Two dimensional materials: to graphene and beyond

Beatrice D’Alò

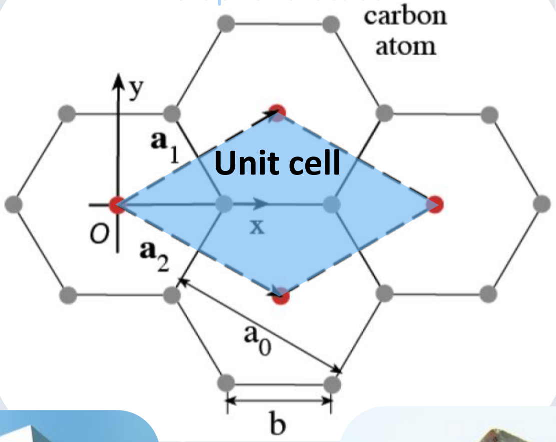
PhD seminars 08-02-2023

Outline

- Introduction to basic concepts of solid state physics;
- Definition of bidimensional materials;
- Graphene;
- Beyond graphene.

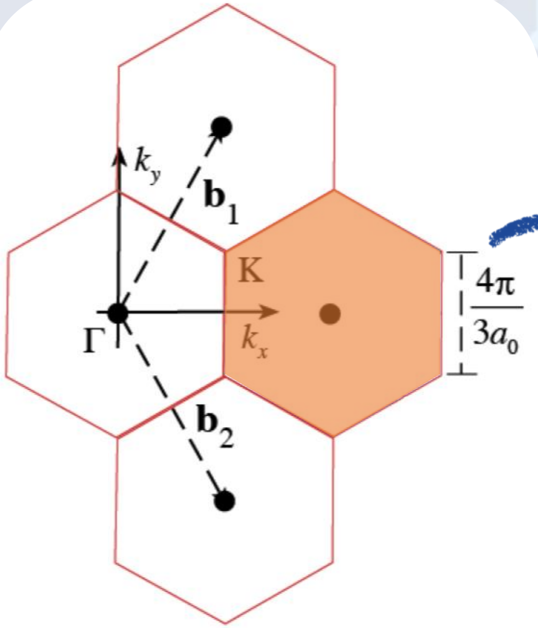
Main concepts of solid state physics

Graphene lattice

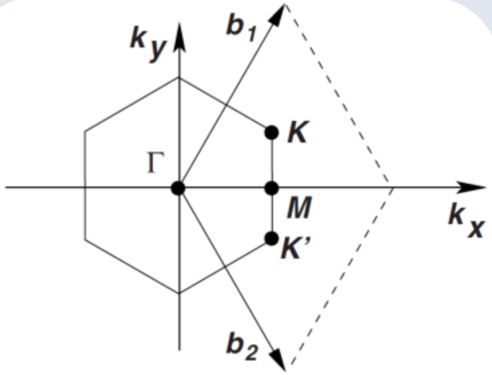


Examples of FeS_2 crystals with cubic lattices

Fourier transform



Graphene (reciprocal lattice)



Brillouin zone of graphene

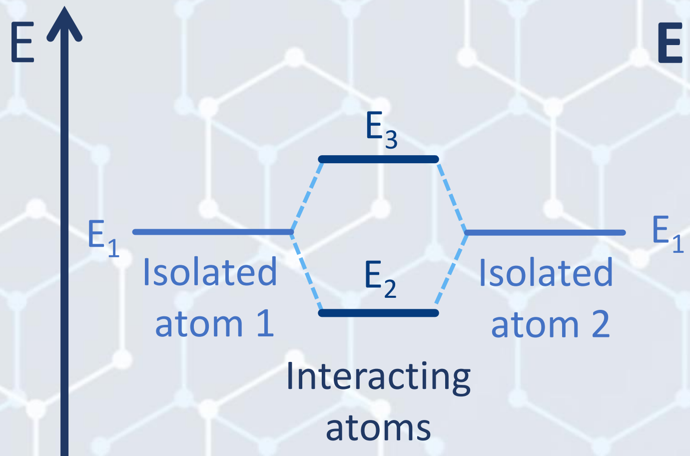
Crystal: solid materials whose constituent are ordered following a **periodic arrangement** (**crystal lattice** or **Bravais lattice**). The lattice describes the crystal in the **real space**.

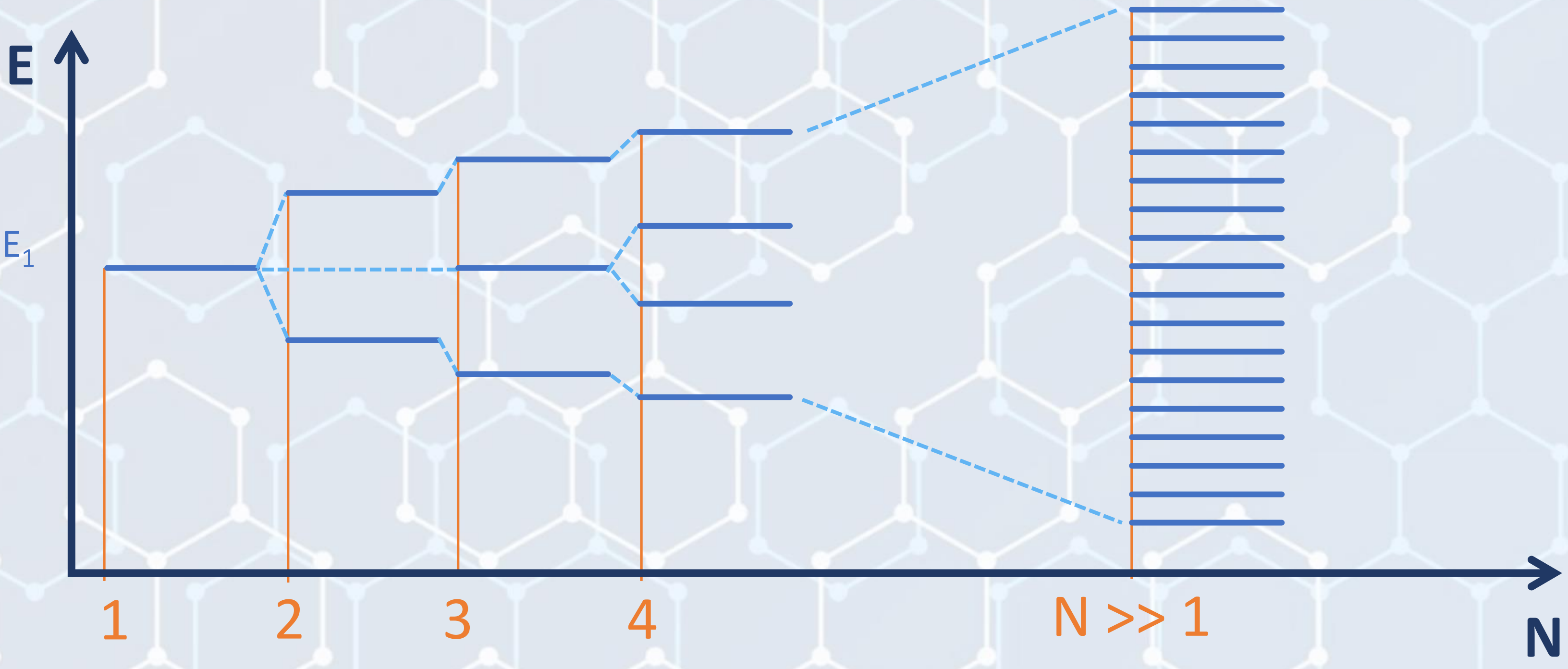
Reciprocal lattice: the Fourier transform of the crystal lattice. It is a lattice in the **momentum k space**!

Brillouin zone: specific choice of unit cell of the reciprocal lattice; it displays many high-symmetry points.

The electronic band structure

An intuitive (not rigorous) derivation of the electronic band structure.





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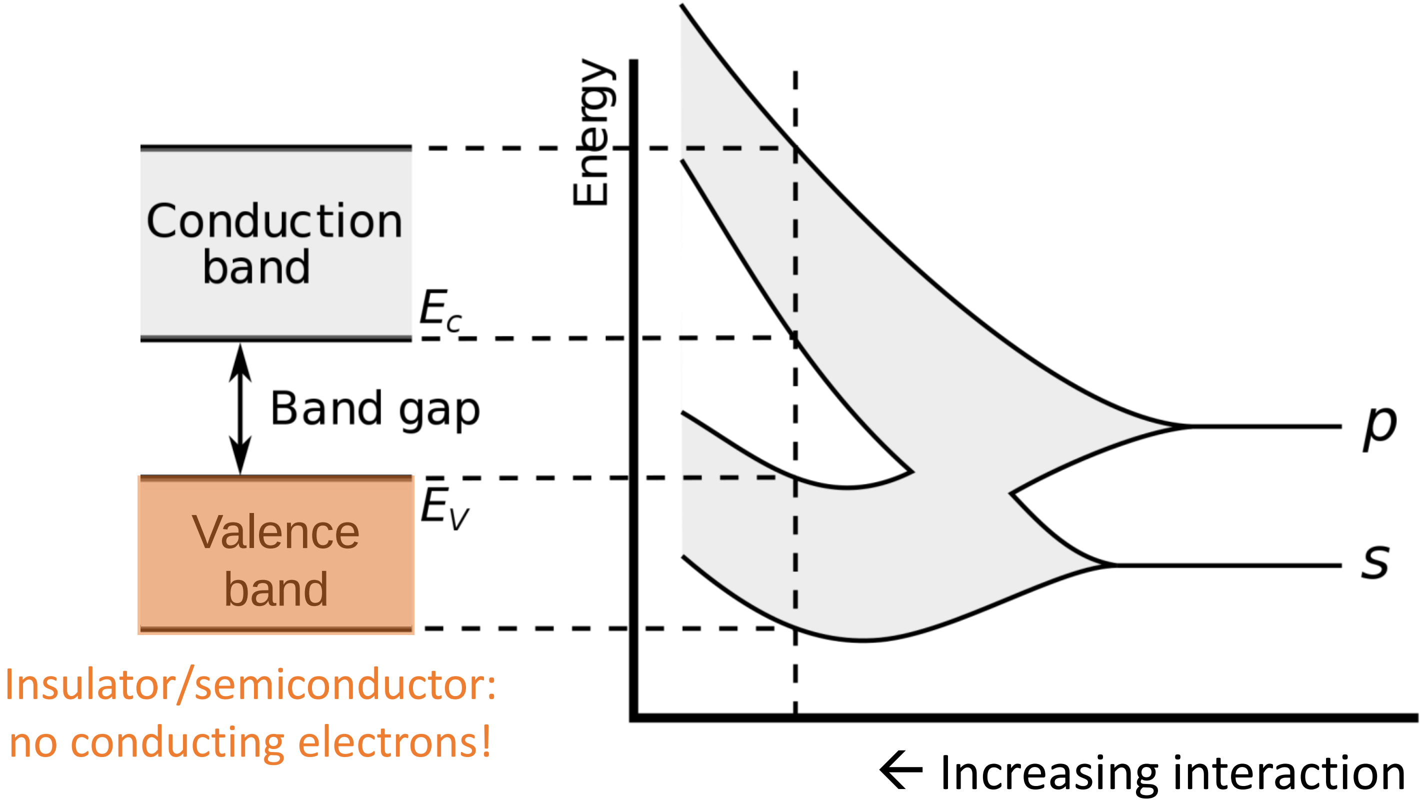

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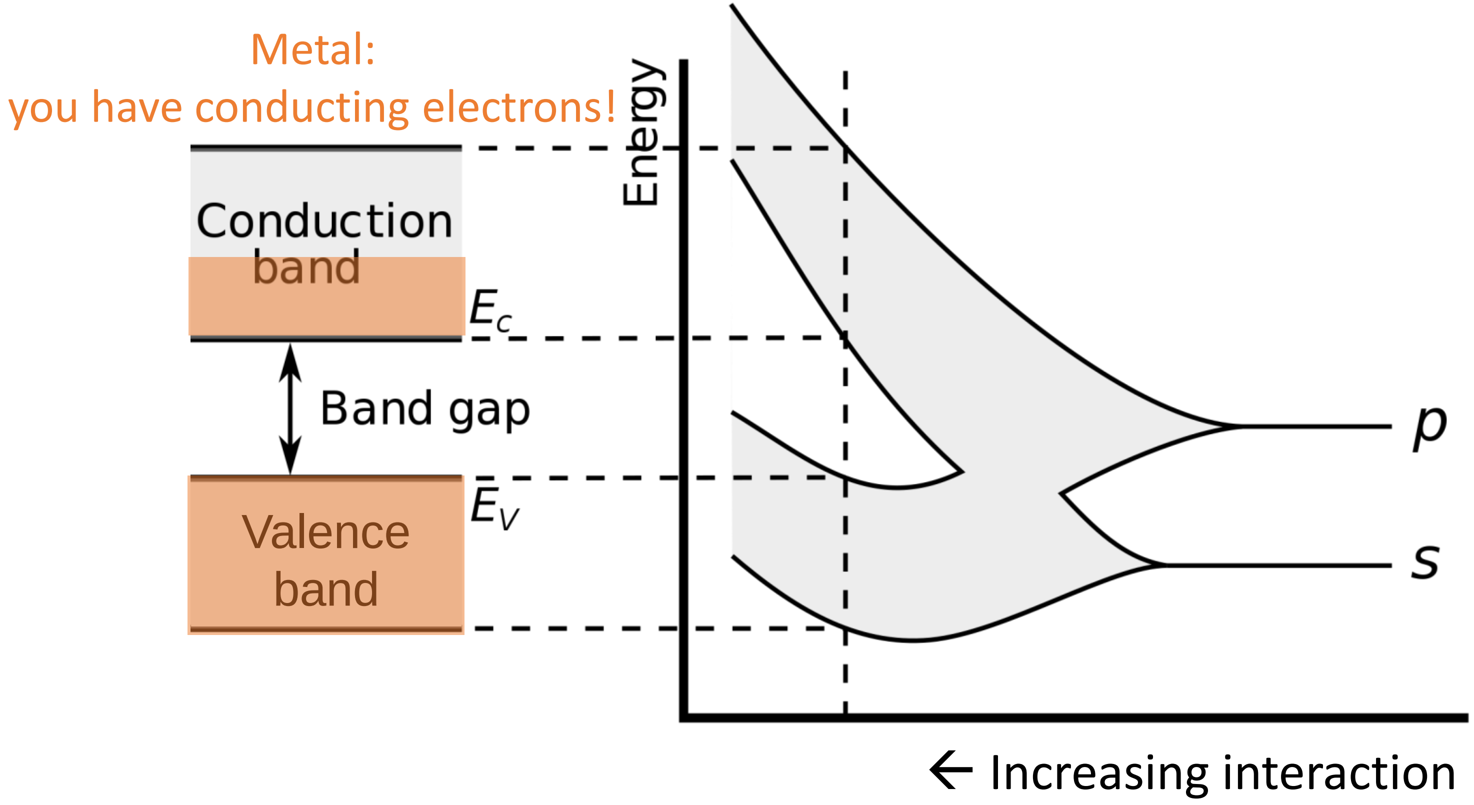
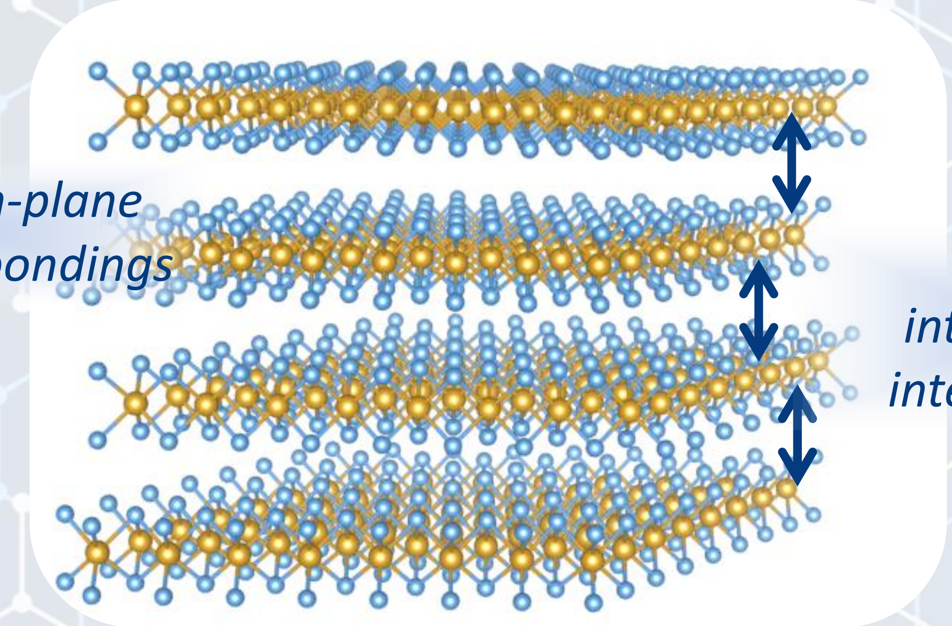


From 3D to 2D single-layer crystals

Bidimensional materials are **monolayer crystals** with a thickness in the atomic scale.

Strong in-plane covalent bondings

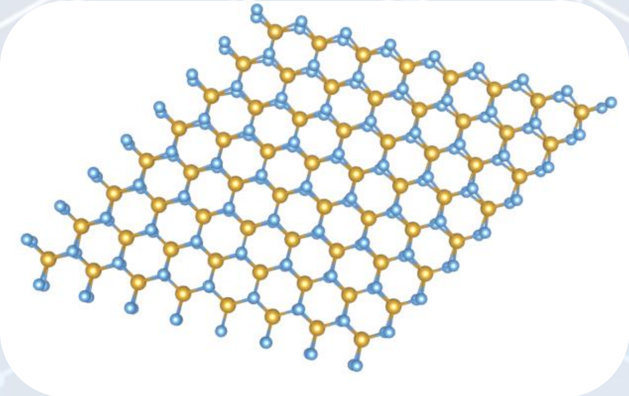


Weak inter-layer interactions

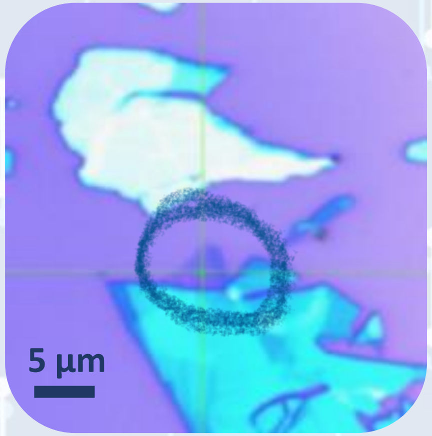
3D crystal

Exfoliation

Transition Metal Dichalcogenides (TMD)



Monolayer crystal

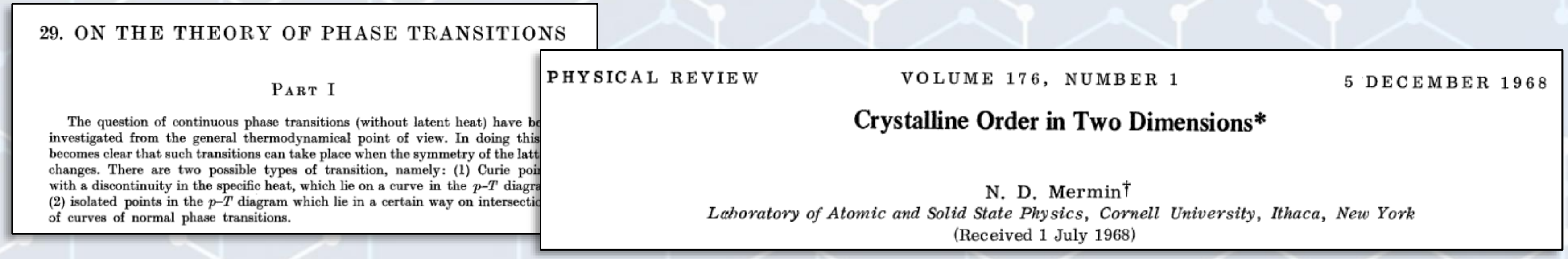


Optical microscope image of a TMD monolayer

The first 2D crystal: graphene

Theoretically, graphene should not exist!

In the 1930s, Peierls and Landau indeed proved that 2D crystals are thermodynamically unstable. Later, in 1968, Mermin arrived to the same results.


29. ON THE THEORY OF PHASE TRANSITIONS

PART I

The question of continuous phase transitions (without latent heat) have be[illegible] investigated from the general thermodynamical point of view. In doing this becomes clear that such transitions can take place when the symmetry of the latt[illegible] changes. There are two possible types of transition, namely: (1) Curie poi[illegible] with a discontinuity in the specific heat, which lie on a curve in the p–T diagra[illegible] (2) isolated points in the p–T diagram which lie in a certain way on intersectio[illegible] of curves of normal phase transitions.

PHYSICAL REVIEW VOLUME 176, NUMBER 1 5 DECEMBER 1968

Crystalline Order in Two Dimensions*

N. D. Mermin†

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

(Received 1 July 1968)

In 2004, Graphene was isolated for the first time by Geim and Novoselov.

Why graphene could be isolated? The previous theories considered a 2D crystal in a 2D world… but we live in a three dimensional world! Out-of-plane deformations along the third dimension can stabilize 2D materials.

N. Mat. 6 (2007) 183-191

The "Friday night experiments" sessions

Geim had the tradition to host regular "Friday night experiments" to try out ideas not necessarily linked to their day jobs. During these sessions, they obtained:

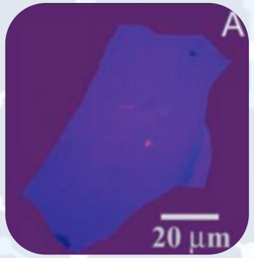
https://www.mub.eps.manchester.ac.uk/graphene/2020/12/the-accidental-nobel-laureates-10-years-on

A levitating frog (1997) - Winned the Ig nobel prize in 2000

Eur. J. Phys. 18 (1997) 307–313

The gecko tape (2003)

N. Mat. 2 (2003) 461–463

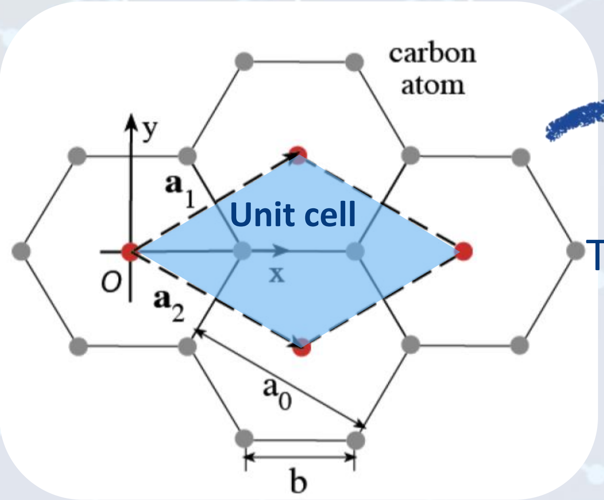


The first isolation of graphene (2004)

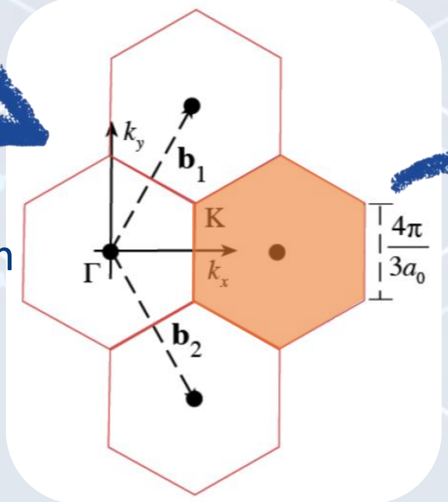
Science 306 (2004) 5696

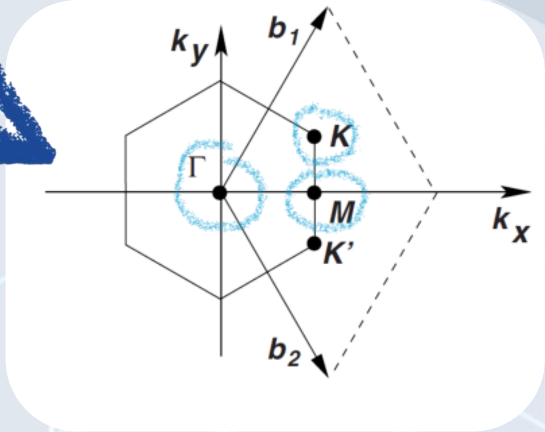
The structure of graphene

Bravais and reciprocal lattices of graphene:



Fourier Transform



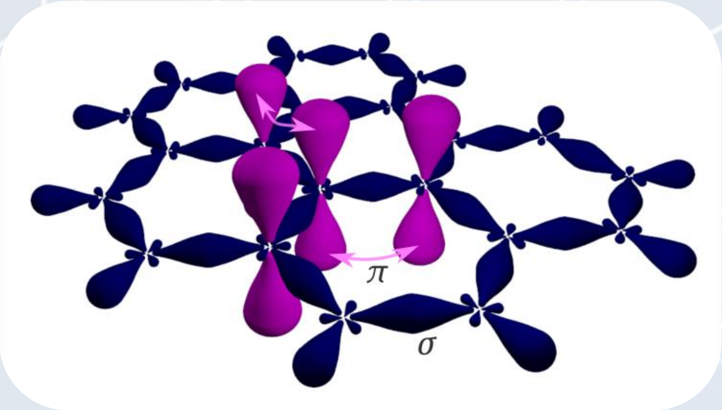


Hexagonal 2D lattice with an honeycomb structure

Hexagonal reciprocal lattice

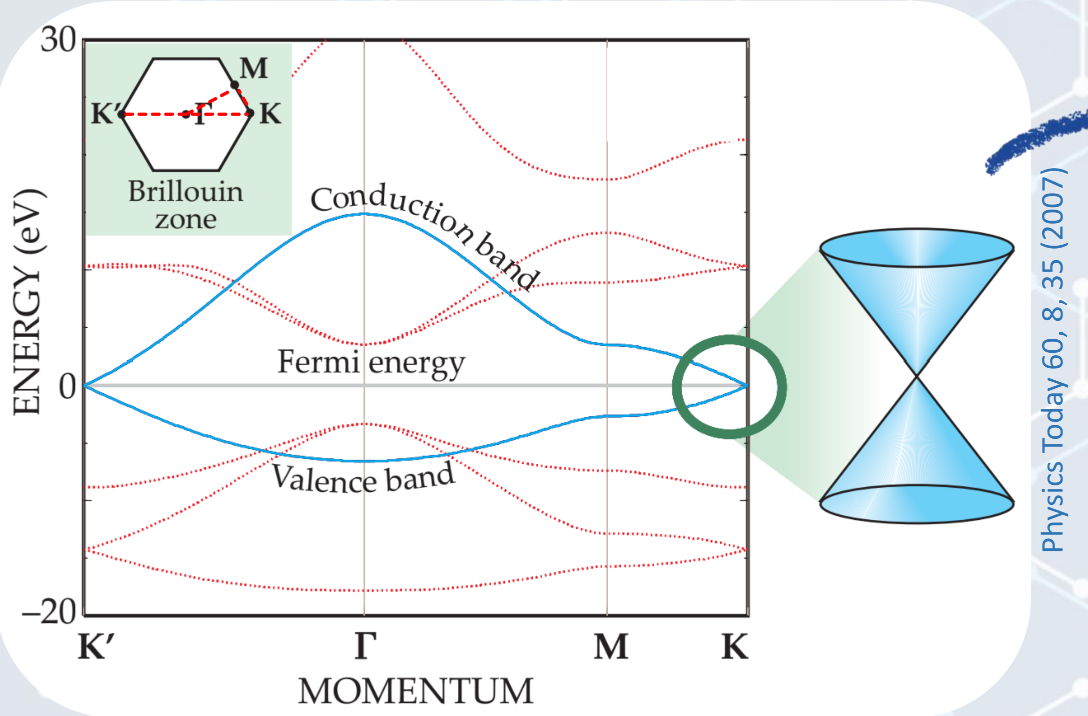
Hexagonal Brillouin zone

About the electrons:



The band structure of graphene

- Zero-gap semiconductor
- Linear dispersion relation around the K points! → Dirac cones



In the Dirac cones, electrons can be described by a Dirac hamiltonian:

$$\hat{H} = \hbar v_F \begin{pmatrix} 0 & k_x - ik_y \\ k_x + ik_y & 0 \end{pmatrix} = \hbar v_F \, \boldsymbol{\sigma} \cdot \mathbf{k}$$

- massless fermions moving at a constant velocity;
- pseudo-spin degree of freedom;
- chirality.

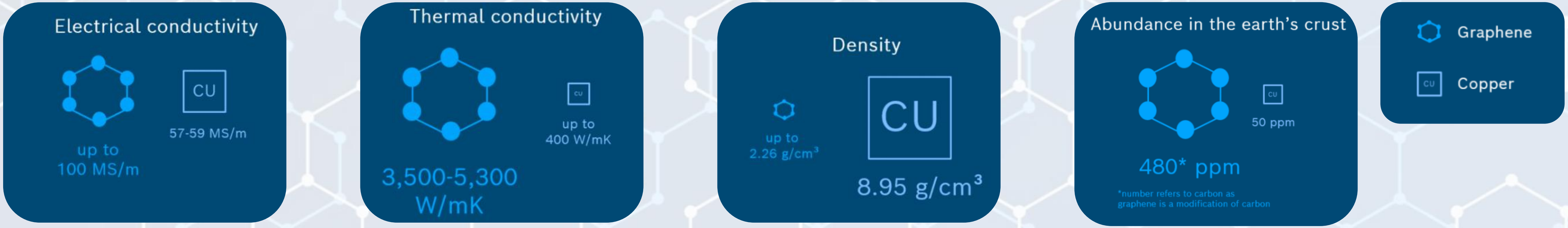
Electrons in graphene ''mimic'' relativistic particles!

N. Mat. 6 (2007) 183-191

Some of the outstanding properties of graphene

- High electrical conductivity (~ double of the copper one!);
- High thermal conductivity (second only to diamond);
- It is a ‘‘light’’ material;
- It is made of carbon, very abundant on the Earth;
- Very ‘‘strong’’ material (10 times stronger than steel)!*

Let’s make a comparison with copper, best known for its thermal and electrical conductivity:



https://www.bosch.com/stories/can-graphene-compete-with-copper-in-electrical-conductivity/

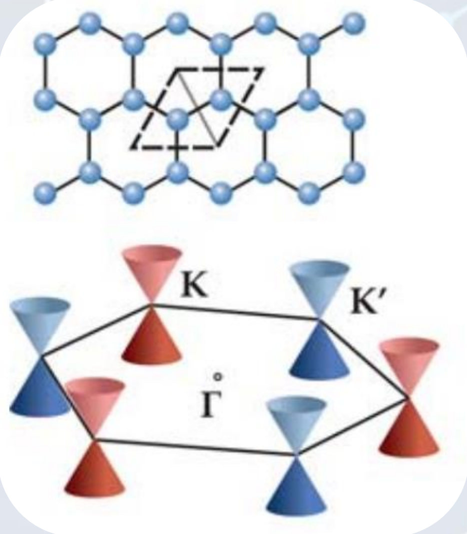
*Strenght is quantified by the Young’s modulus E = stress (σ)/strain(ε). For graphene, $E \approx 10^{12}$ Pa, while steel has $E \approx 2*10^{11}$ Pa. (from wikipedia)

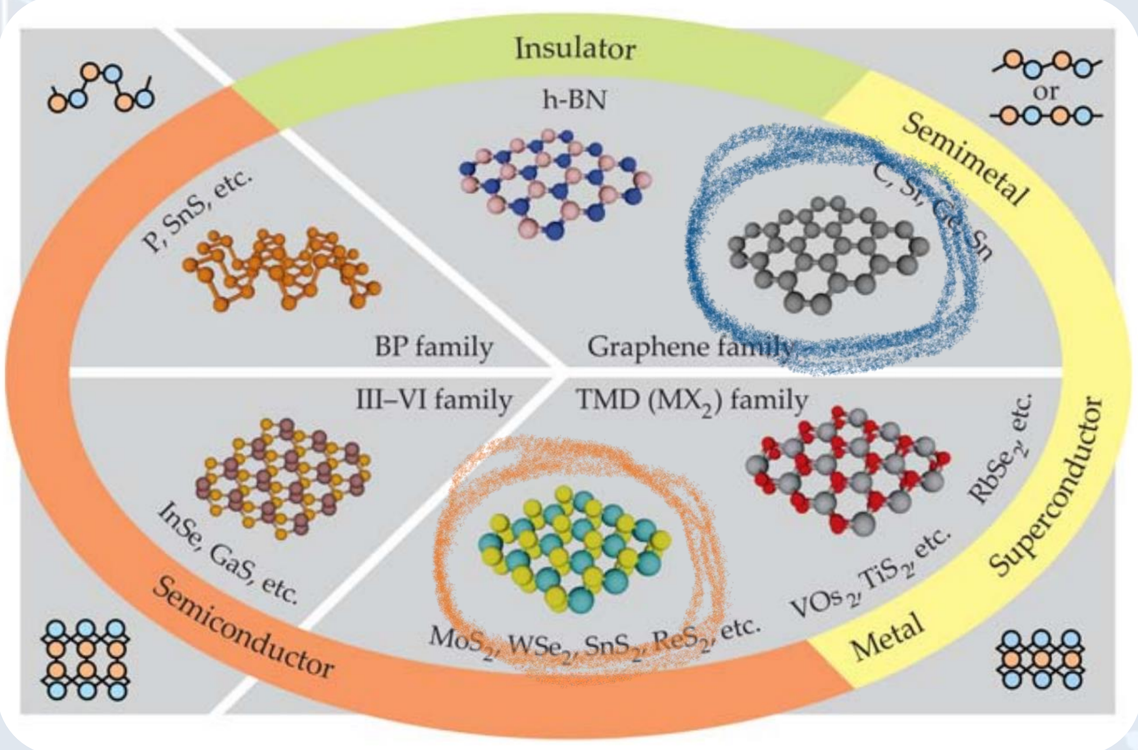
Beyond graphene

There is a shortcoming for the use of graphene in optical and electronic devices: it has a zero bandgap!

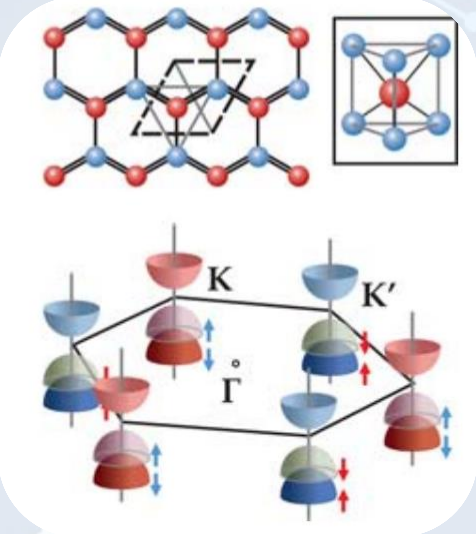
Luckily, there are many bidimensional crystals which span the full range of electronic properties.

Graphene





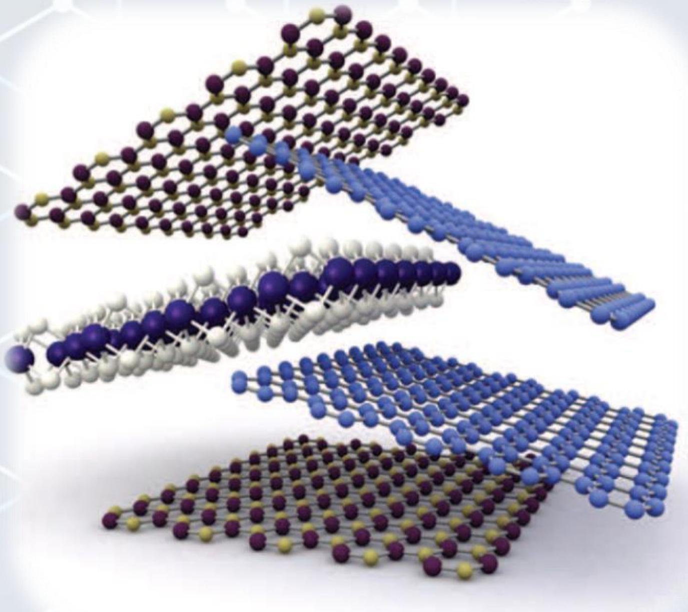
Transition metal dichalcogenides (TMDs)



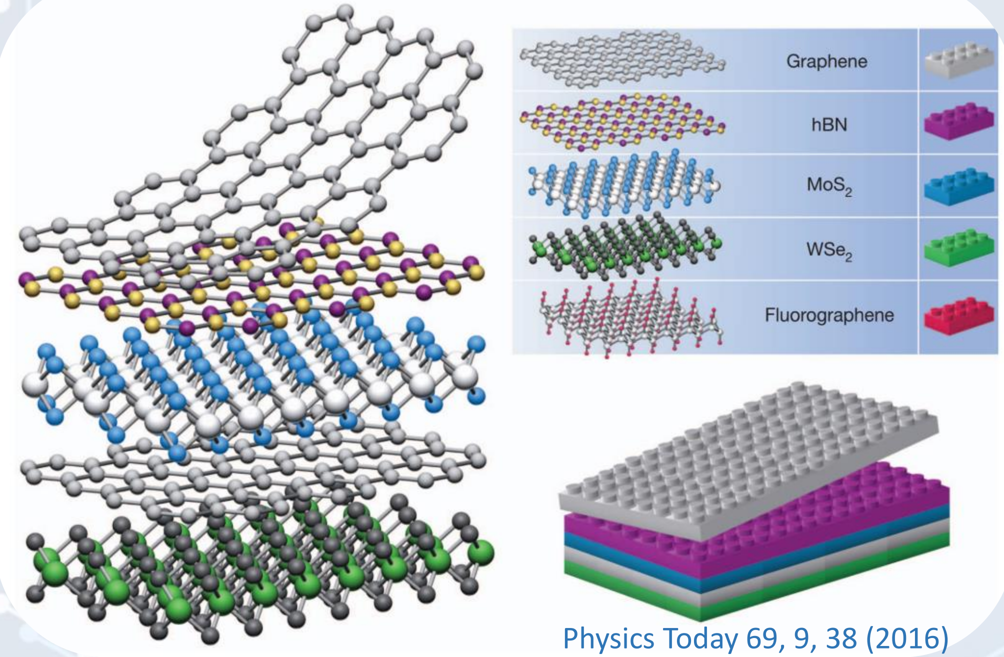
Physics Today 69, 9, 38 (2016)

Stacking 2D crystals: the heterostructures

- Piling different 2D crystals gives rise to **new electronic structures**!
- Many degrees of freedom in stacking 2D crystals: chemical composition, twist-angles;



Science 353, 6298 (2016)



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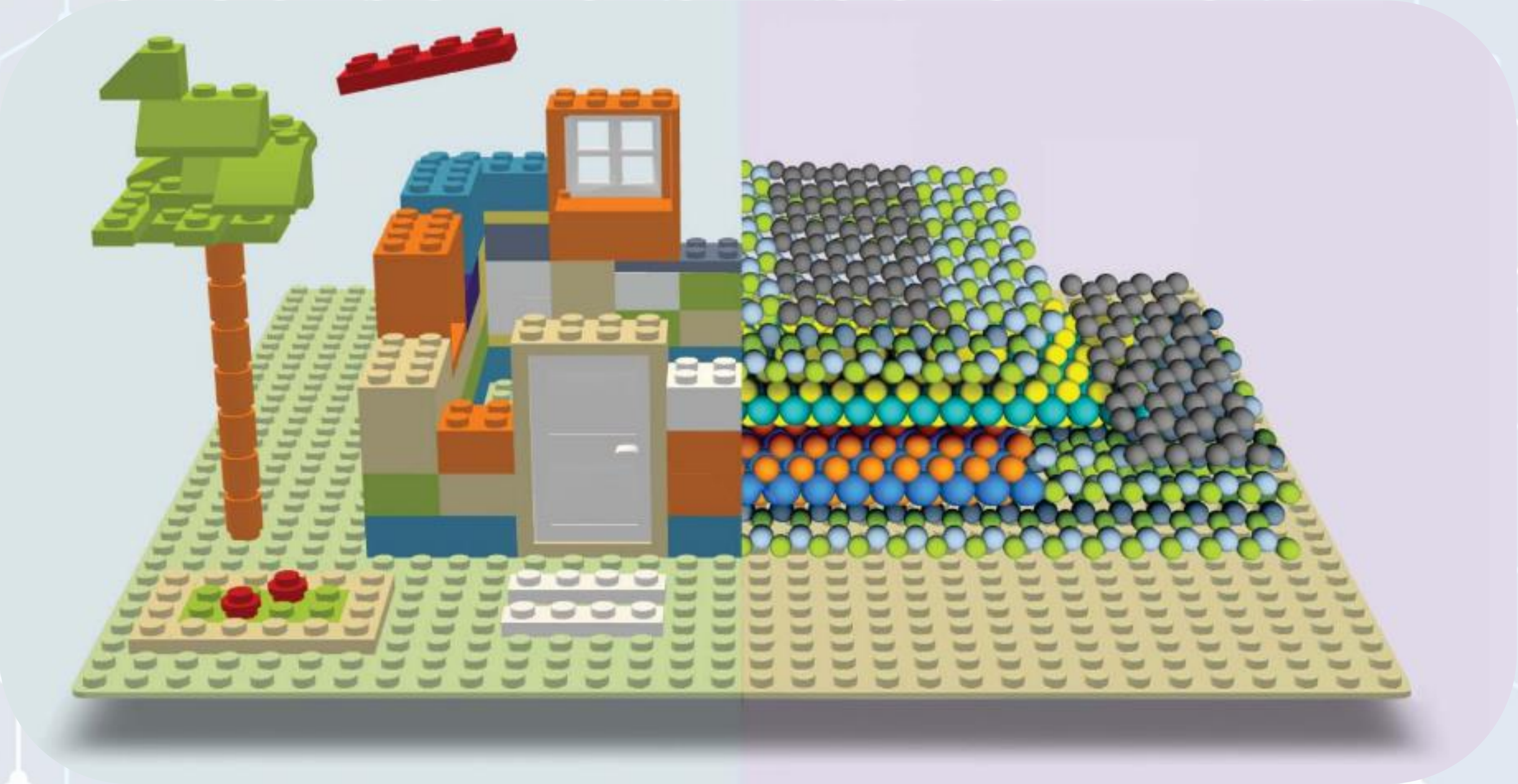

You can build new artificial systems with one-atom-thick Lego bricks!

Physics Today 69, 9, 38 (2016)

Thank you for your attention!