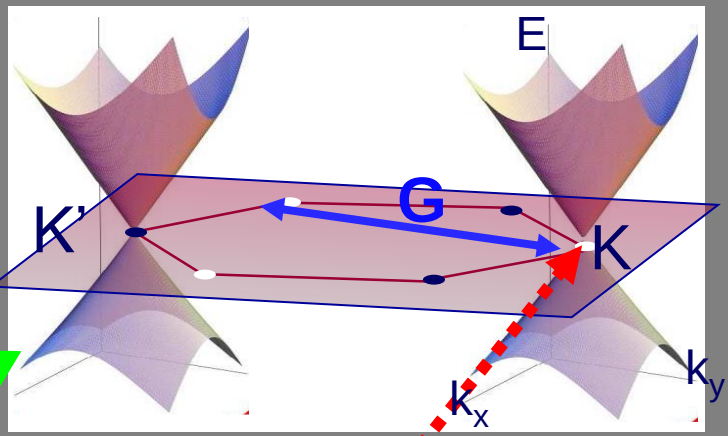
New degree of Freedom

- Pseudospin



Low energy excitations

Dirac cones



Dirac point

6 Dirac points, but only 2 independent points K and K', others can be derived with translation by reciprocal lattice vectors.

The Dirac points are protected by 3 discrete symmetries: $\mathbb{T}$, I, C_3

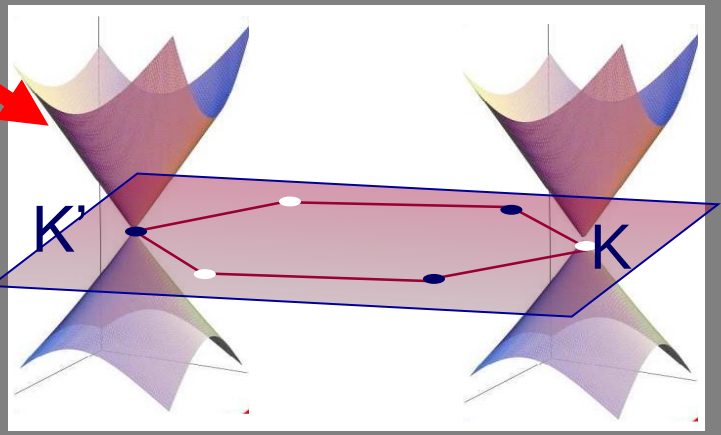
Low energy band structure

Conduction band ⇨ electrons

Fermi energy E_F
Fermi "surface" =2 points

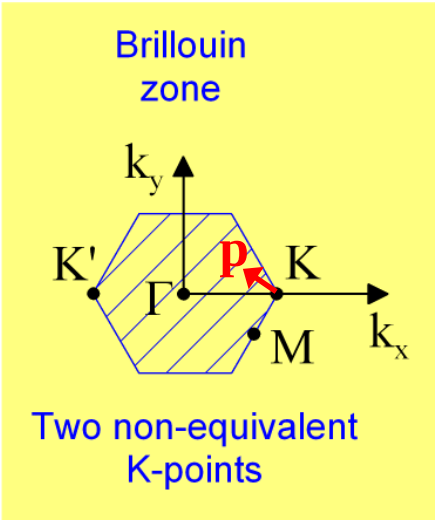
Valence band ⇨ holes

Dirac cones



Low energy band structure

1 Linear expansion near the K point



Consider two non-equivalent K points:

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

and small momentum near them:

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

$$p_x \equiv -i\hbar\frac{\partial}{\partial x};\ p_y \equiv -i\hbar\frac{\partial}{\partial y}$$

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

Linear expansion in small momentum: $$f\left(\vec{k}\right) = -\frac{\sqrt{3}a}{2\hbar}\left(\xi p_x - ip_y\right) + O\left(pa/\hbar\right)^2$$

$$H = \begin{pmatrix} 0 & -tf\left(\vec{k}\right) \\ -tf^*\left(\vec{k}\right) & 0 \end{pmatrix} \approx v_F \begin{pmatrix} 0 & \xi p_x - ip_y \\ \xi p_x + ip_y & 0 \end{pmatrix}$$

$$v_F = \frac{\sqrt{3}at}{2\hbar} \approx 10^6\, m/s$$

Low energy band structure

2. Dirac-like equation with Pseudospin

For one K point (e.g. ξ=+1) we have a 2 component wave function,

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

with the following effective Hamiltonian (Dirac Weyl Hamiltonian):

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

$$\sigma_x =; \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

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

Pauli Matrices
- Operate on sublattice degree of freedom

Low energy band structure

2. Dirac-like equation with Pseudospin

To take into account both K points (ξ=+1 and ξ=-1) we can use a 4 component wave function,

$$\psi = \begin{pmatrix} \psi_{AK} \\ \psi_{BK} \\ \psi_{AK'} \\ \psi_{BK'} \end{pmatrix}$$

Note: real spin not included.
Including spin gives 8x8 Hamiltonian

with the following effective Hamiltonian:

$$H = v_F \begin{pmatrix} 0 & p_x - ip_y & 0 & 0 \\ p_x + ip_y & 0 & 0 & 0 \\ 0 & 0 & 0 & -p_x - ip_y \\ 0 & 0 & -p_x + ip_y & 0 \end{pmatrix}$$

H(K) H(K')

$$H_K = v_F \vec{\sigma}.\vec{p} \qquad H_{K'} = -v_F \vec{\sigma}^*.\vec{p}$$

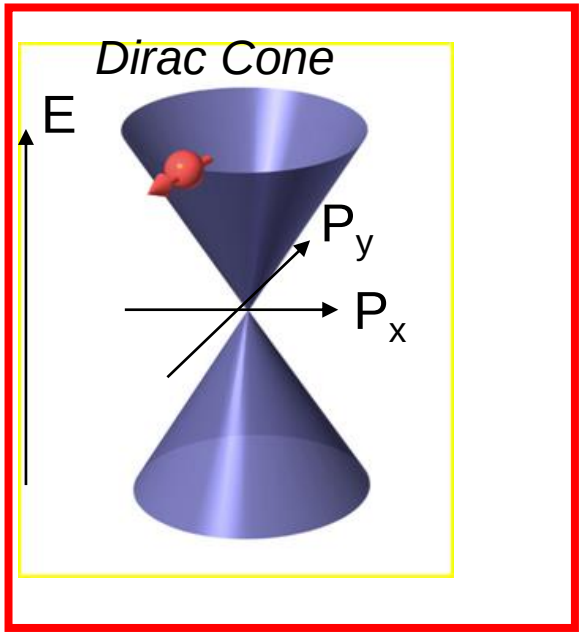
H_K and $H_{K'}$ are related by time reversal symmetry

Massless Dirac fermions

3. Massless Dirac Fermions

Hamiltonian near K point:

$$H = \hbar v_F \begin{pmatrix} 0 & -i\partial_x + \partial_y \\ -i\partial_x - \partial_y & 0 \end{pmatrix} = \hbar v_F \left(-i\sigma_x \partial_x - i\sigma_y \partial_y\right)$$



$$E = s v_F p \quad \Leftrightarrow \quad \psi = \frac{1}{\sqrt{2}} e^{i\vec{k}\cdot\vec{r}} \begin{pmatrix} 1 \\ s e^{i\varphi} \end{pmatrix}$$

$\varphi = \arctan(p_y / p_x)$ *polar angle*

$s = band \quad index$

Pseudospin vector

- Is parallel to the wave vector k in upper band
- Antiparallel to k in lower band (s=-1)

Massless particle : m=0

..Photons, neutrinos..

$$E = cp$$

➢ But 300 times slower

$$v_F \approx 10^6 m/s$$

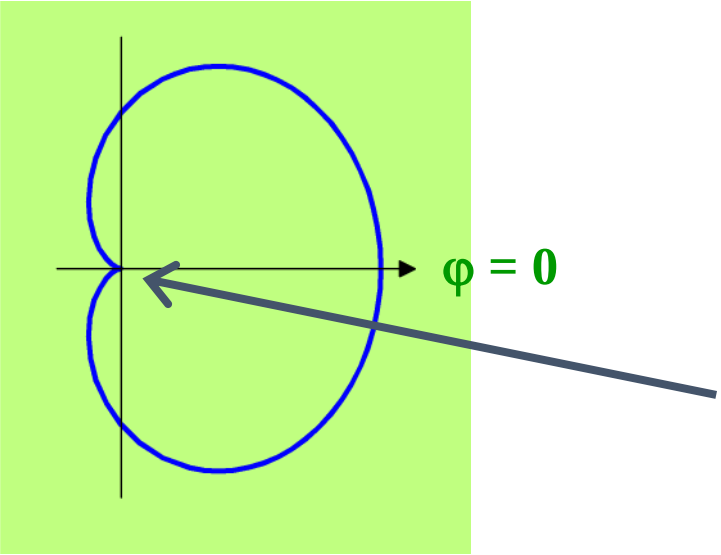
E.Y. Andrei

No backscattering within Dirac cone

4. Absence of backscattering within a Dirac cone

$$\psi = \frac{1}{\sqrt{2}} e^{i\vec{k}\cdot\vec{r}} \begin{pmatrix} 1 \\ s e^{i\varphi} \end{pmatrix}$$

angular scattering probability:



$$\left| \langle \psi(\varphi) | \psi(\varphi = 0) \rangle \right|^2 = \cos^2(\varphi/2)$$

under pseudospin conservation, backscattering within one valley is suppressed

Helicity (Chirality)

5. Helicity

Hamiltonian at K point:

$$H(K) = v_F \vec{\sigma} \cdot \vec{p} = v_F\, p \vec{\sigma} \cdot \vec{n}$$

Helicity operator: $\hat{h} = \vec{\sigma} \cdot \vec{n}$

$$H(K) = v_F\, p \hat{h}$$

Helicity is conserved

Helical electrons

pseudospin direction is linked to an axis determined by electronic momentum.

for conduction band electrons,

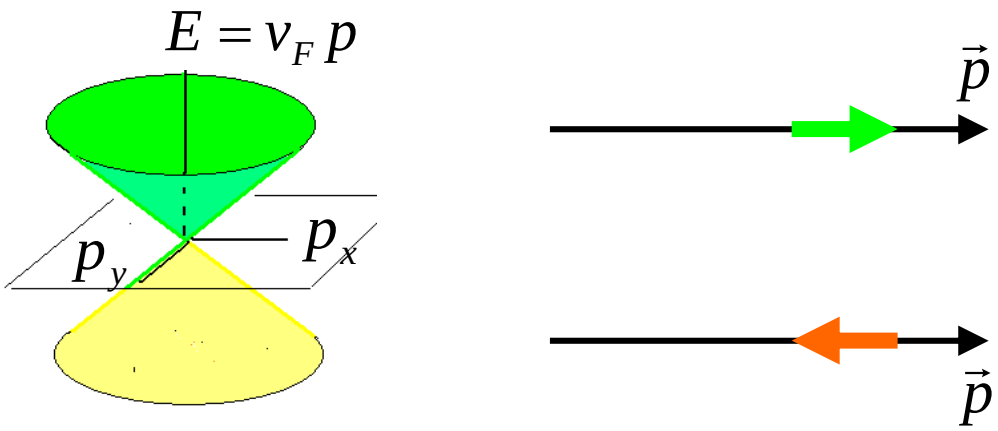
$$\vec{\sigma} \cdot \vec{n} = 1$$

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

valence band ('holes')

Helicity (Chirality)

5. Helicity



Note: Helicity is reversed in the K' cone

Helical electrons

pseudospin direction is linked to an axis determined by electronic momentum.

for conduction band electrons,

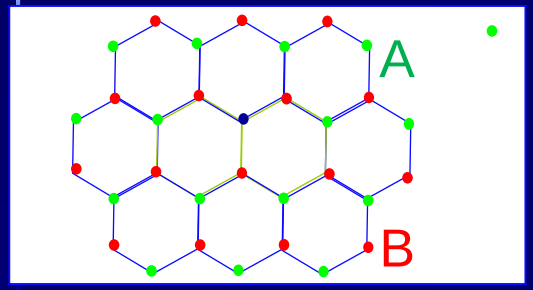
$$\vec{\sigma} \cdot \vec{n} = 1$$

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

valence band ('holes')

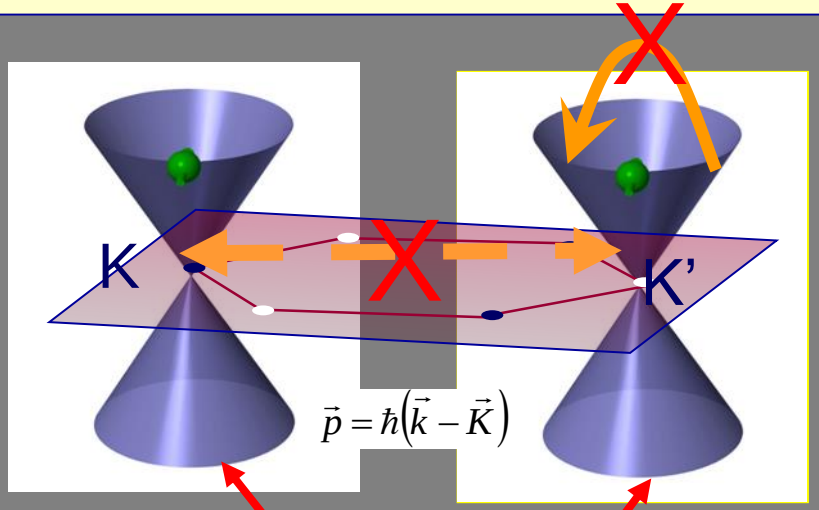
Helicity conserved $\mapsto$ No backscattering between cones

No Backscattering



No backscattering between cones

No backscattering within cones



Dirac Weyl Hamiltonian

$$H = v_F \begin{pmatrix} 0 & \vec{\sigma}.\vec{p} \\ -\vec{\sigma}^*.\vec{p} & 0 \end{pmatrix}$$

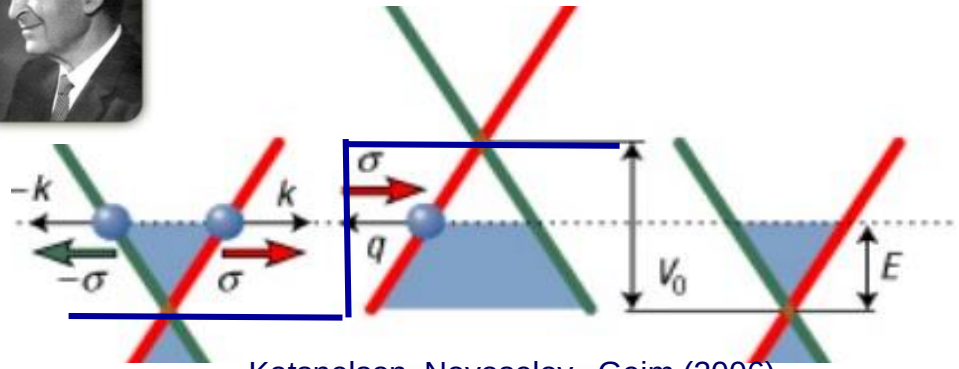
conserved Helicity $\vec{\sigma}.\vec{p} \propto \vec{h}$

- No backscattering
- High carrier mobility

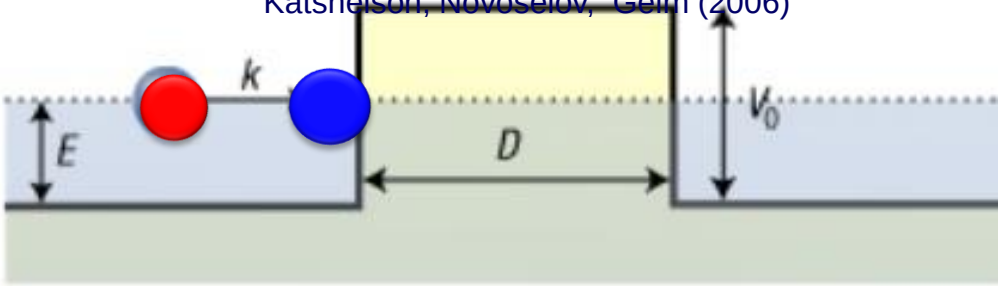
Pristine graphene

Pseudospin + chirality $\mapsto$ Klein tunneling

Klein Tunneling



Katsnelson, Novoselov, Geim (2006)

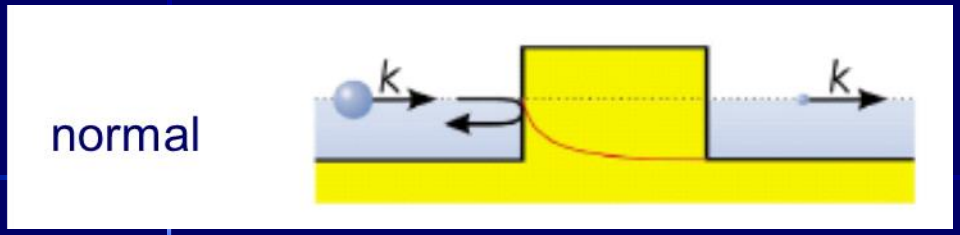


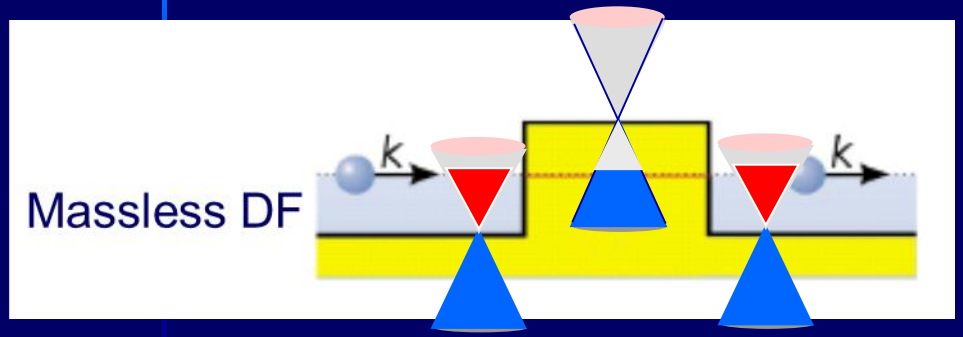
Katsnelson, Novoselov, Geim (2006)

No electrostatic confinement

- No quantum dots
- No switching
- No guiding

Klein tunneling



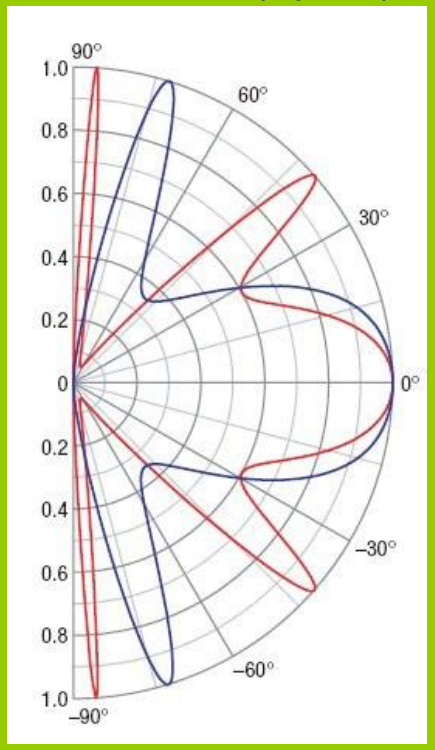


Klein “paradox”

- Transmission of relativistic particles unimpeded even by highest barriers
- Physical picture: particle/hole conversion

Angular dependence of transmission

Katsnelson et al Nature physics (2006)



Carrier density outside the barrier is 0.5 x 10^{12} cm^{-2} . Inside the barrier, hole concentrationn is 1 x 10^{12} and 3 x 10^{12} cm^{-2} for the red and blue curves.

The Berry phase

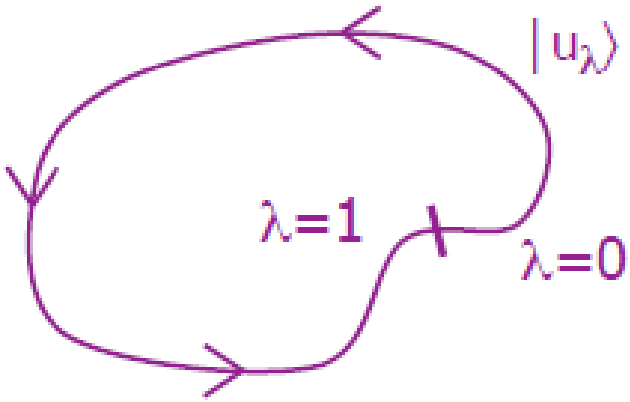
Proc. R. Soc. Lond. A **392**, 45–57 (1984)
Printed in Great Britain

Quantal phase factors accompanying adiabatic changes

By M. V. Berry, F.R.S.

Imagine a quantal sy… effects of an un-
changing environmen… te. If the environ-
ment, and hence $\hat{H}$, is s… theorem (Messiah
1962) that at any insta… e instantaneous $\hat{H}$.
In particular, if the H… m the system will
return to its original st… actor is observable
by interference if the … hat was separated
from it at an earlier ti… tant.

My purpose here is … circuit-dependent
component exp (iγ) in… nent exp ($-$i$Et/\hbar$)
which accompanies th… eral formula for γ
in terms of the eigens… ircuit is close to a
degeneracy in the spe… orm which will be
derived in § 3; this cor… ound a degeneracy
of the eigenstates of … well as Hermitian

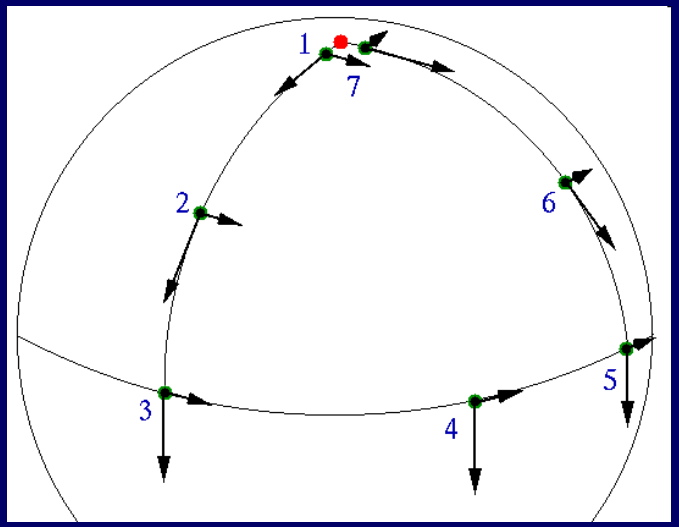


$$\phi = -\mathrm{Im} \oint d\lambda \, \langle u_\lambda | \frac{du_\lambda}{d\lambda} \rangle$$

$$\phi = -\mathrm{Im} \oint d\lambda \, \langle u_\lambda | \frac{d}{d\lambda} | u_\lambda \rangle$$

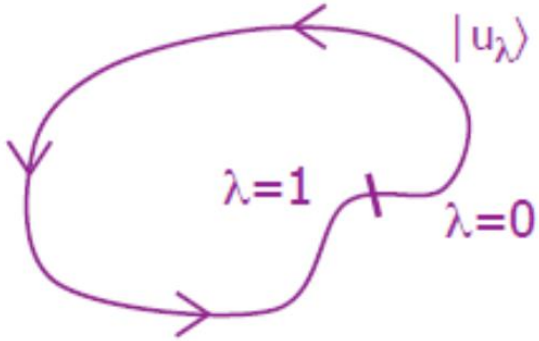
Berry phase

- Examples
  - Curved space
  - Mobius strip
  - Twisted optical fiber
  - Bohm Aharonov phase
  - Dirac belt



Berry Phase Tutorial:
https://www.physics.rutgers.edu/grad/682/textbook/ch-3.pdf

Berry phase



$$\phi = -\mathrm{Im}\oint d\lambda \langle u_\lambda | \frac{du_\lambda}{d\lambda} \rangle$$

$$\phi = -\mathrm{Im}\oint d\lambda \langle u_\lambda | \frac{d}{d\lambda} | u_\lambda \rangle$$

$$\psi(\varphi) = \frac{1}{\sqrt{2}} e^{i\vec{k}\cdot\vec{r}} \begin{pmatrix} 1 \\ e^{i\varphi} \end{pmatrix}$$

$$\varphi \equiv 2\pi\lambda \Rightarrow \varphi[0,2\pi] \rightarrow \lambda[0,1]$$

$$\psi_\lambda = \frac{1}{\sqrt{2}} e^{ikr\cos(2\pi\lambda)} \begin{pmatrix} 1 \\ e^{i2\pi\lambda} \end{pmatrix}$$

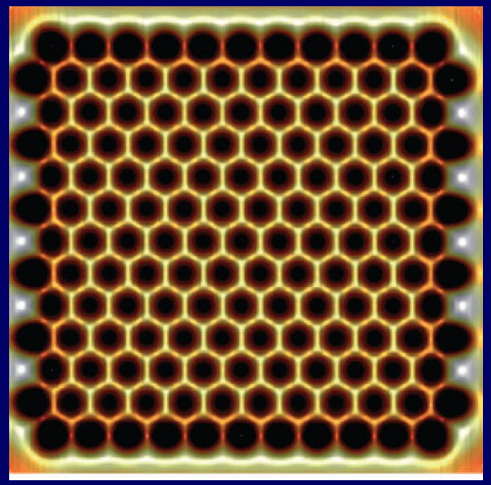
$$Berry \quad phase = -\mathrm{Im}\oint_\lambda d\lambda \left[\psi_\lambda \frac{d\psi_\lambda}{d\lambda} \right] = \pi$$

Homework:
Prove this relationship

Graphene Relatives

- Many natural materials have Dirac cones in their bandstructure (e.g. highTc compnds). But the Fermi surface of these materials contains many states that are not on a Dirac cone. As a result the electronic properties are controlled by the normal electrons and the Dirac electrons are invisible.

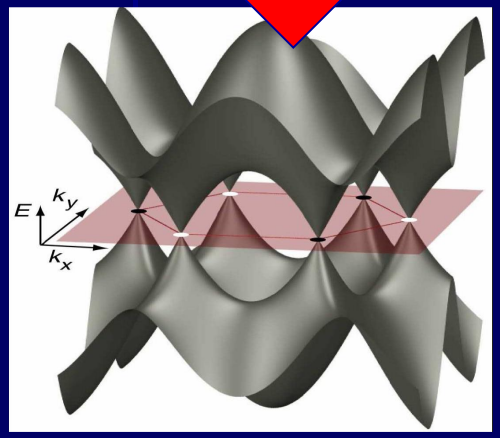
- Graphene is the ONLY naturally occurring material where the Fermi surface consists of Dirac points alone. As a result all its electronic properties are controlled by the Dirac electrons.



Graphene – bifishcotsture

Ingredients

1. 2D
2. Honeycomb structure
3. 2 identical atoms/cell



Graphene (2005)

Silicene (2010)

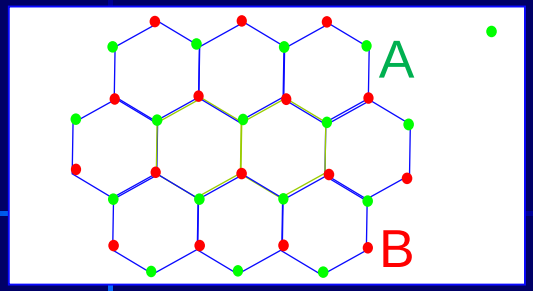
Germanine (2014)

Stanene (2013)

Phosphorene *(2014)*

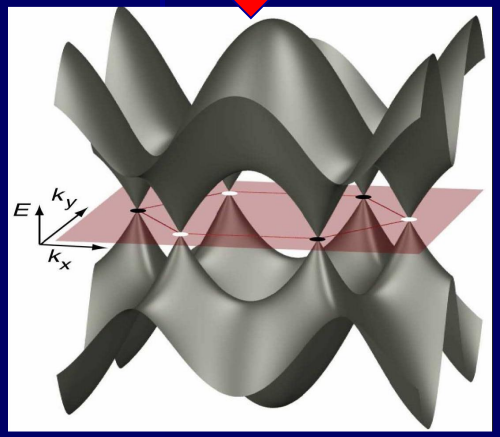
Borophene B_{36} *(2014)*

Artificial Graphene



Ingredients:

1. 2D
2. Honeycomb structure
3. Identical populations

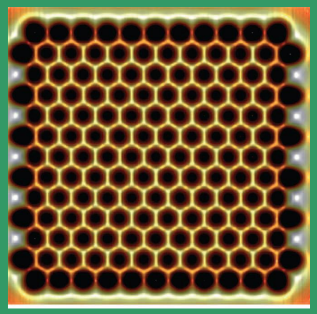


LETTER

doi:10.1038/nature10941

Designer Dirac fermions and topological phases in molecular graphene

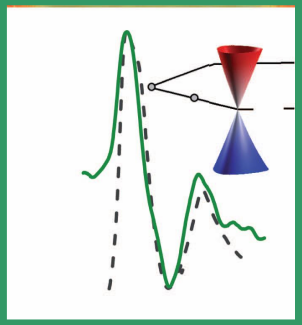
Kenjiro K. Gomes[1,2]*, Warren Mar[2,3]*, Wonhee Ko[2,4]*, Francisco Guinea[5] & Hari C. Manoharan[1,2]



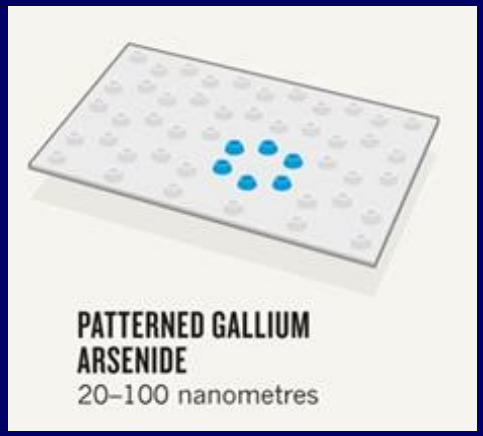
$a \sim 2nm$

$$t \propto \frac{\hbar^2}{m^* a^2} \approx 120meV$$

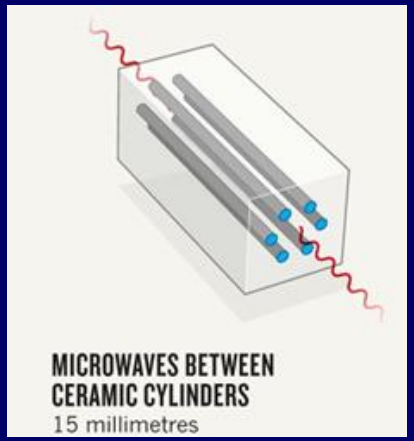
$$v_F = t\frac{3a}{2\hbar} \approx 3\times10^5 m/s$$



Also:

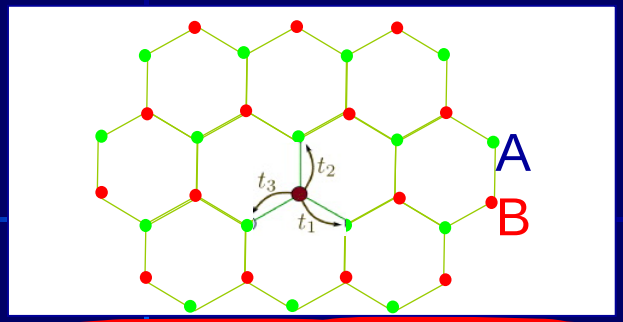


PATTERNED GALLIUM ARSENIDE
20–100 nanometres

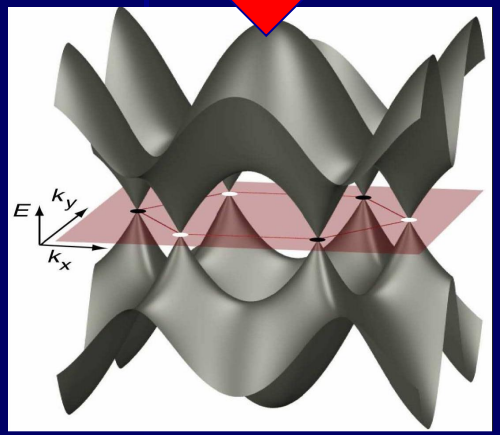


MICROWAVES BETWEEN CERAMIC CYLINDERS
15 millimetres

Graphene bandstructure



1. 2D
2. Honeycomb structure
3. 2 identical atoms/cell
4. $t_1=t_2=t_3= t$



Can one control/manipulate the bandstructure?

- Relax the condition: $t_1=t_2=t_3$
  - ✓ Strain
  - ✓ Impose external potential
  - ✓ Hybridization
- Electrostatic potential
- Defects

E.Y. Andrei

Summary

1. 2D
2. Honeycomb structure (non-Bravais)
3. 2 identical atoms/cell

$$H = v_F \vec{\sigma}.\vec{p}$$

$$E = sv_F p \quad ; \quad \psi = \frac{1}{\sqrt{2}} e^{i\vec{k}\cdot\vec{r}} \begin{pmatrix} 1 \\ se^{i\varphi} \end{pmatrix}$$

$$s = \pm 1 \quad band \quad index$$

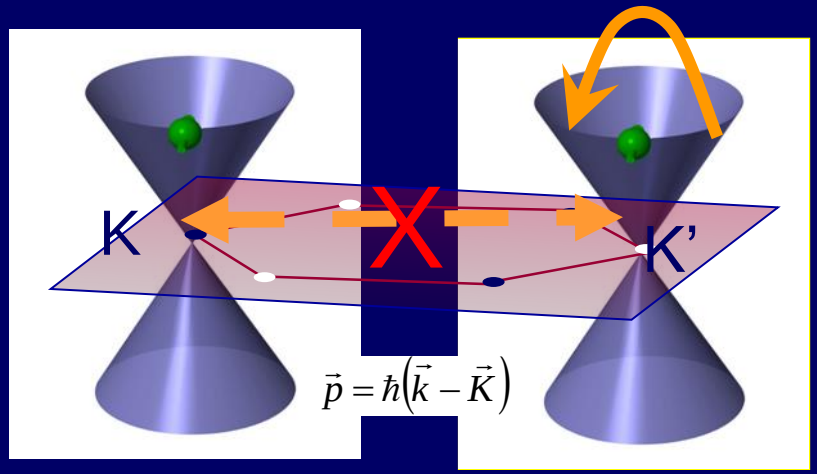
Pseudospin ; Helicity

- Chiral quasiparticles
- No backscattering

Berry phase π

Density of states

$$g(E) = 2\frac{L^2}{\pi(\hbar v_F)^2}|E|$$



E.Y. Andrei