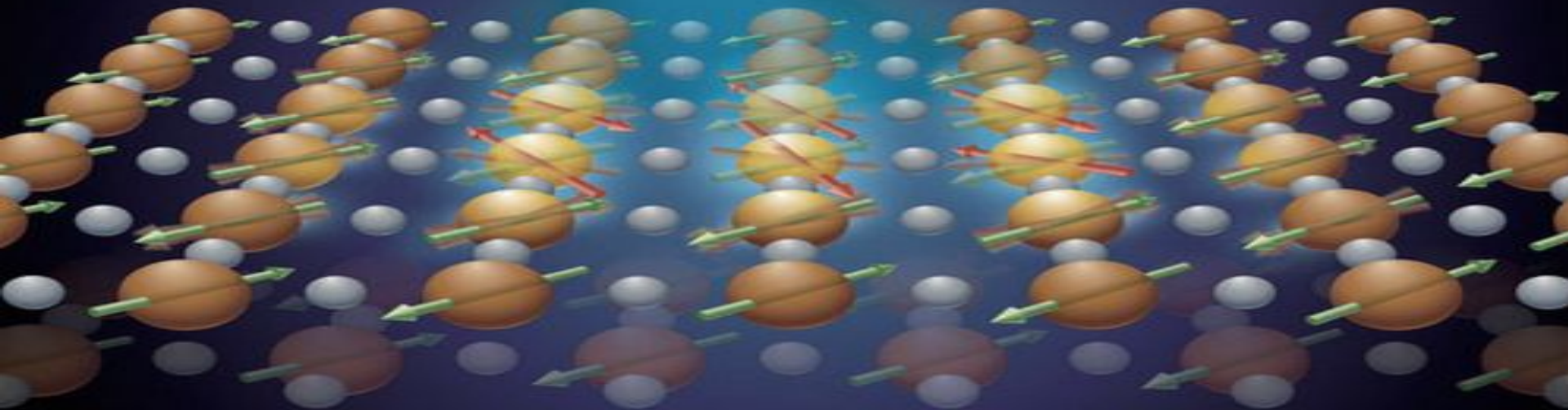


# Introduction to Solid State Physics

Sonia Haddad

Laboratoire de Physique de la Matière Condensée  
Faculté des Sciences de Tunis, Université Tunis El Manar



# Outline

## Lecture I: Introduction to Solid State Physics

- **Brief story...**
- **Solid state physics in daily life**
- **Basics of Solid State Physics**

## Lecture II: Electronic band structure and electronic transport

- **Electronic band structure: Tight binding approach**
- **Applications to graphene: Dirac electrons**

## Lecture III: Introduction to Topological materials

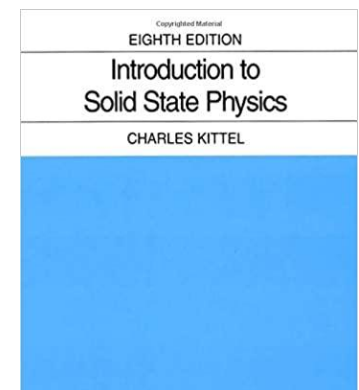
- **Introduction to topology in Physics**
- **Quantum Hall effect**
- **Haldane model**

It's an online lecture, but...stay focused...  
there will be **Quizzes** and **Assignments**!

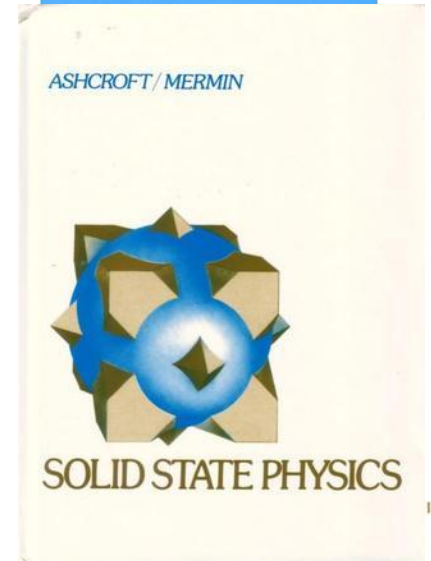


## References

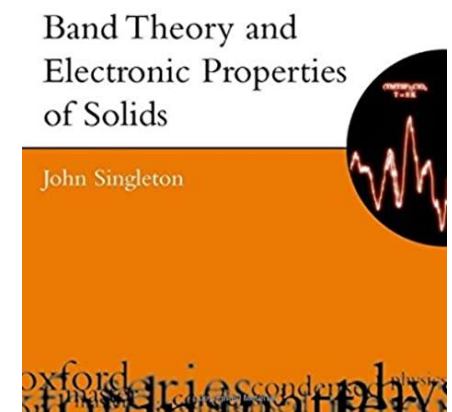
### Introduction to Solid State Physics, Charles Kittel



### Solid State Physics Neil Ashcroft and N. Mermin



### Band Theory and Electronic Properties of Solids, John Singleton



# Outline

## Lecture I: Introduction to Solid State Physics

- A Brief story...
- Solid state physics in daily life
- Basics of Solid State Physics

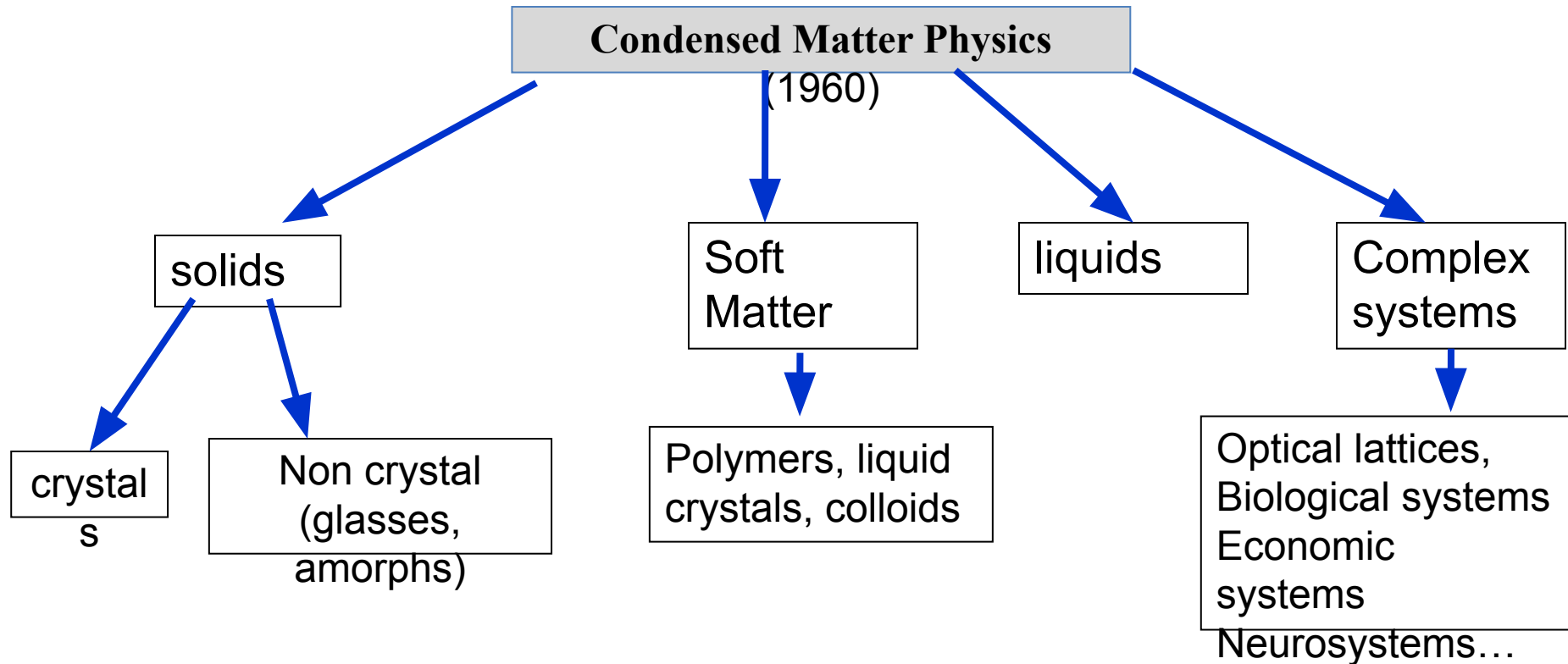
## Lecture II: Electronic band structure and electronic transport

- Tight binding approach
- Applications to graphene: Dirac electrons

## Lecture III: Introduction to Topological materials

- Introduction to topology in Physics
- Quantum Hall effect
- Haldane model

## What is solid state Physics?

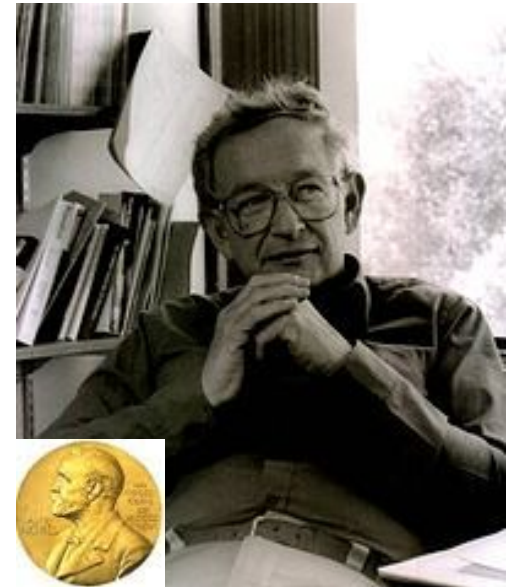


## What is condensed Matter Physics?

*"More is different!"*

*P.W. Anderson*

$$1+1 \neq 2$$





## What is Condensed Matter Physics?

Condensed matter physics deals with systems of **large number of interacting particles** (constituents)

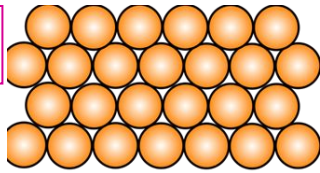
Explores macroscopic behavior of matter based on its **microscopic properties**



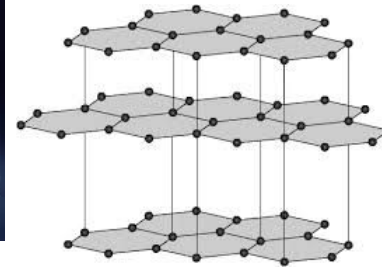


## What is solid state Physics?

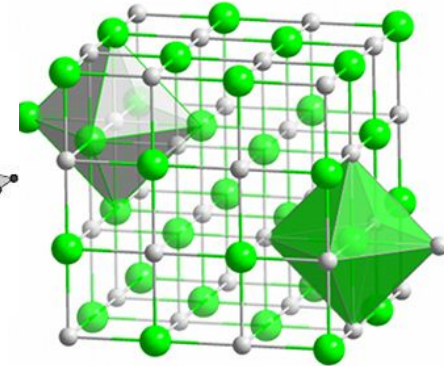
Crystalline  
solids



quartz

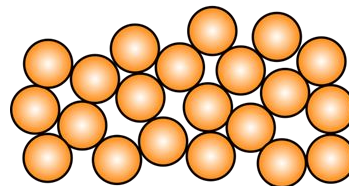


graphite

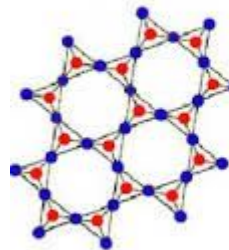


Na  
Cl

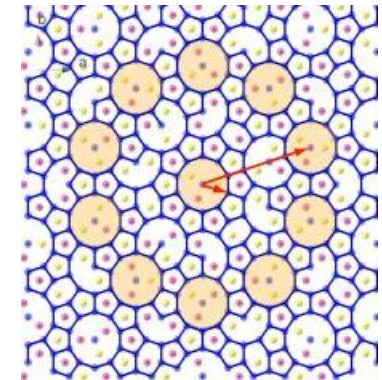
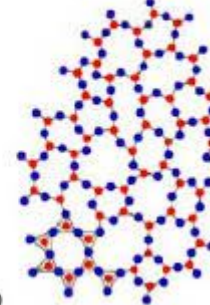
Non crystalline  
solids



Crystalline  $\text{SiO}_2$   
(Quartz)



Amorphous  $\text{SiO}_2$   
(Glass)



Quasi-crystals:  
Ordered at large scale but are  
not periodic

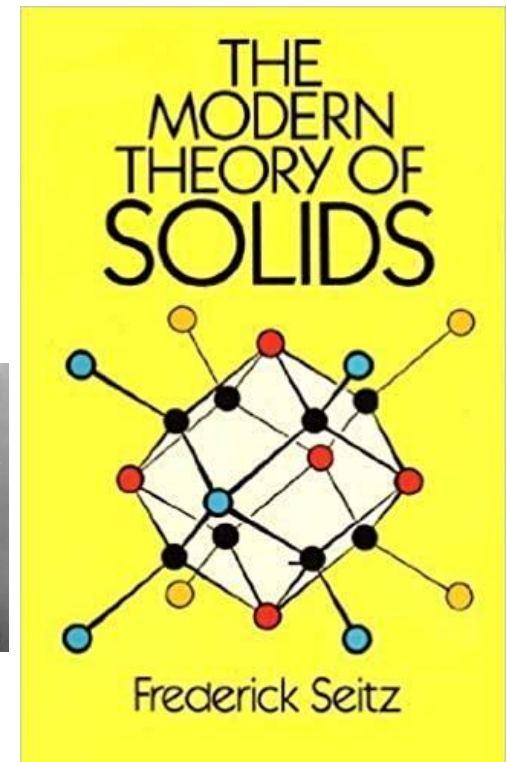
## What is solid state Physics?

- Study the microscopic properties (electrical, thermal, magnetic...) of solids
- Solid: system with a large number of particles (atoms, molecules, ions) **in strong interaction** (contrary to a gas)

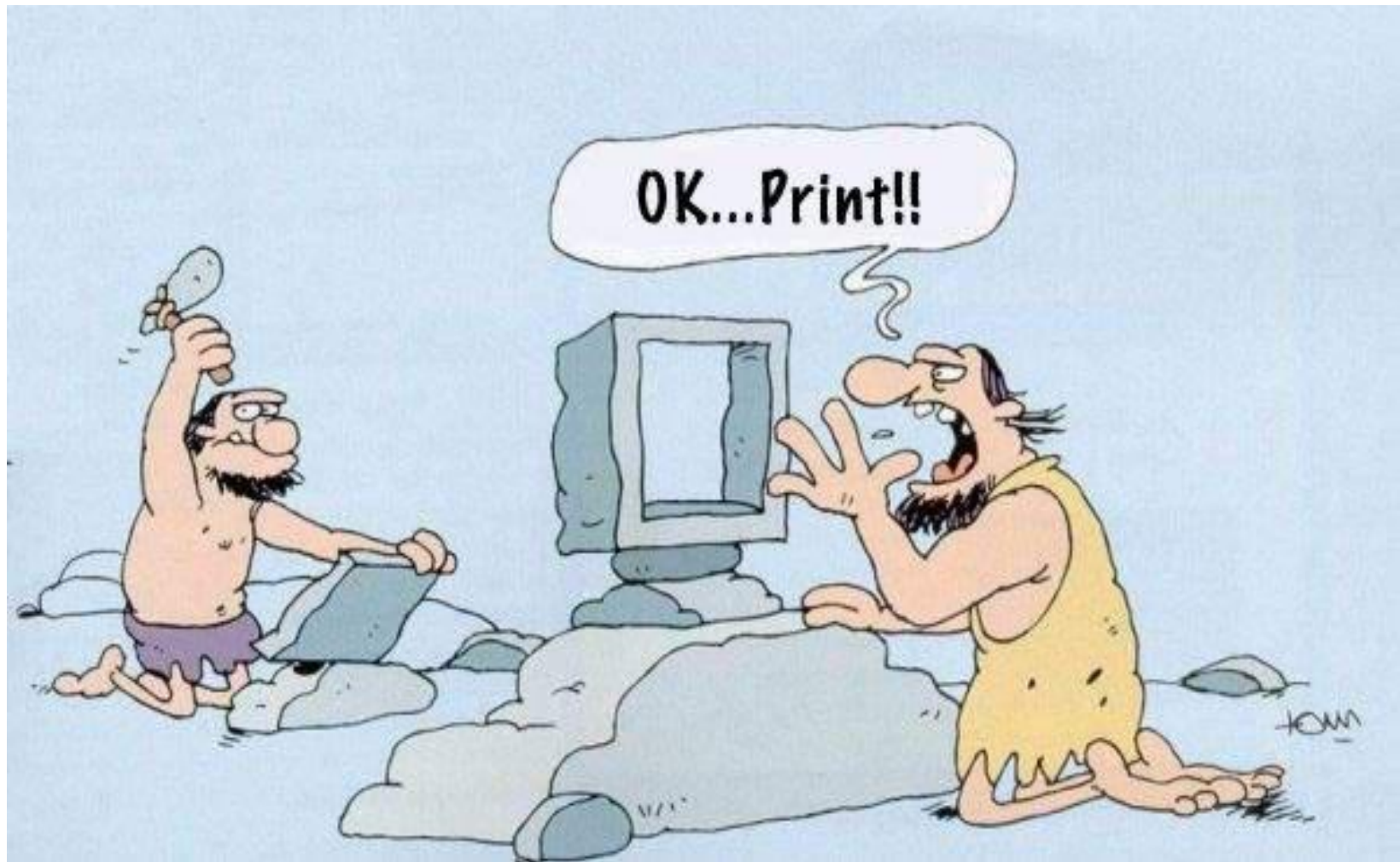
Birth of Solid state Physics:

publication of Fredrick Seitz  
book

*Modern Theory of Solids (1940)*



## Solid state and Materials Physics: a Brief story...





## Brief story...

More than 2.6 millions years ago



## a Brief story...

## The stone age

More than 2.6 millions years ago in Africa



**Flint**  
(contains crystals of quartz  $\text{SiO}_2$ )

**Knapping process of a flint**





## a Brief story...

## The stone age





## a Brief story...

Bronze: alloy of copper.

## The bronze age

3000 to 1000 BC





## a Brief story...

à 1100 BC



## The iron age



## a Brief story...

1400 to 50 BC



1320 BC



**Lycurgus Cup**  
**Glass+ gold nanoparticles**

4th-century





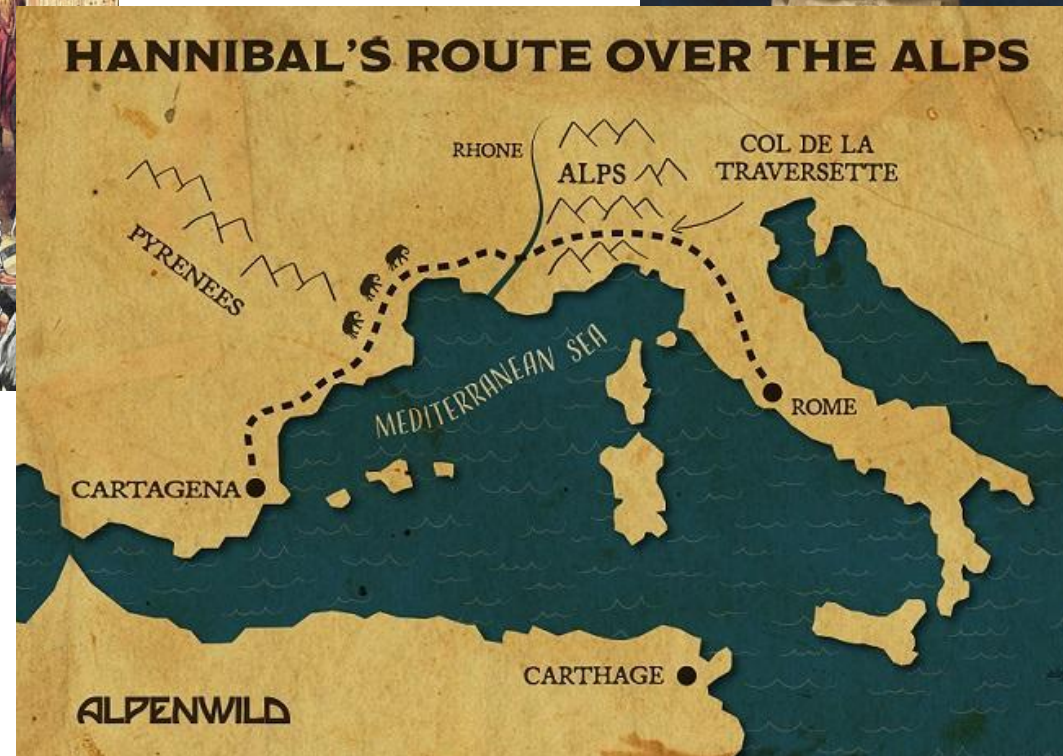
## a Brief story...

**Hannibal Barca**  
Carthaginian general

2sd punic war 218 BC



**Quiz:** Did Hannibal use African or Indian Elephants?





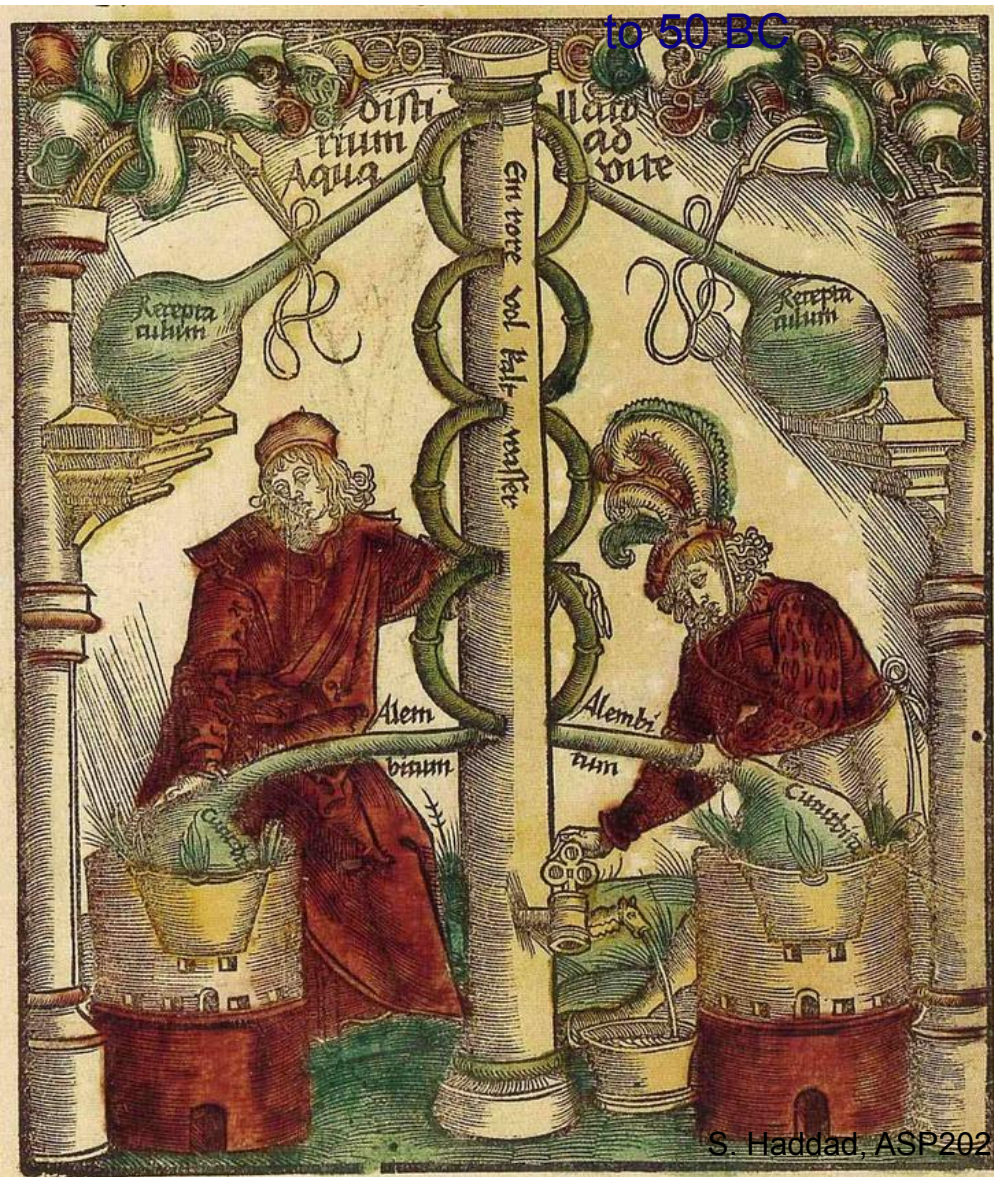
## Materials Physics: a Brief story...

Middle age:  
500 to 1500

### Use of:

Gold (Au), silver (Ag), iron (Fe), tin (Sn), mercury (Hg), , copper (Cu), lead (Pb), carbon (C), sulfur (S)...

Alchemy:  
transform metals in gold !





## Materials Physics: Birth of crystallography...

Modern period  
1500 to 1800

Discovery of crystallographic order

1781

René Just Haüy





## Materials Physics: Birth of crystallography...

Modern period  
1500 to 1800



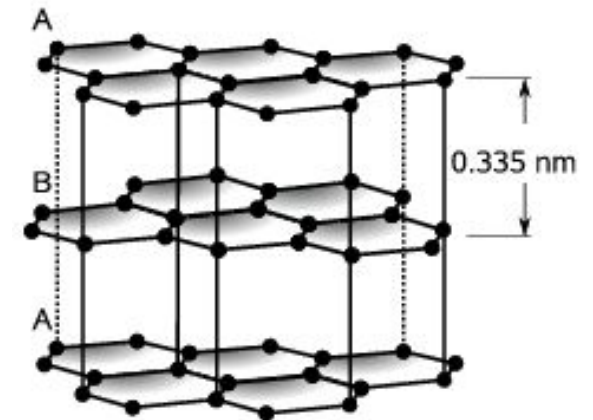
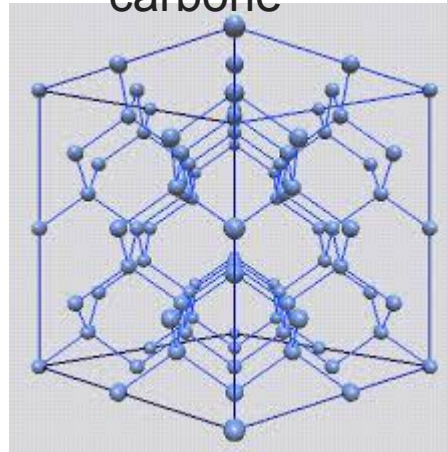
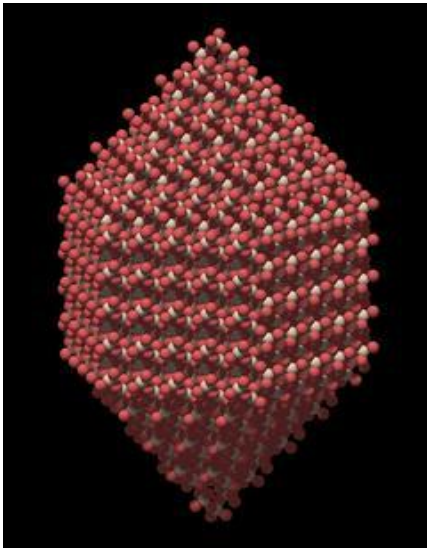
Quartz  
 $\text{SiO}_2$



Diamond  
d  
carbone



Graphite  
carbone



## Materials Physics: Birth of crystallography... 1895

How to observe the crystallographic order ?

X rays

1st Nobel prize in Physics 1901



**Wilhelm Conrad Röntgen**



## Materials Physics: Birth of crystallography... 1895

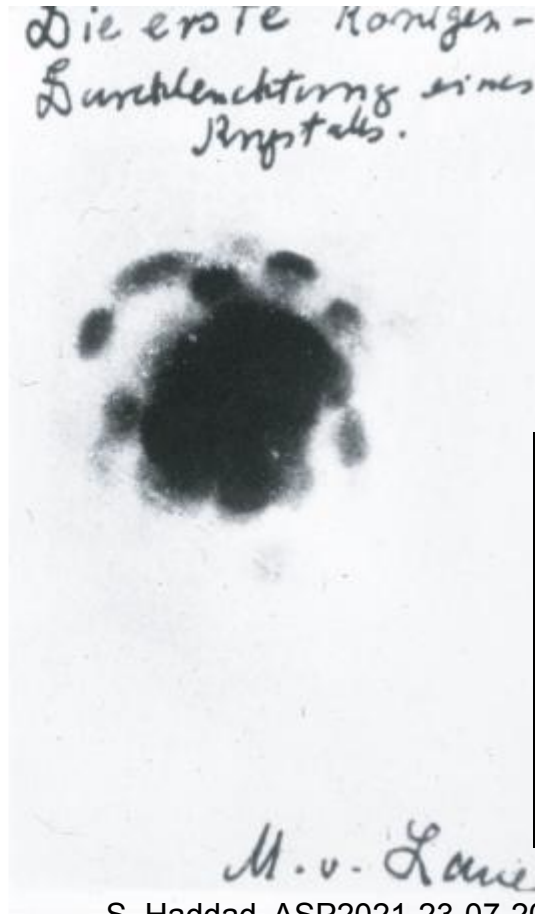
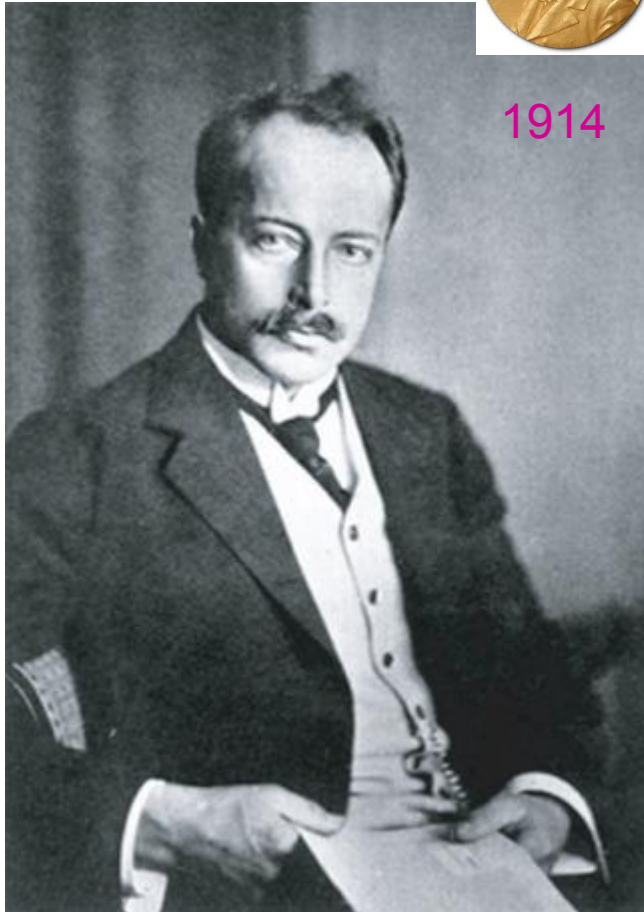
How to observe the crystallographic order ?

X rays

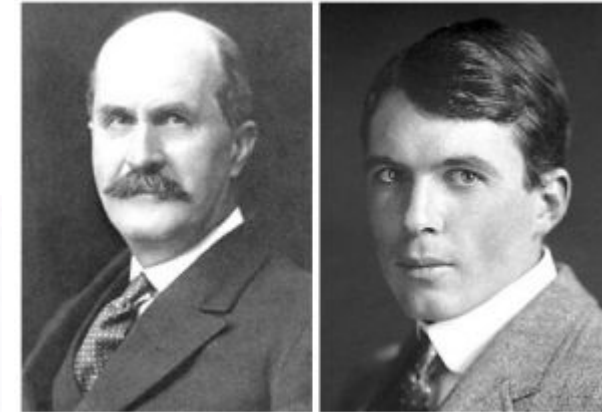
Max von Laue



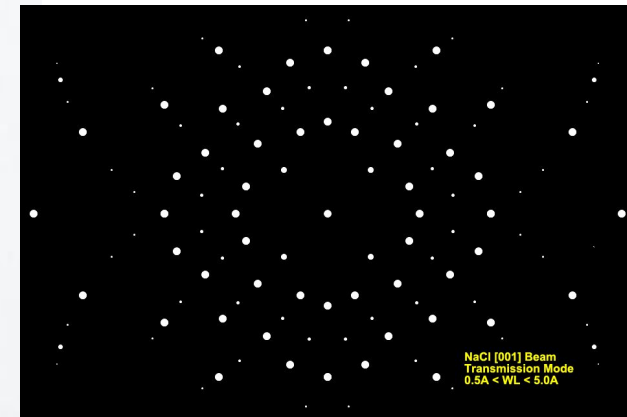
1914



1915



William Henry Bragg  
William Lawrence  
Bragg





## Emergence of Materials Physics

How to observe the crystallographic order ?

Electron Microscopy (1931)  
Max Knoll and Ernst Ruska...

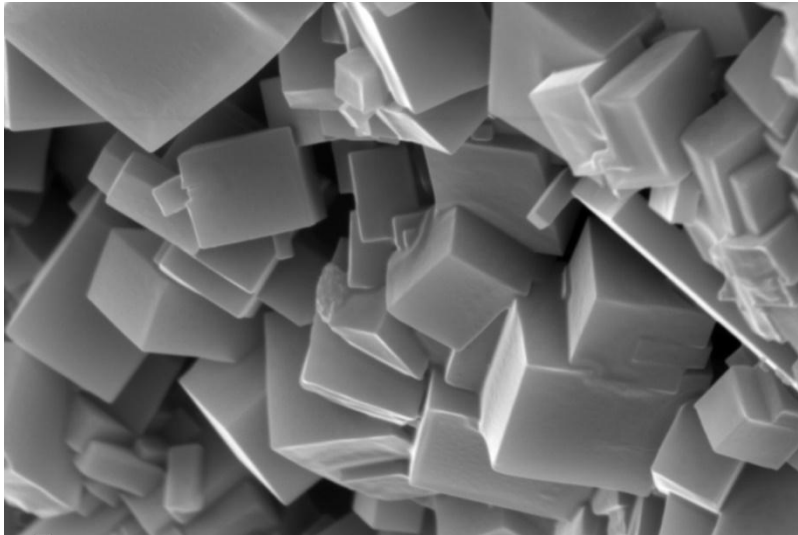


<https://www.youtube.com/watch?v=wMLvodIVYNI>

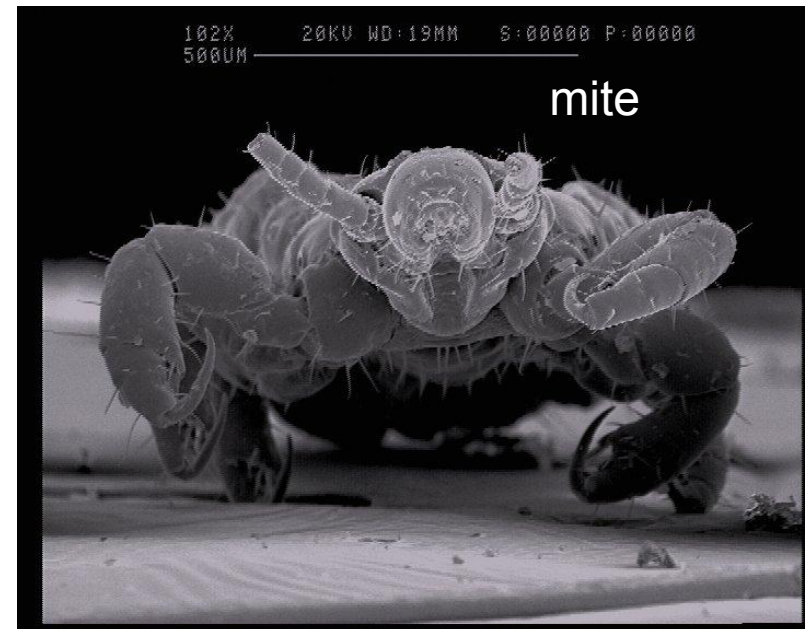
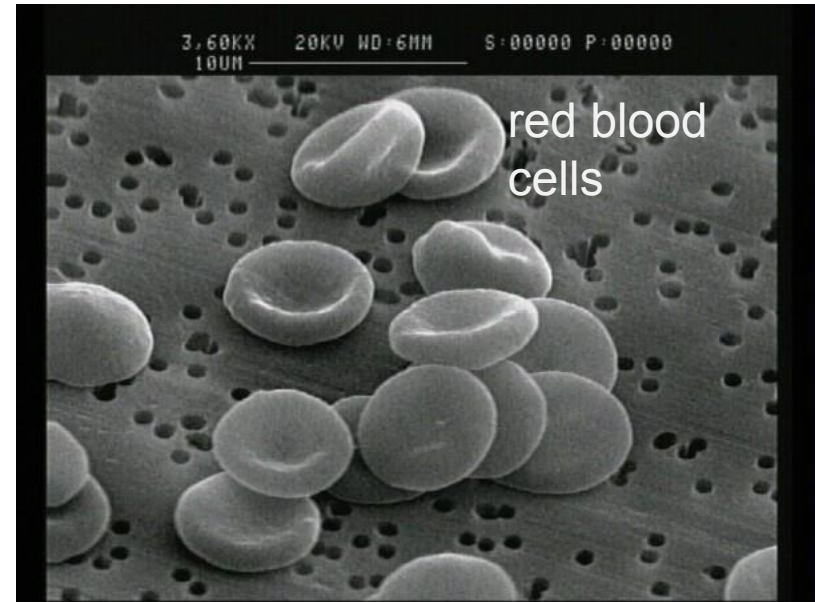


## Emergence of Materials Physics

### Electron Microscopy



Salt crystals



# Lecture I: Introduction to solid state Physics

## Some milestones

1897: Discovery of the electron by Thomson



Joseph John Thomson

1900: Quanta theory of Max Planck



1900: Drude model: 1<sup>st</sup> model of metals



Paul Drude

1924: De Broglie duality



Louis de Broglie

1926: Fermi – Dirac statistics



Enrico Fermi



Paul Adrien Maurice Dirac

1926: Sommerfeld model of electrons in metals



Arnold Johannes Sommerfeld

1926: Schrödinger equation



Erwin Schrödinger

1928: Bloch theorem and electronic band theory



Felix Bloch

1948: Invention of transistor



William Bradford Shockley



John Bardeen



Walter Houser Brattain



## Emergence of Materials Physics

Fabrication 1<sup>st</sup> transistor in 1949 based on Germanium



1956



John Bardeen, William Shockley  
et Walter Brattain

**Starting of la microelectronics**

## Emergence of Advanced Materials Physics



## Emergence of Materials Physics

### Materials for technology: how to rise the challenge?

"DO IT YOURSELF  
MATERIALS SYNTHESIS"



Design a material *à la carte* !

Analytical, Simulations,  
Machine learning

DESIGN

OBSERVATION

ENGINEERING

ADVANCED  
MATERIALS

MANIPULATION

ATOMIC SCALE

MICRO SCALE

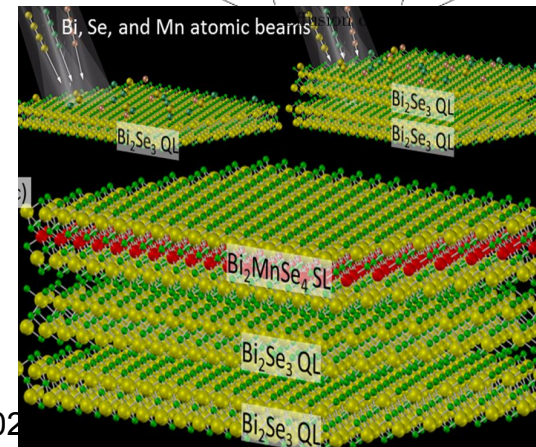
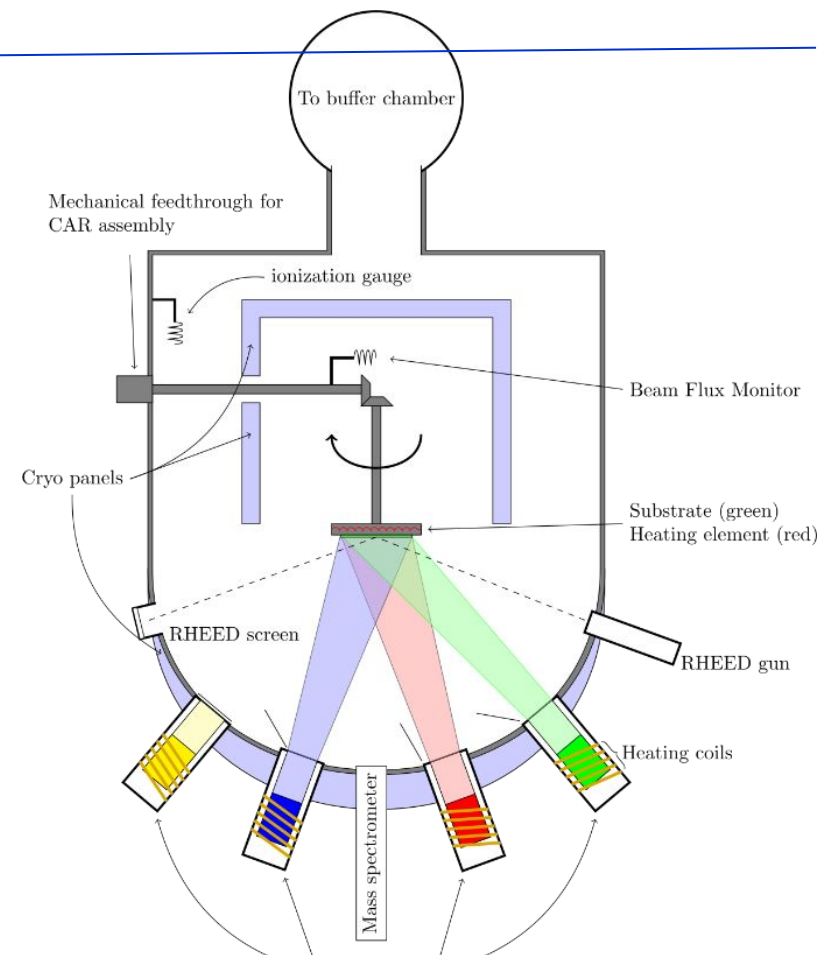
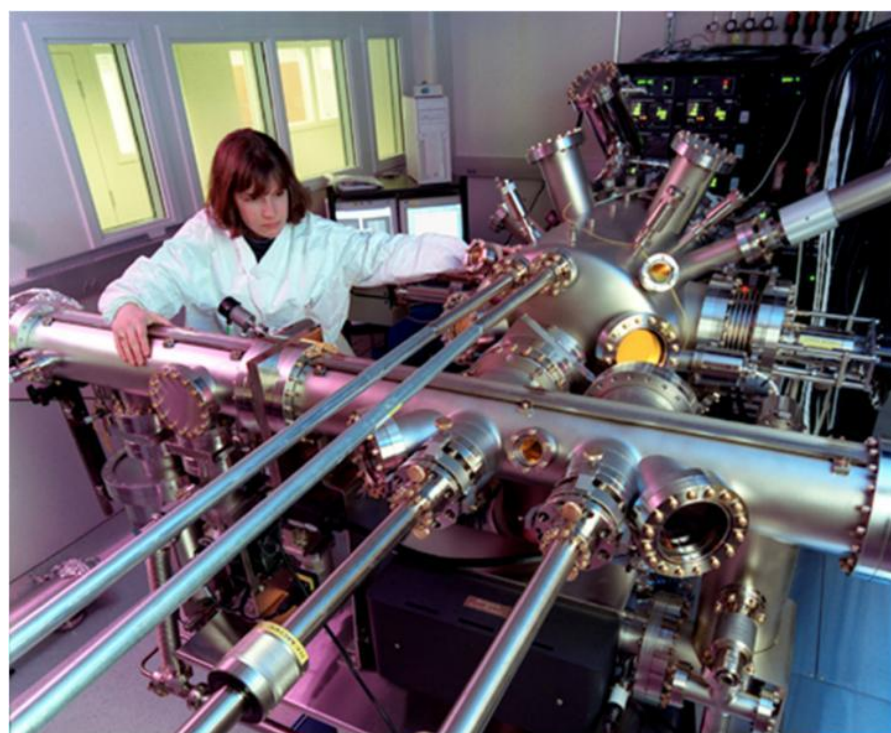
MACRO SCALE

MEGA SCALE

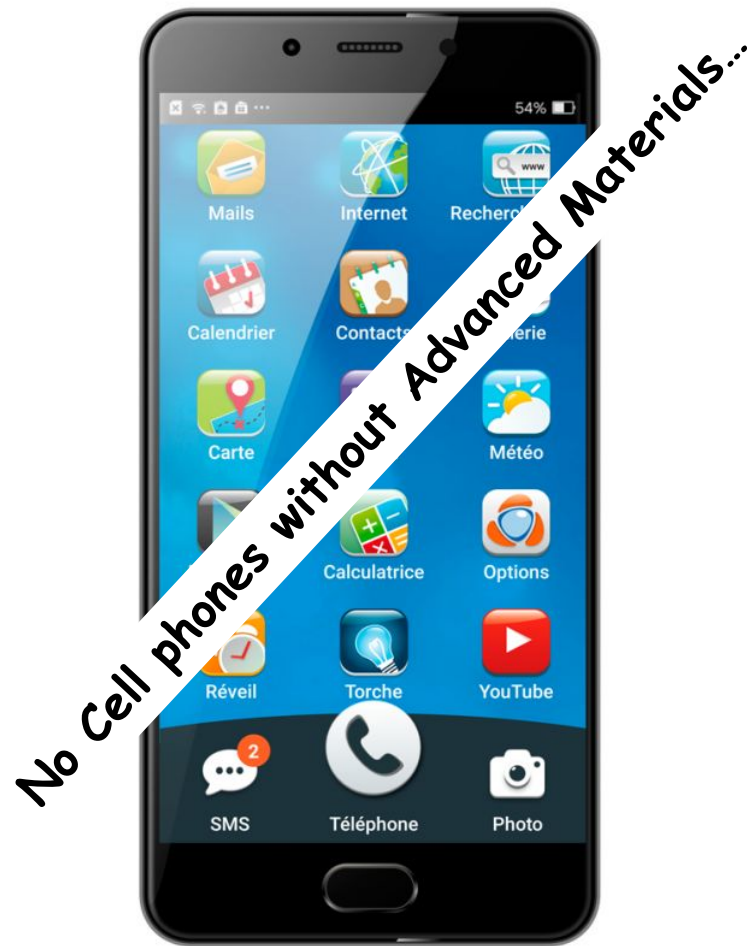


## Advanced Materials Physics

molecular beam  
epitaxy

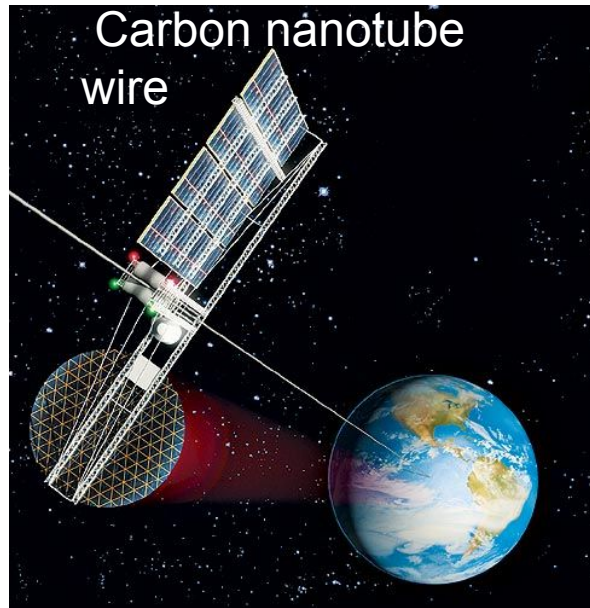


## Advanced Materials Physics

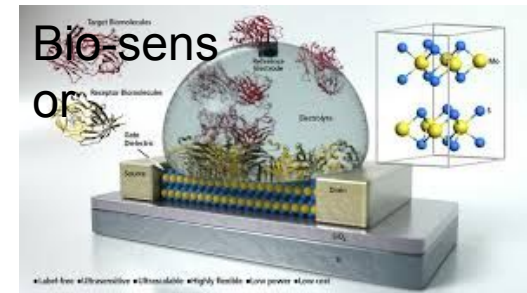
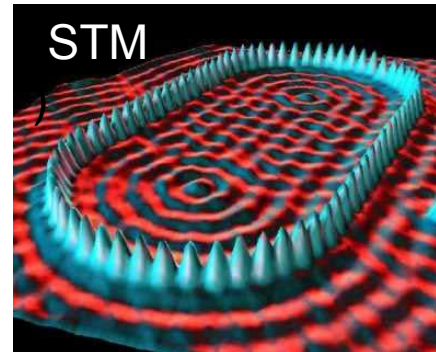




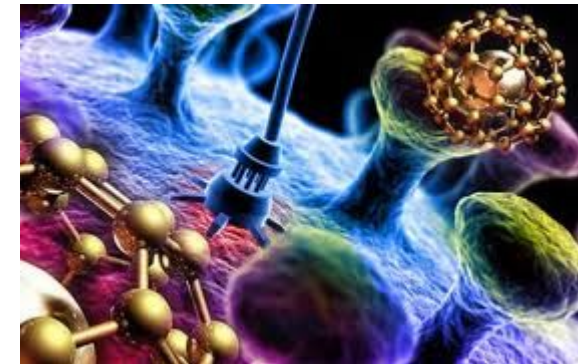
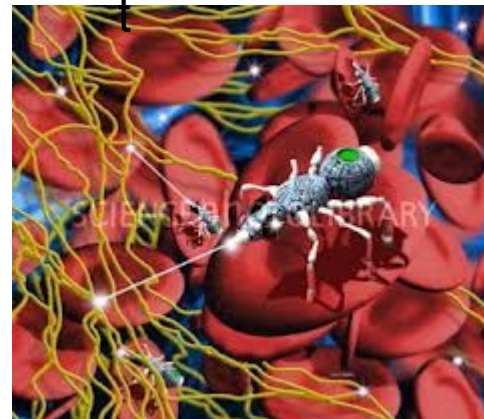




It is not Science-fiction  
!



Nano-robo









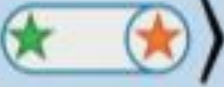



Meta-material

s




# QUANTUM COMPUTING

Material System	$ 0\rangle$	$ 1\rangle$
Ion traps		
Defects in solids		
Semiconductor quantum dot		
Superconducting		
Topological nanowire		

# Lecture I: Introduction to solid state Physics

Solid state physics :

- New **fundamental concepts** (composite fermions, topology...)
- **New phenomena**: superconductivity, quantum Hall effect, spin Hall effect...
- **New class of materials**: multiferroics, 2D materials, Dirac electrons systems, topological insulators, Weyl semi-metals
- Playground for fundamental concepts: **Higgs mechanism**, **Majorana fermions**, **Dirac fermions**...

Higgs Bosons in Particle Physics and in Condensed Matter  
G. E. Volovik  & M. A. Zubkov  
*Journal of Low Temperature Physics* **175**, 486–497 (2014) | [Cite this article](#)

## Topological materials move from the world of theoretical physics to experimental chemistry

These exotic materials could find applications in electronics, catalysis, and quantum computing

*by Neil Savage, special to C&EN*

June 23, 2018 | A version of this story appeared in **Volume 96, Issue 26**

International Journal of Modern Physics B | Vol. 30, No. 19, 1630012 (2016)

| Review Paper

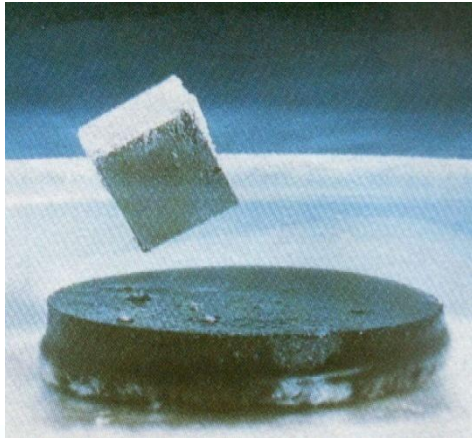
## Majorana fermions in condensed-matter physics

A. J. Leggett



# Lecture I: Introduction to solid state Physics

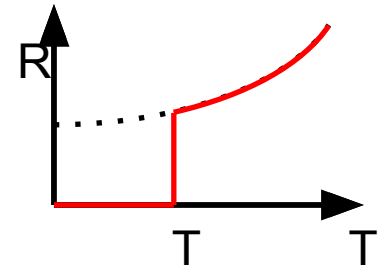
## Superconductivity and its applications



1911 :

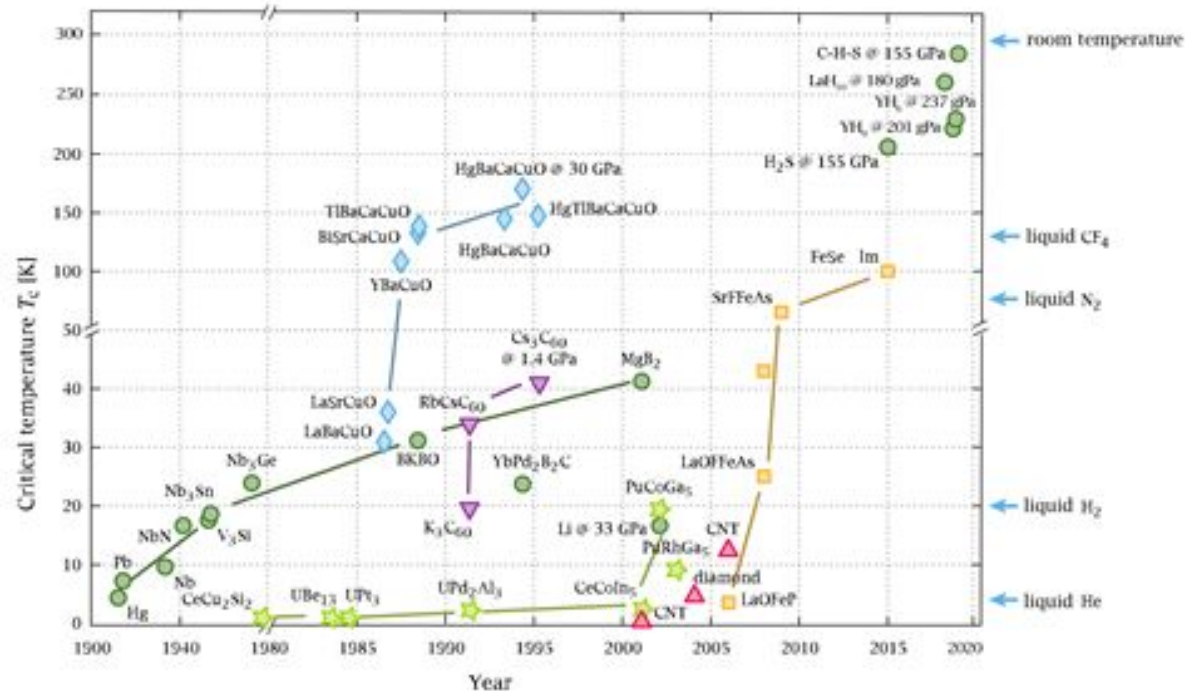
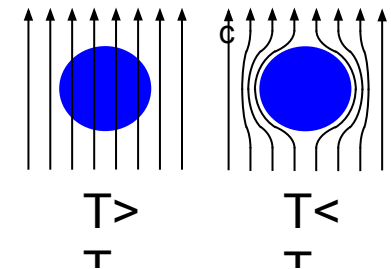
H. Kamerlingh Onnes

Electrical resistivity drops to zero at a critical temperature



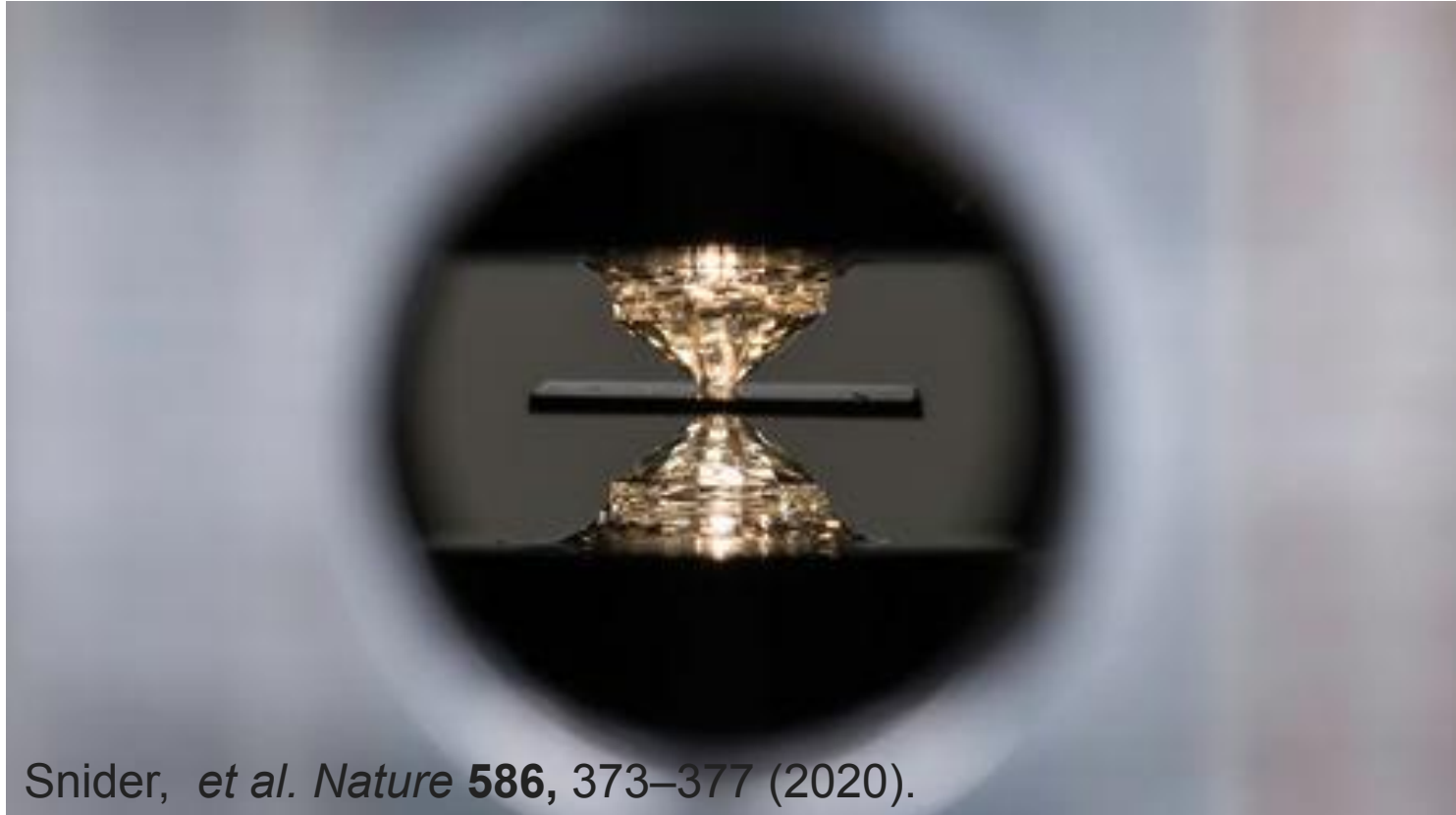
1933 : W. Meissner et R. Ochsenfeld

Total diamagnetism below  $T_c$  and  $H_c$



# After decades, room temperature superconductivity achieved

14 octobre 2020

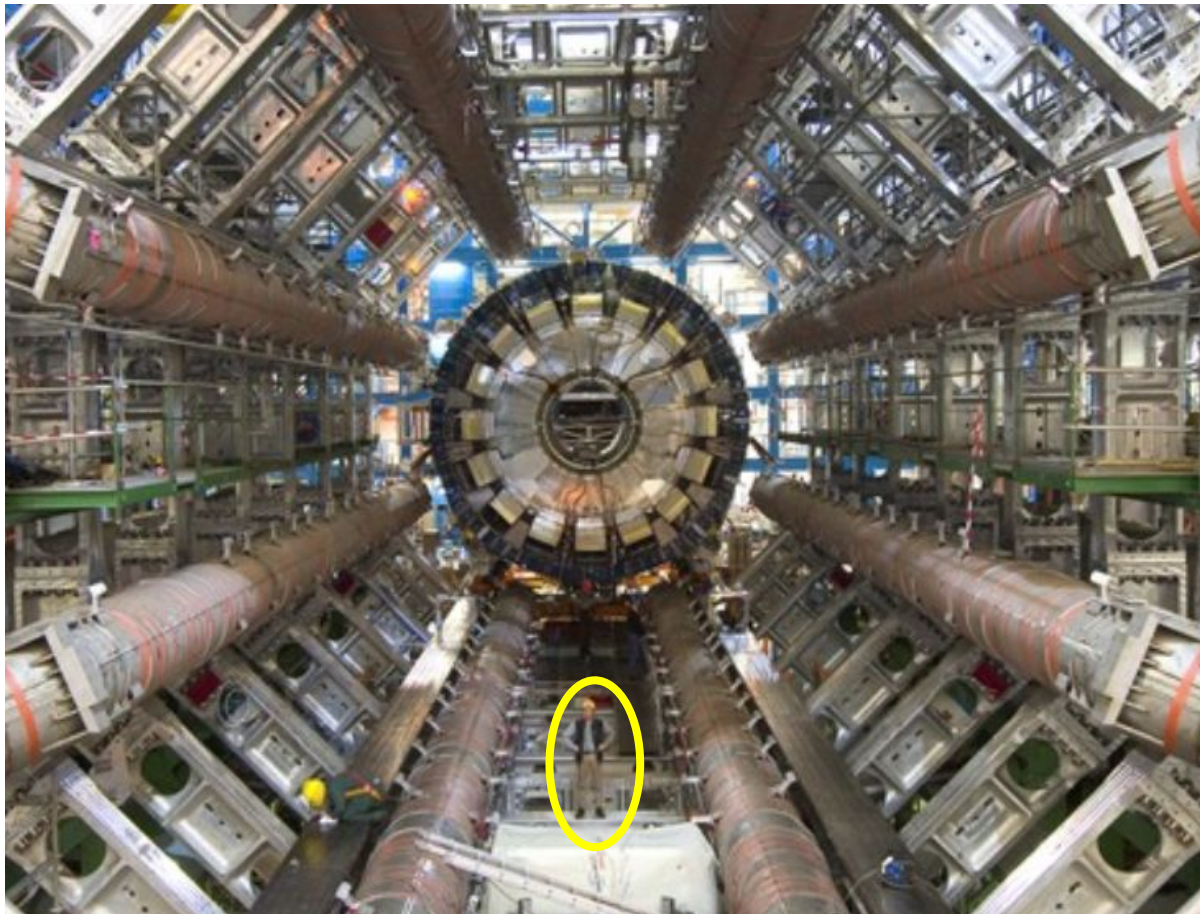


Snider, *et al. Nature* **586**, 373–377 (2020).

Crushed between two diamonds, a compound of hydrogen, sulfur, and carbon superconducts at room temperature.

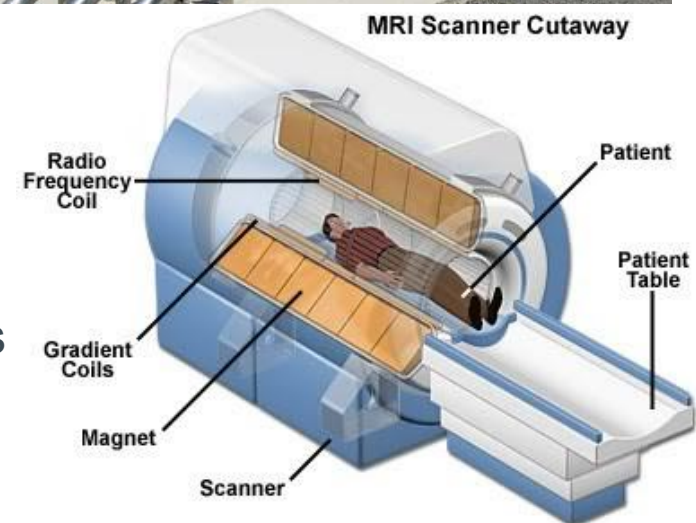
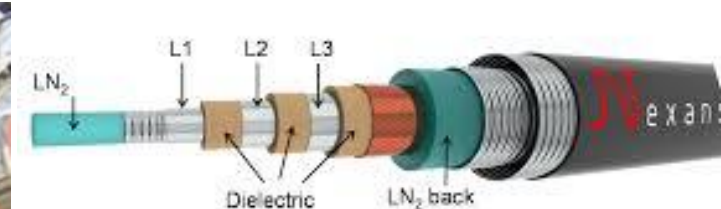
**Mechanism of high temperature superconductivity is still under debate!**





Central view of the ATLAS detector with its eight toroids around the calorimeter (Image: CERN)

, 10 kV, 1 km superconducting cable in  
t current limiter



## Advanced Materials Physics

### Superconductors

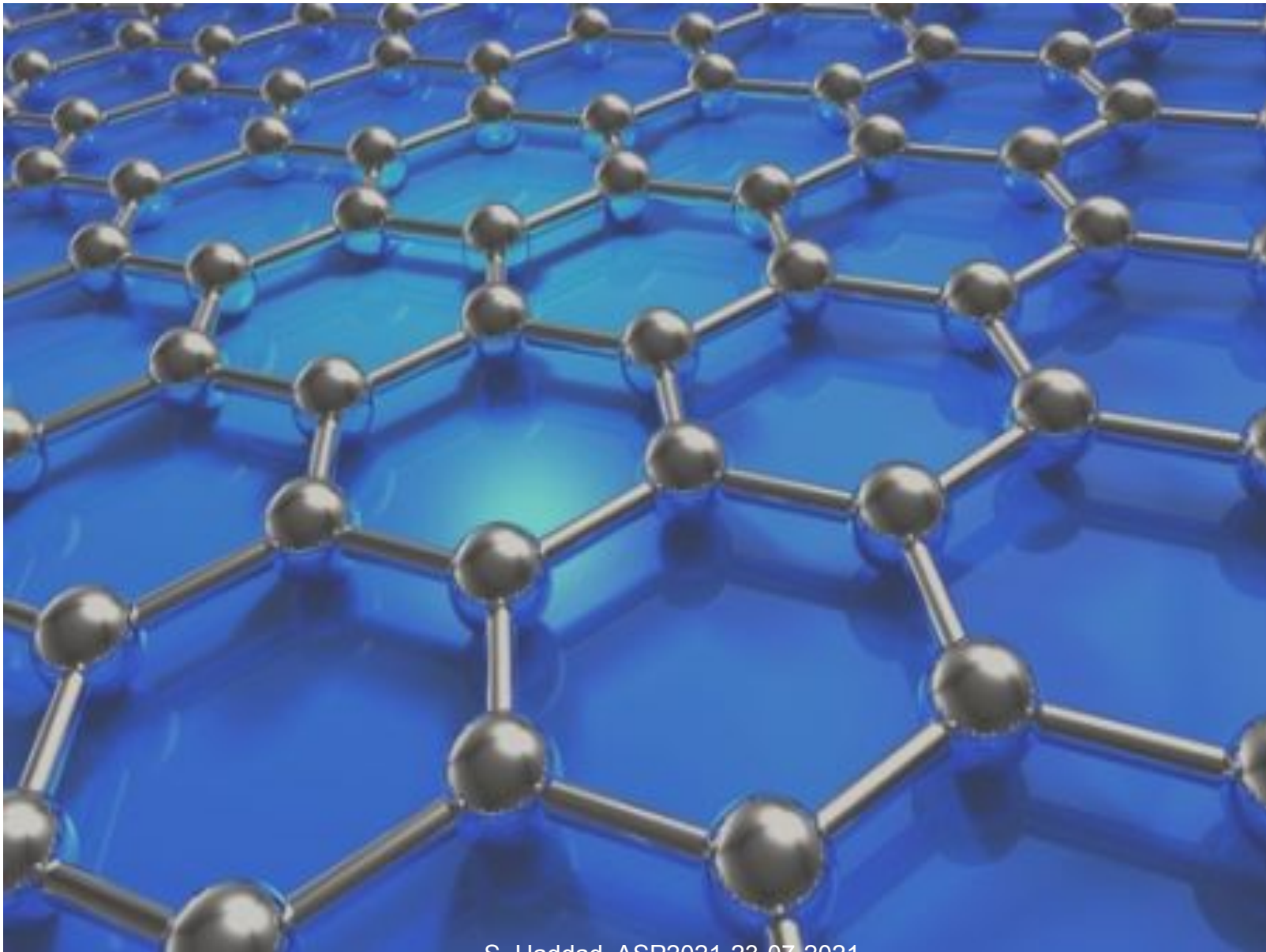




## Superconductors

**Applications...**

## Graphene, the wonder material



# WELCOME TO THE GRAPHENE AGE



George Osborne on a visit to the Manchester University lab of Professors Geim and Novoselov

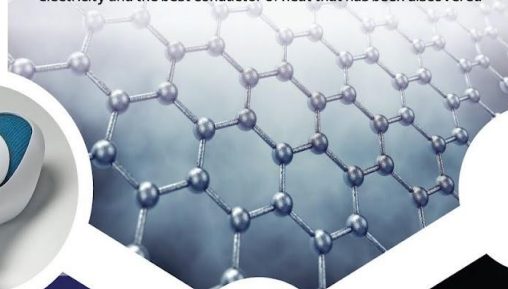
## SOLAR PANELS

MIT professors have shown how graphene could be used to make the electrodes in organic solar cells cheaper, lighter and more flexible than in current systems



## A CLOSER LOOK AT GRAPHENE

Graphene is a one-atom thick form, or allotrope, of carbon – other allotropes include diamond and graphite. It is often described as an atomic-scale chicken wire constructed of carbon atoms and their bonds. When graphene sheets are stacked, three million sheets would be needed to create a 1mm thickness. It's been claimed that it is the strongest material known to man, that a clingfilm-thick layer could support an elephant. Despite its strength it can be stretched by 20% without being damaged. It is also an excellent conductor of electricity and the best conductor of heat that has been discovered



## AIR TRAVEL

Using graphene would enable aeroplane manufacturers to develop extremely strong yet light components – bringing down weight and therefore reducing fuel costs



## MOBILE PHONES

Nokia is exploring the potential uses of graphene in mobile devices. Aside from smaller, more flexible phones, it may allow built-in solar power and transparent electronics



## FLEXIBLE SCREENS

Researchers in South Korea have produced a continuous layer of graphene 63cm wide. This has opened up possibilities in electronics, "You could theoretically roll up your iPhone and stick it behind your ear like a pencil," claims one scientist



## PROSTHETICS

Aside from allowing for the construction of stronger, more flexible and lighter limbs, its conductivity opens up new possibilities for its use in the electrodes used to turn brain signals into movement

## COMPUTER CHIPS

Geim and Novoselov have been working on demonstrating how graphene could replace silicon as the key material in electronic circuits. IBM is one of many electronics firms experimenting with graphene conductors



## DNA SEQUENCING

Researchers at British firm Oxford Nanopore, building on discoveries made at Harvard, claim that using graphene could reduce the cost and speed up the process of DNA sequencing





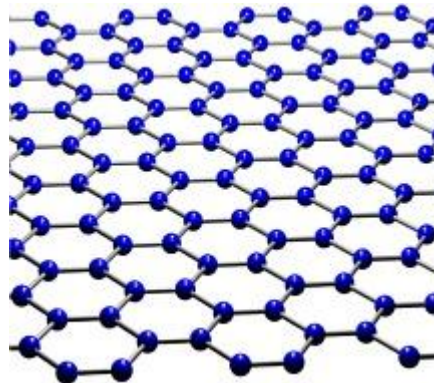
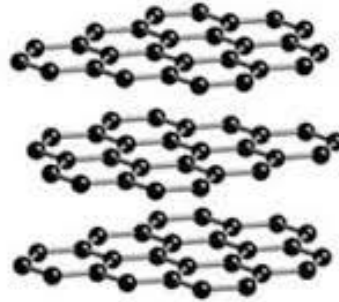
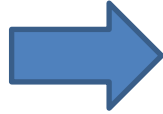
# Graphene, the wonder material



Graphite



Exfoliation (scotch)



Graphene discovered in  
2004



Geim et Novoselov  
Nobel prize of Physics

2010



## Graphene, the wonder material

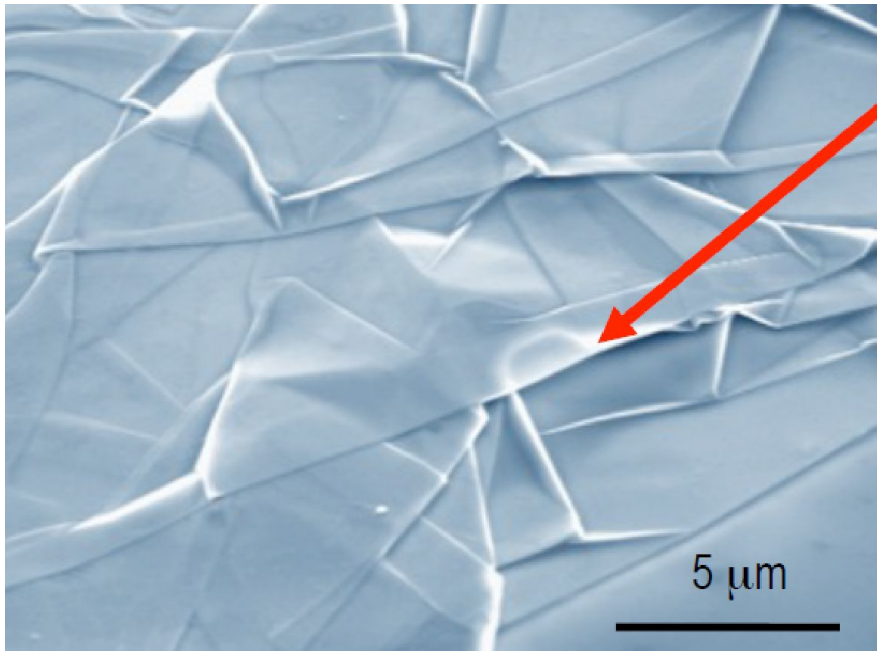
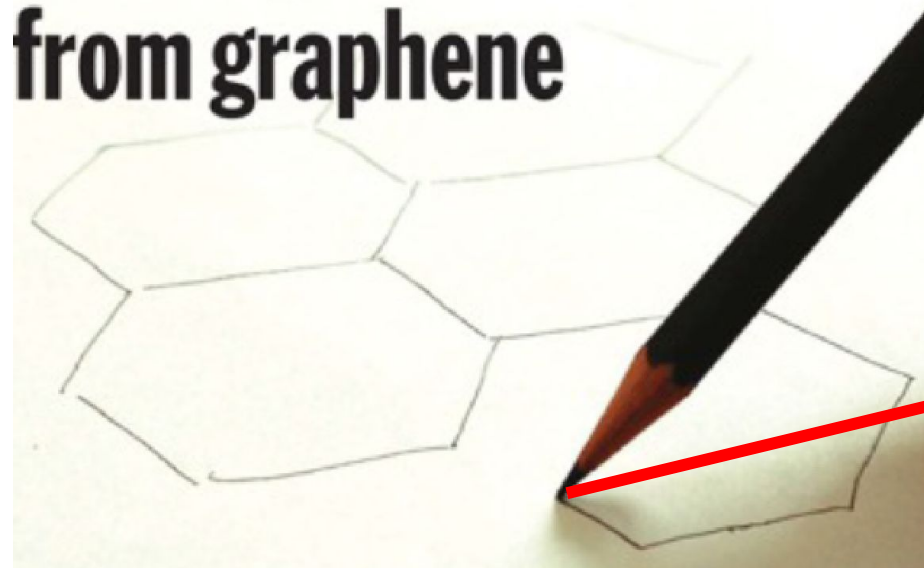
# Friday scribble yields Nobel Prize

By David Bradley | 1 January 2011

The work by Geim and Novoselov on graphene is equally bizarre and unexpected. Geim explains that the pair discovered how to make graphene in a 'fun Friday afternoon experiment' where they used adhesive tape to peel off the top layer of carbon atoms from a pencil mark on a glass surface and, with repeated folding and peeling of the sticky tape, were able to whittle the deposit down to a layer one single atom thick. Of course, the fine details of this 'cleavage' technique and its implications for science were published in research papers with rather esoteric, yet intriguing, titles such as *Electric Field Effect in Atomically Thin Carbon Films*<sup>1</sup> in the journal *Science* in October 2004 and *Two-dimensional atomic crystals* in *Proceedings of the National Academy of Sciences*<sup>2</sup> in 2005.



# Drawing conclusions from graphene

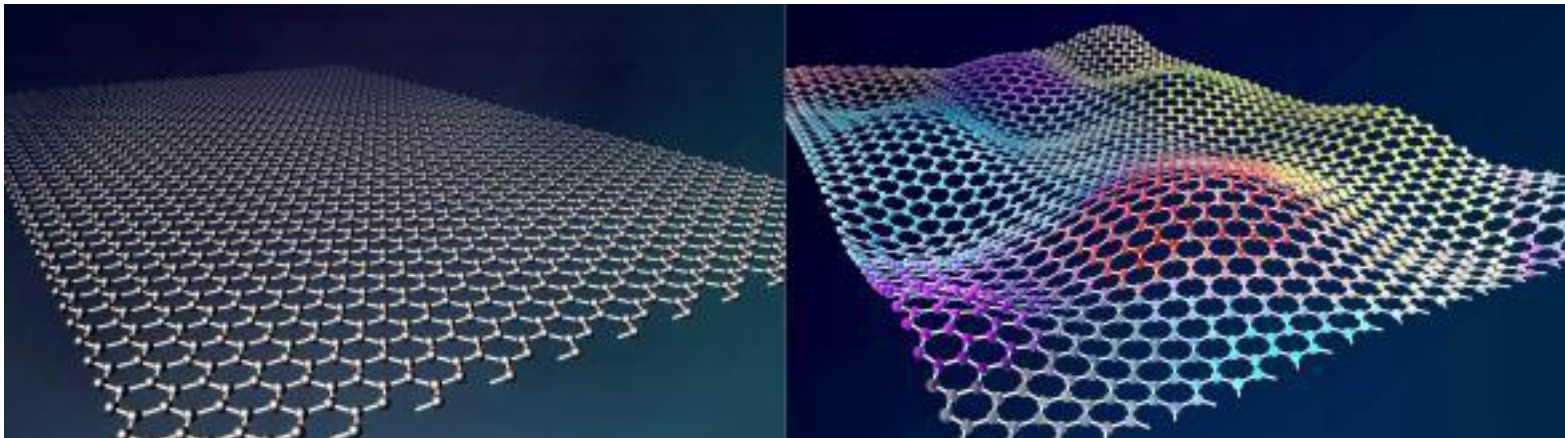


***Pencil used in England since 1560  
(Angleterre)!***



### Graphene: 2D or not 2D?

It was long believed that strictly two dimensional (2D) arrangements of atoms would be unstable (Mermin-Wigner theorem)



Ideal 2D graphene

Real graphene: ripples heights  
are of atomic size

graphene is 2D material

Wonder nanomaterial which may one-day enable faster and tinier computational and electronic devices.

MacGyver in the physics lab



+



=



Scotch tape

piece of graphite

Nobel prize  
2010

[www.strippedscience.com](http://www.strippedscience.com)

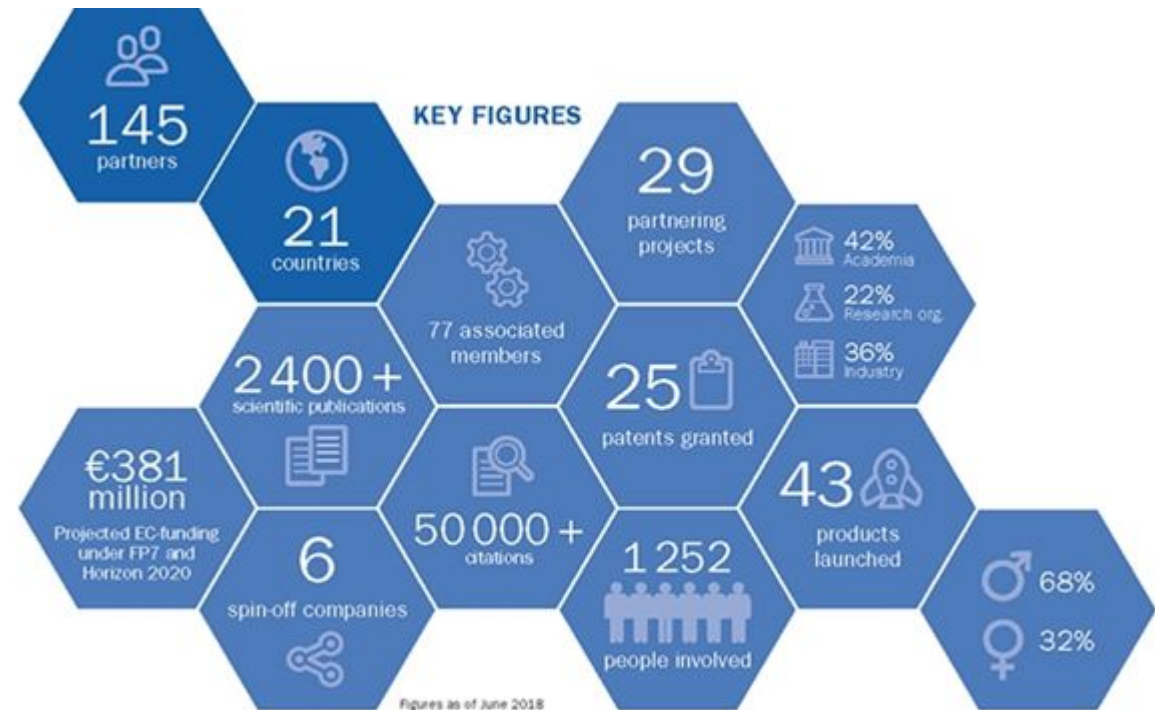
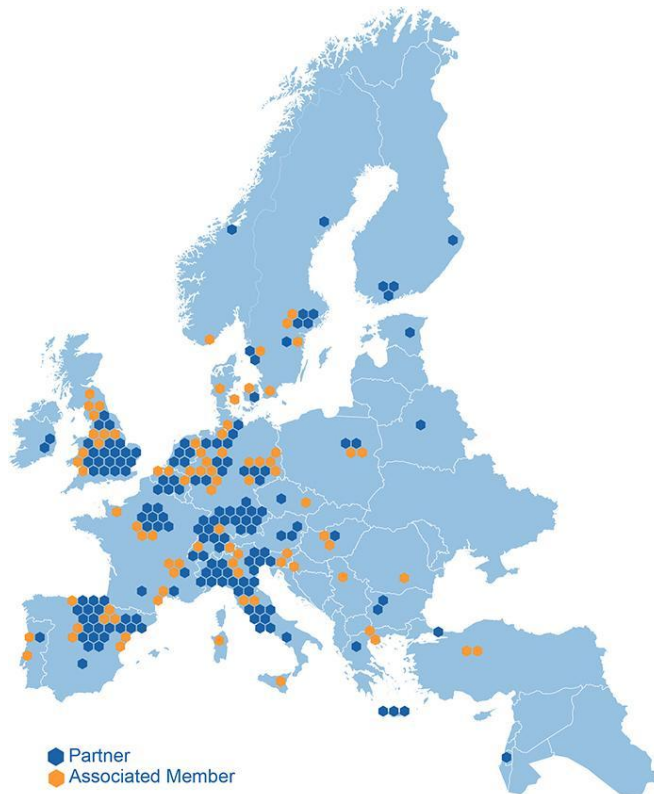
06:59:59

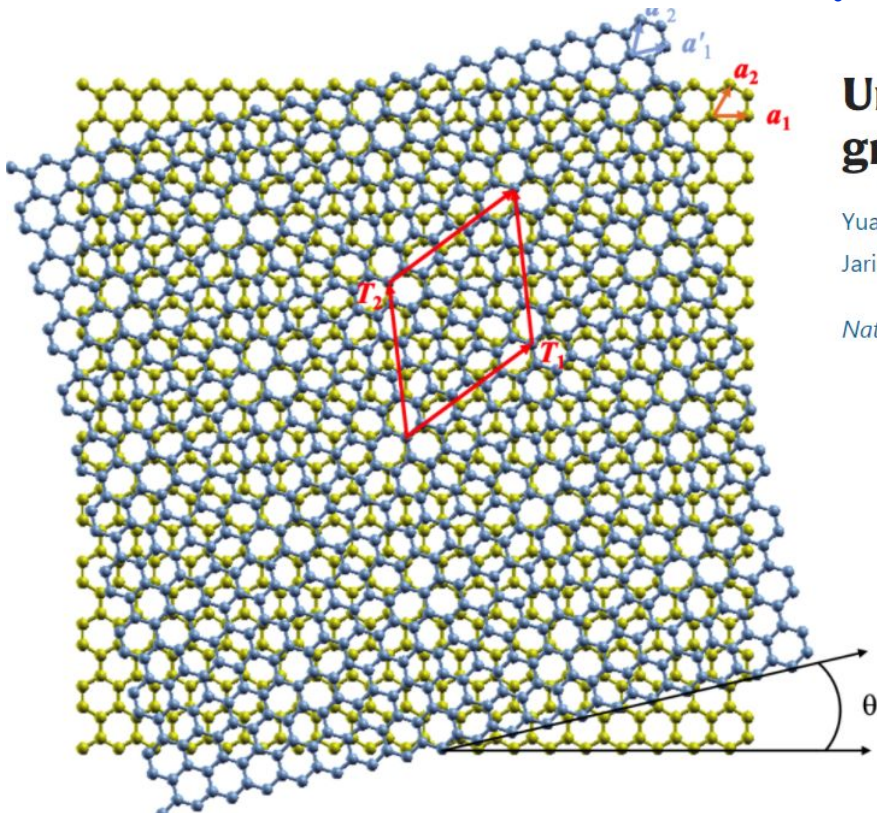






## GRAPHENE FLAGSHIP

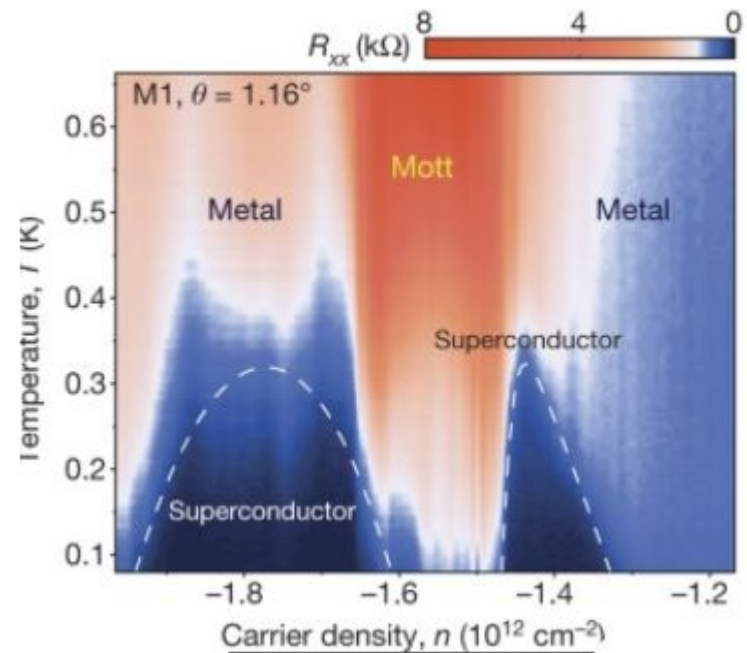
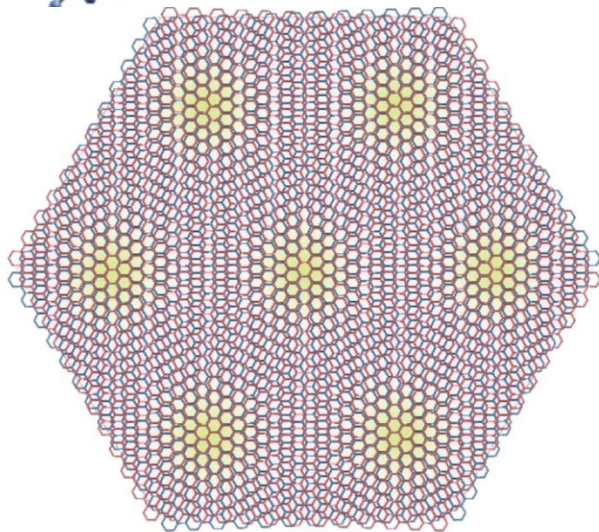
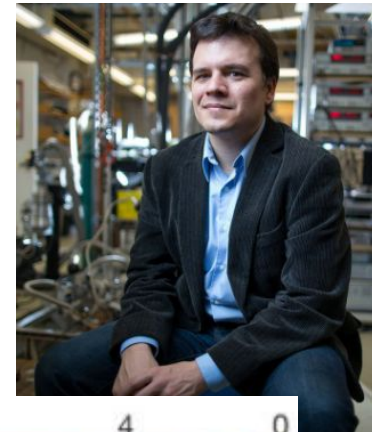




## Unconventional superconductivity in magic-angle graphene superlattices

Yuan Cao , Valla Fatemi, Shiang Fang, Kenji Watanabe, Takashi Taniguchi, Efthimios Kaxiras & Pablo Jarillo-Herrero 

*Nature* **556**, 43–50 (2018) | [Cite this article](#)





# How to model electronic properties in crystals?



Real  
system



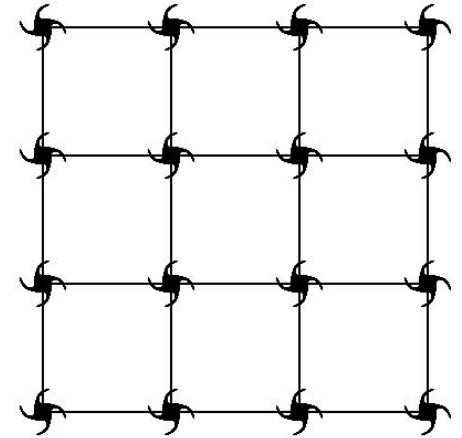
Physics  
Model



## Overview of basic concepts

### Crystal:

- regular arrangement of a **unit structure** (atoms, molecules...) in the space.
- Can be described by a lattice



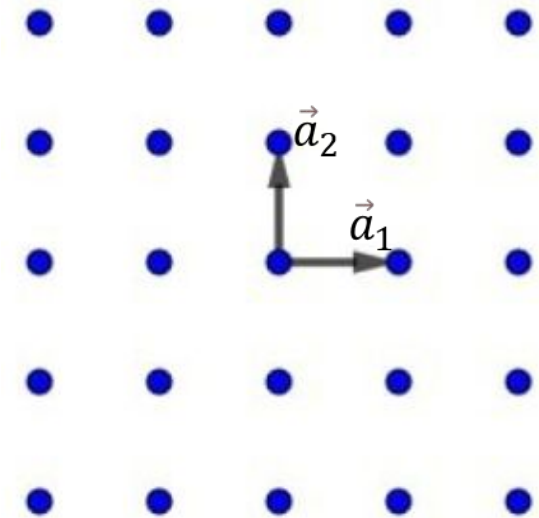
### Lattice:

- Set of points arranged periodically, in the space, in the same way as the unit structure
- Each lattice point correspond to a unit structure
- Lattice is purely geometric

**Crystal = Lattice + unit structure**

**Lattice:** described by an origin + **basis**

Each point of lattice :  $\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3, n_i \in \mathbb{Z}$



## Unit cell:

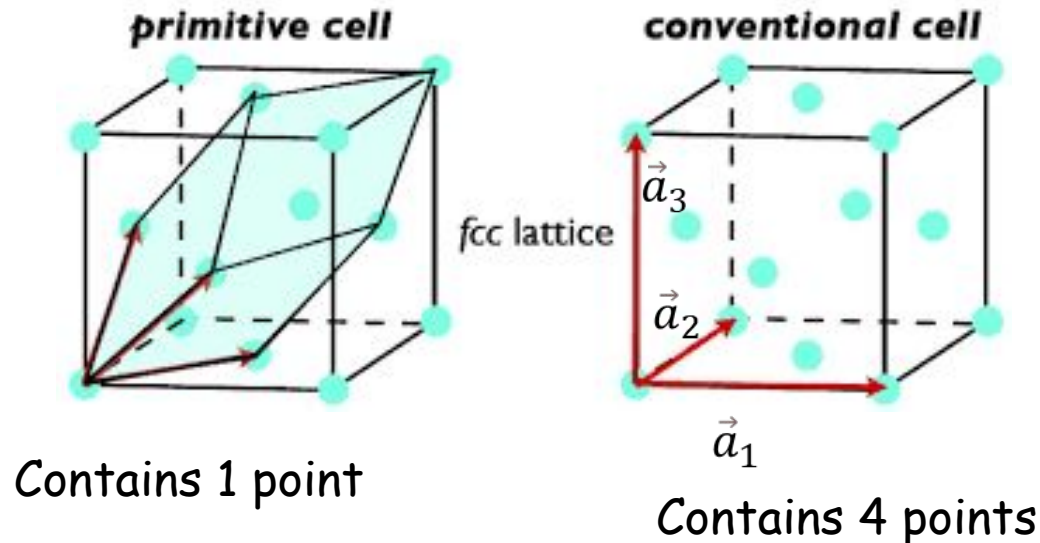
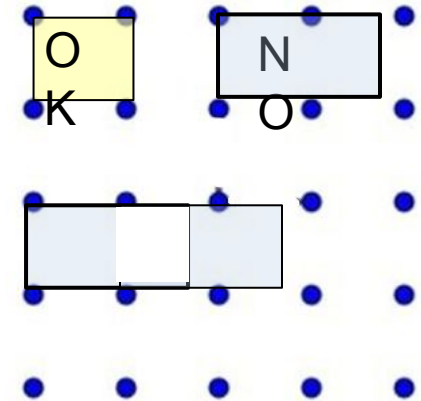
- Volume which, under translations, **fills up all the space without any overlapping**

## Primitive cell:

- unit cell with the **smallest volume**
- Contains **one lattice point**

## Conventional unit cell:

- may contain **more than a lattice point**
- brings out the **symmetry** of the crystal



**2D:** 5 Bravais Lattices

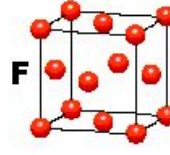
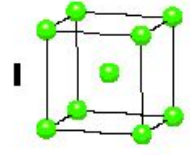
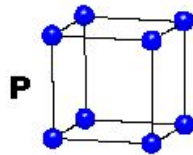
**3D:** 7 crystalline classes

14 Bravais Lattices

## CUBIC

$$a = b = c$$

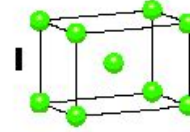
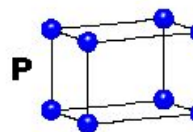
$$\alpha = \beta = \gamma = 90^\circ$$



## TETRAGONAL

$$a = b \neq c$$

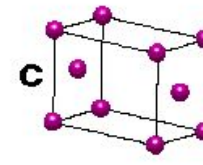
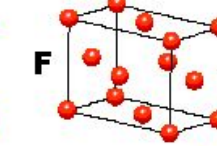
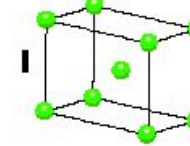
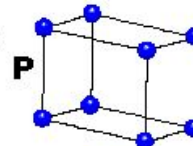
$$\alpha = \beta = \gamma = 90^\circ$$



## ORTHORHOMBIC

$$a \neq b \neq c$$

$$\alpha = \beta = \gamma = 90^\circ$$

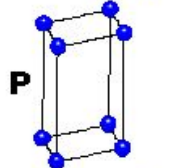


## HEXAGONAL

$$a = b \neq c$$

$$\alpha = \beta = 90^\circ$$

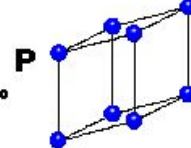
$$\gamma = 120^\circ$$



## TRIGONAL

$$a = b = c$$

$$\alpha = \beta = \gamma \neq 90^\circ$$

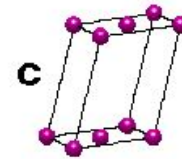
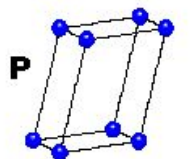


## MONOCLINIC

$$a \neq b \neq c$$

$$\alpha = \gamma = 90^\circ$$

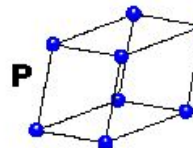
$$\beta \neq 120^\circ$$



## TRICLINIC

$$a \neq b \neq c$$

$$\alpha \neq \beta \neq \gamma \neq 90^\circ$$



(a) Linear 	(b) Square 	(c) Rectangular 
$ a $	$ a  =  b , \phi = 90^\circ$	$ a  \neq  b , \phi = 90^\circ$
(d) Oblique 	(e) Hexagonal 	(f) Centered Rectangular 
$ a  \neq  b , \phi \neq 90^\circ$	$ a  =  b , \phi = 120^\circ$	$ a  \neq  b , \phi = 90^\circ$

### 4 Types of Unit Cell

P = Primitive

I = Body-Centred

F = Face-Centred

C = Side-Centred

+

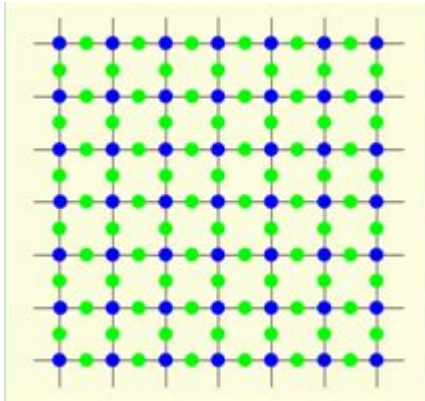
7 Crystal Classes

→ 14 Bravais Lattices



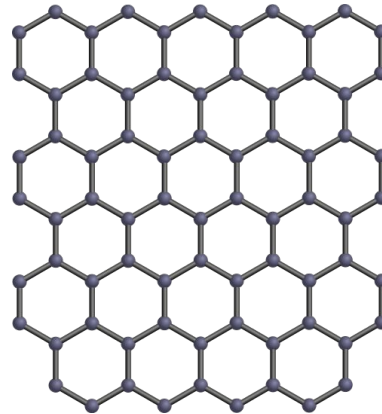
# Assignment 1

1/ Find the Bravais Lattice of the following structure

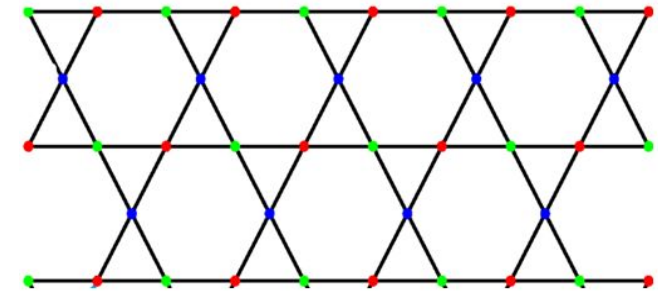


Copper oxide plane of cuprates  
(high temperature  
superconductors)

Blue dot : copper, green: oxygen

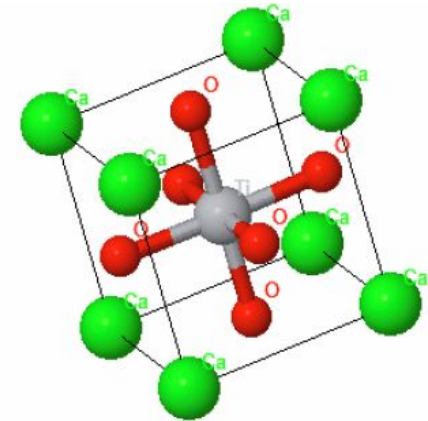


graphene



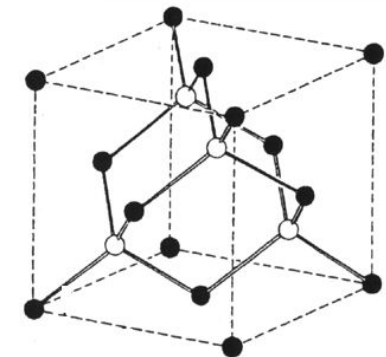
Kagome Lattice

2/ Find the unit structure and the chemical formula of this crystal



3/ The crystal of GaAs has a zinc blende structure. Ga atoms are in the sites (0,0,0) and As atoms As are at sites (1/4,1/4,1/4). The lattice parameter is 5.65 Å

Calculate the density of atoms of Ga et As per cm<sup>3</sup>.



**To observe the crystalline order:** diffraction of photons, neutrons and electrons

X ray diffraction

$$\lambda = \frac{hc}{E}, \quad \lambda(\text{\AA}) = \frac{12.4}{E(\text{eV})}$$

**Quiz 1:** Why X rays ?

Neutron diffraction

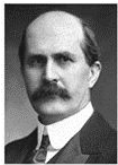
$$\lambda = \frac{h}{\sqrt{2m_n E}}, \quad \lambda(\text{\AA}) = \frac{0.28}{\sqrt{E(\text{eV})}}$$

Electron diffraction

$$\lambda = \frac{h}{\sqrt{2m_e E}}, \quad \lambda(\text{\AA}) = \frac{12}{\sqrt{E(\text{eV})}}$$

**Bragg Law**

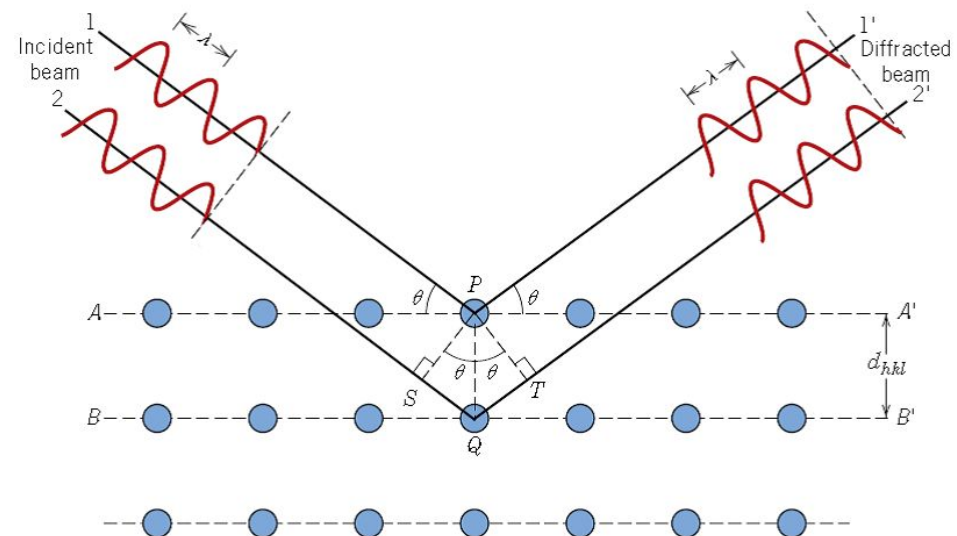
$$n\lambda = 2d \sin \theta \quad (1)$$



**Bragg Law**  $\Leftrightarrow$  von Laue Law

$$e^{i\vec{K} \cdot \vec{R}} = 1 \quad (2)$$

**Quiz 2:** Show the equivalence between (1) and (2)



$$\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3, \quad n_i \in \mathbb{Z}$$

# Reciprocal lattice

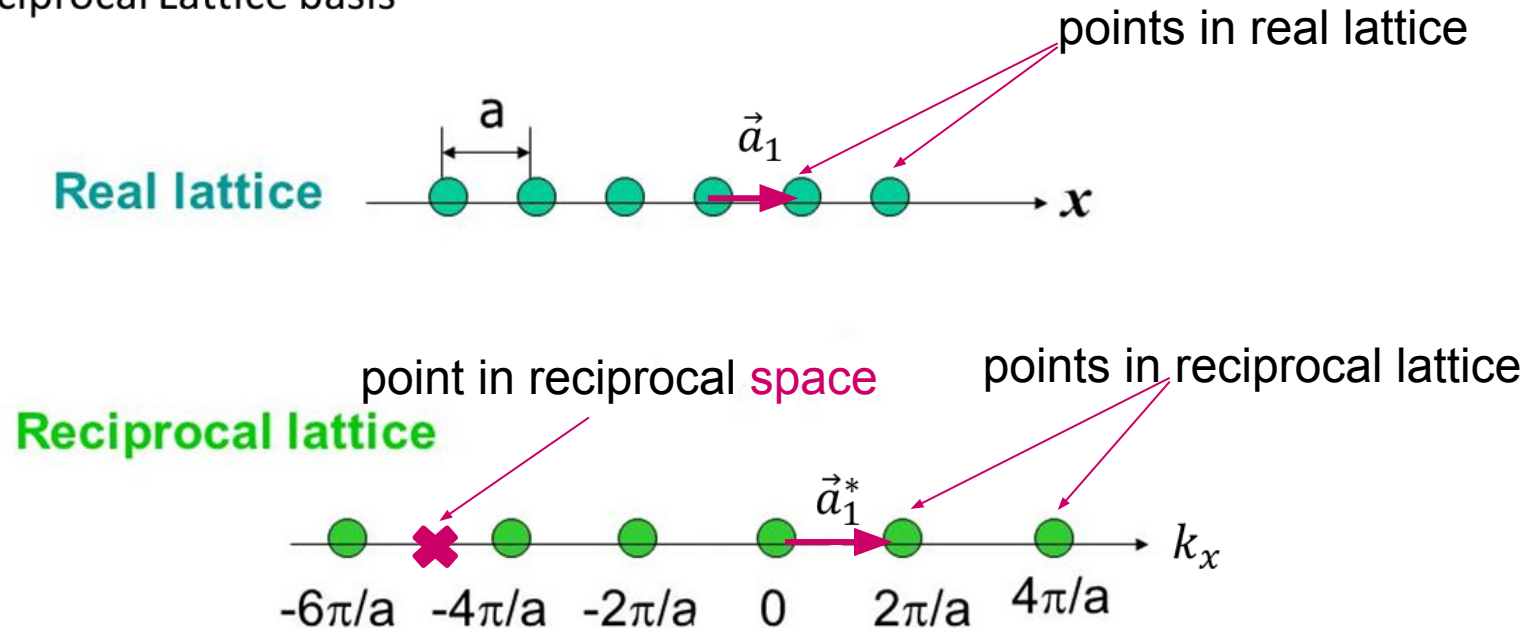
$$e^{i\vec{K} \cdot \vec{R}} = 1$$

$$\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3, n_i \in \mathbb{Z}$$

$$\vec{K} = m_1 \vec{a}_1^* + m_2 \vec{a}_2^* + m_3 \vec{a}_3^*, m_i \in \mathbb{Z} \quad \text{point in the reciprocal Lattice}$$

$$\vec{a}_i^* \cdot \vec{a}_j = 2\pi \delta_{ij}$$

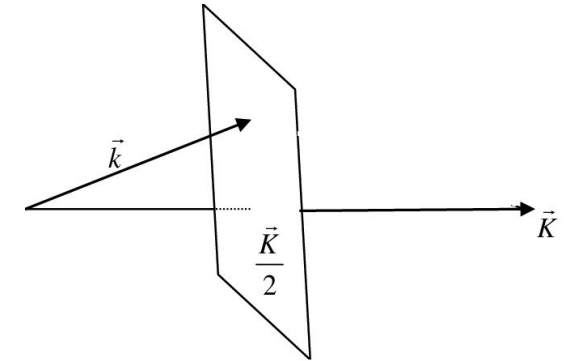
$(\vec{a}_1^*, \vec{a}_2^*, \vec{a}_3^*)$  Reciprocal Lattice basis



**Quiz 3:** Write  $\vec{K}$  (reciprocal lattice) and  $\vec{k}$  (reciprocal space)

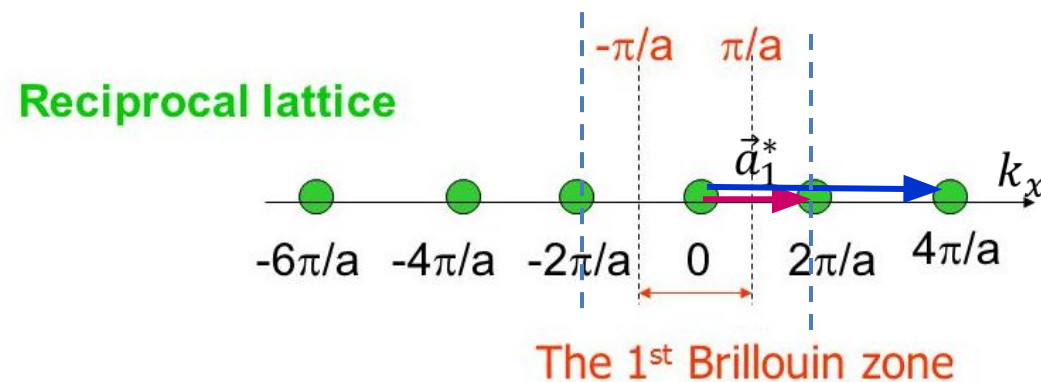


**Bragg plane:** bisecting plane of  $\vec{K}$ :  $|\vec{k} \cdot \vec{K}| = \frac{K^2}{2}$



**1<sup>st</sup> Brillouin zone:** set of reciprocal space points which can be reached from the origin without crossing any Bragg plane (0 plane)

**n<sup>th</sup> Brillouin zone:** set of reciprocal space points which can be reached from the origin by crossing (n-1) Bragg planes



$$1D: 1st\ BZ\ is\ k_x \in \left] -\frac{\pi}{a}, \frac{\pi}{a} \right]$$

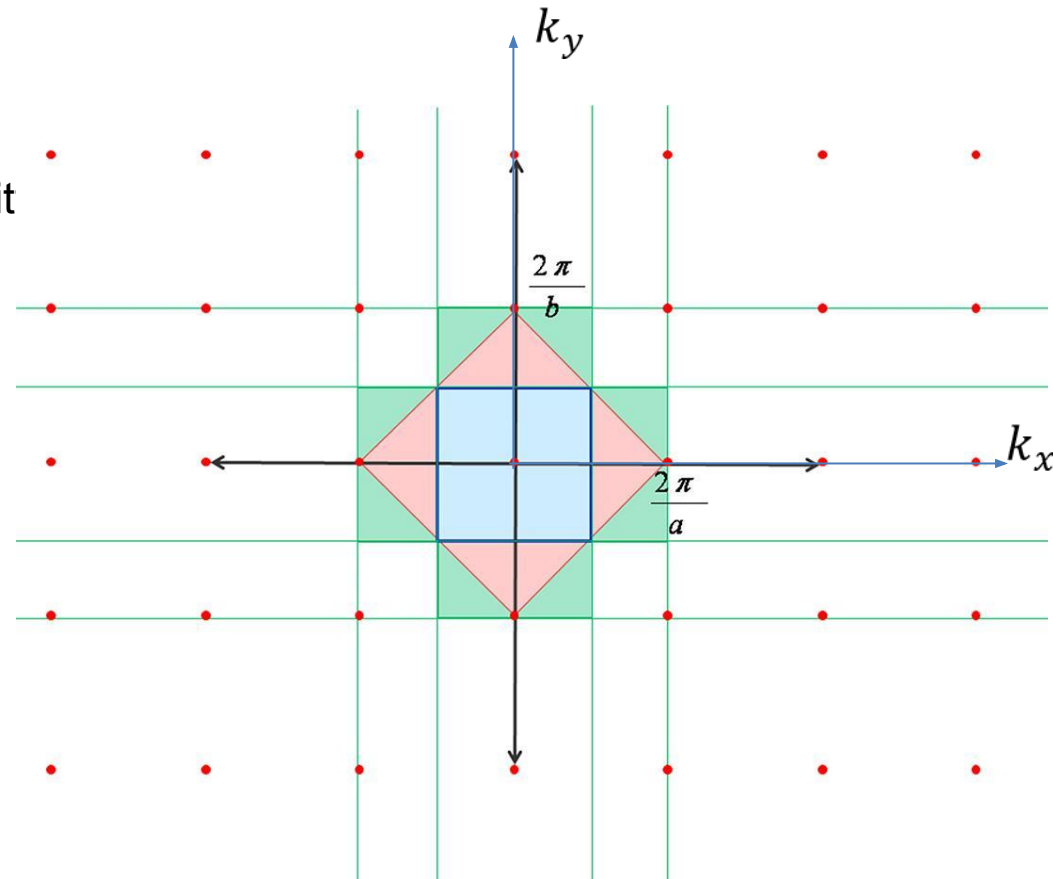
$$2sd\ BZ\ is\ k_x \in \left] -\frac{2\pi}{a}, -\frac{\pi}{a} \right] \cup \left] \frac{\pi}{a}, \frac{2\pi}{a} \right]$$

## BZ of square lattice

- All BZ have the same volume
- Each vector from nth zone can be writ

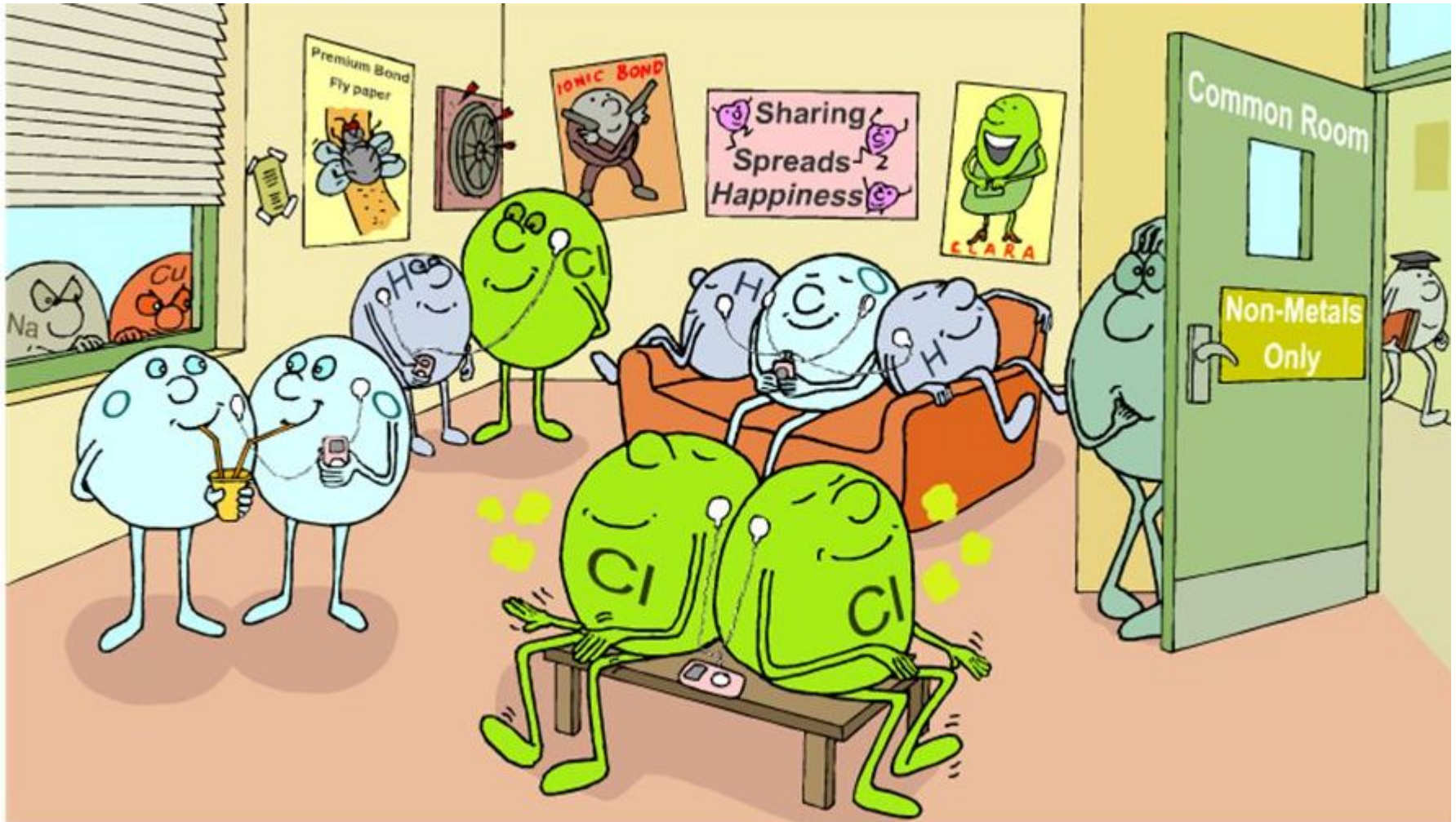
$$\vec{k}_n = \vec{k} + \vec{K}, \vec{K} \in RL, \vec{k} \in 1st\ BZ$$

$\vec{k}$  and  $\vec{k}_n$  are equivalent



**Assignment 2:** Draw the 1st and 2nd BZ of triangular lattice

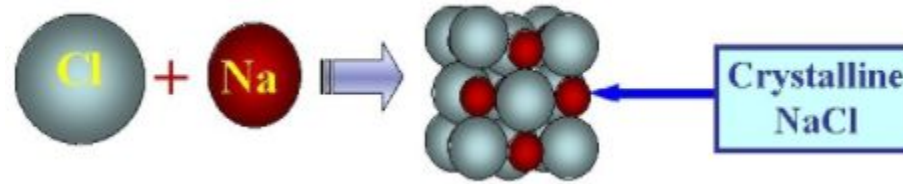
## What makes atoms bond to form crystals?





## Bonding energy

## Ionic crystals

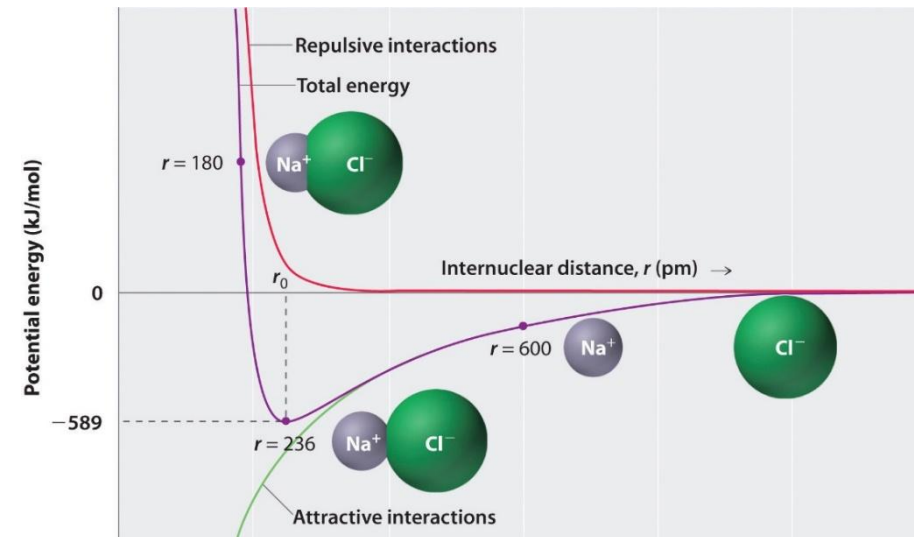


## Electrostatic interaction

Total bonding energy of ionic crystal with  $2N$  ions

repulsive attractive

$$U_{total} = NU_i = N \left( z\lambda e^{-\frac{R}{\rho}} - \frac{\alpha q^2}{R} \right)$$



$q$ : ion charge

$R$ : distance between 1st nearest neighbor atoms

$z$ : nb of 1st nearest neighbor ions

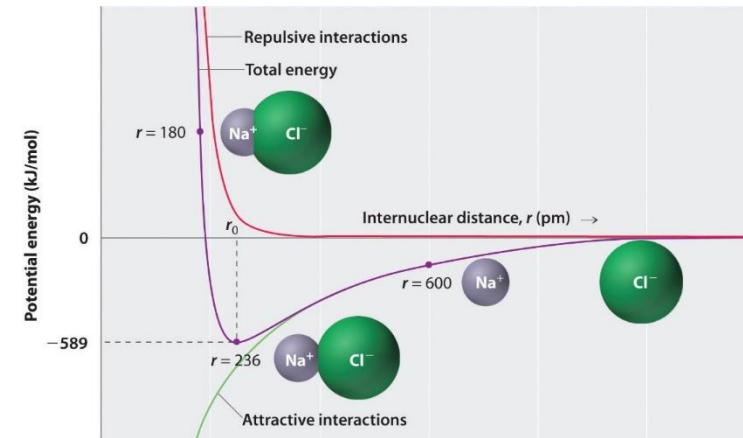
$\alpha$ : Madelung constant, depends on the crystal structure

$\lambda$  and  $\rho$ : empirical parameters

# Bonding energy

## Ionic crystals

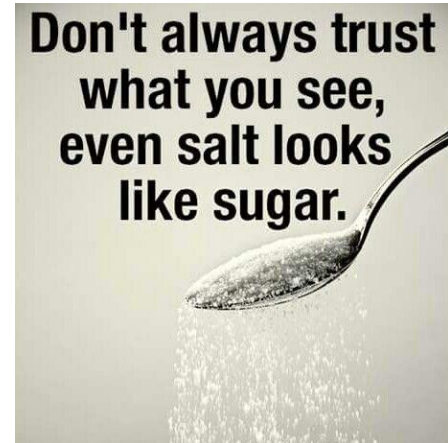
$$U_{total} = NU_i = N \left( z\lambda e^{-\frac{R}{\rho}} - \frac{\alpha q^2}{R} \right)$$



**Cohesive energy** = crystal energy- energy of free atoms

$$\frac{dU}{dR_{R_0}} = 0 \quad \Rightarrow \quad U_{tot}(R_0)$$

The atomic cohesive energy of NaCl per ion pair  $\approx -6$  eV



**Quiz 4:** how could you distinguish between salt and sugar without tasting?

## Bonding energy

## Molecular crystals

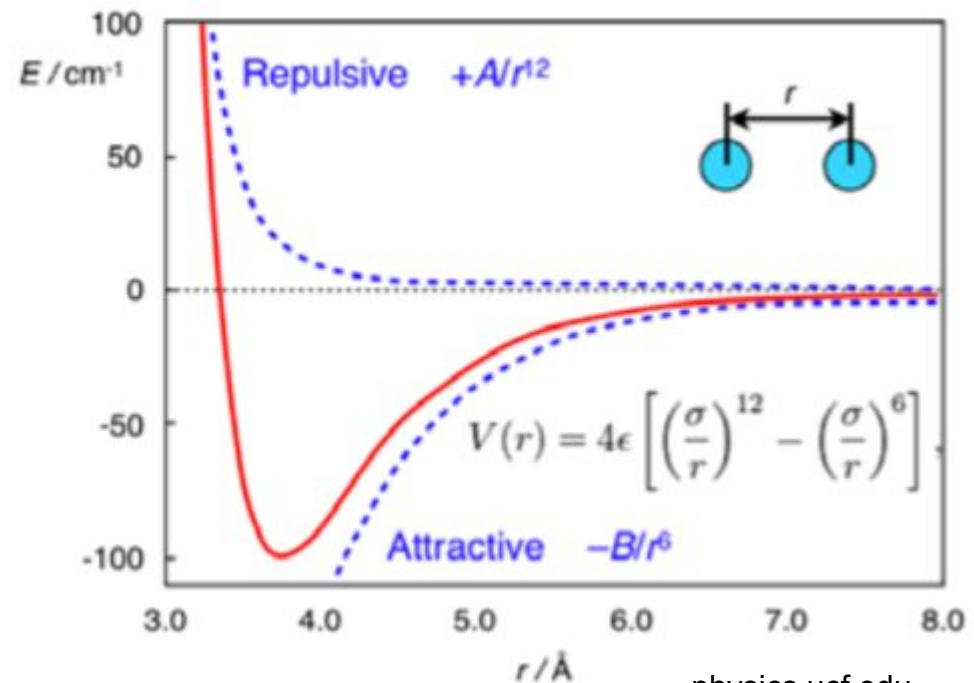
noble gas crystals (Ne, Ar, Kr, Xe)

Attractive interaction due to **van der Waals** forces (force between electric dipoles)

Total bonding energy per atom

$$U(R) = 4\epsilon \left[ \left( \frac{\sigma}{R} \right)^{12} - \left( \frac{\sigma}{R} \right)^6 \right]$$

$R$  : distance between 1st nearest neighbors  
 $\sigma$ : depends on the crystal structure  
 $\epsilon$ : empirical parameter

Cohesive energy **meV**

physics.ucf.edu



### Bonding energy

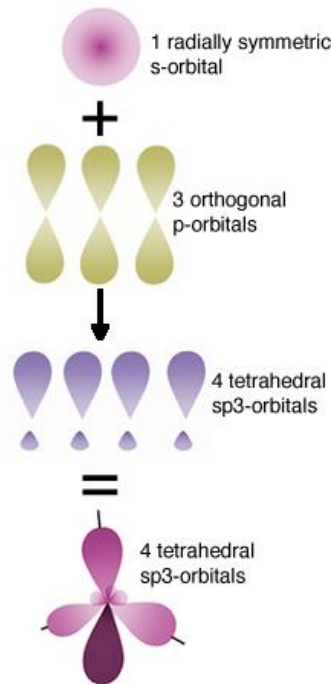
### Covalent crystals

Attractive interaction due to covalent bonding

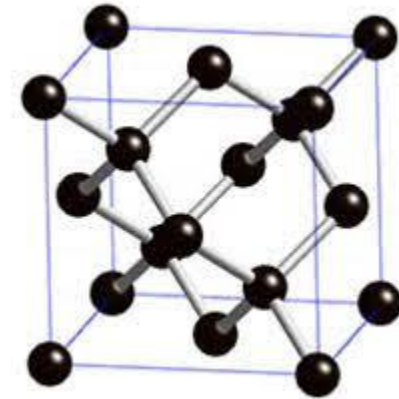
- Need **Quantum Mechanics**
- **Hybridization and overlap** of the electron wave function between atoms
- **Exchange energy** (spin dependent interaction)

Carbon C: [He]  $2s^2 2p^2$

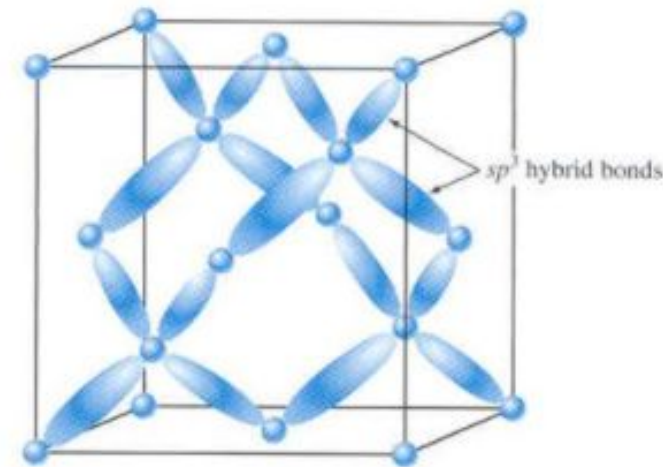
hybridation  $sp^3$



Natural Diamond



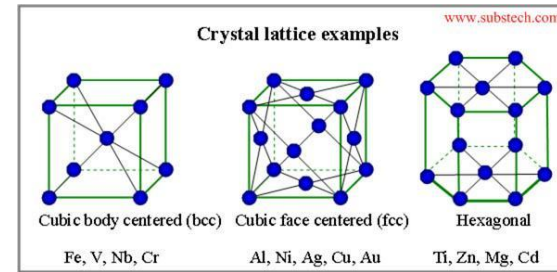
Zinc Blende crystal structure



Cohesive energy/atom **eV**

# Bonding energy

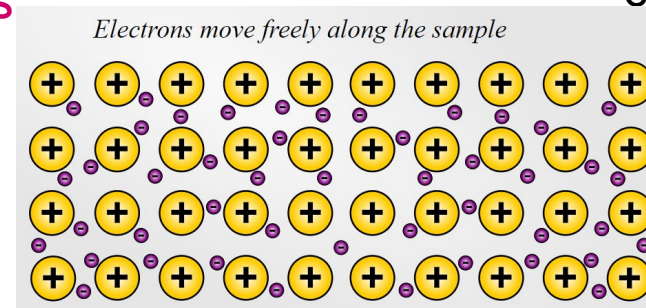
## Metallic crystals



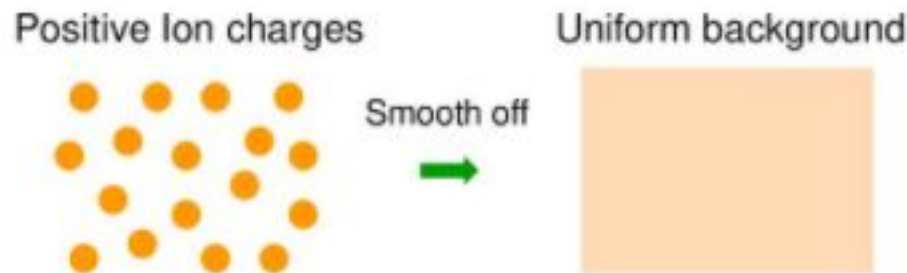
Copper crystal

Attractive interaction due to metallic bonding

- Need **Many-body Quantum Mechanics**



**Jellium model:** positive charges are assumed to be uniformly distributed in space and the electron density is a uniform quantity in space.



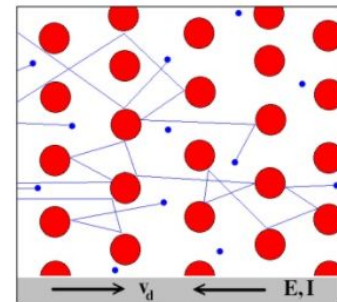
Cohesive energy/atom 0.5 eV

## Drude Model (1900):

- 1st microscopic model to interpret the electronic conductivity of metals
- Conducting electrons described by classical gas (Maxwell-Boltzmann statistics)
- Electrons undergo collisions with positive ions
- Explain the increase of resistivity with temperature 😊
- BUT discrepancies for heat capacity ☹️



Paul Karl Ludwig Drude (1863–1906)



Arnold Johannes Sommerfeld

## Sommerfeld Model (1928):

- Conducting electrons described by quantum gas (Fermi-Dirac statistics)
- Explain the contribution of electrons to the heat capacity of metals 😊
- BUT did not explain why there are insulating, semi-conducting crystals? ☹️

What did they miss?



There are symmetries in the crystal!  
Translations



What are the consequences of the translational symmetry on the electronic properties?

## Electron in crystals: classical or quantum?

Characteristic temperature in metals  $T_F \approx 10^4 \text{K} \gg T_{\text{ambient}}$   $\Rightarrow$  Quantum Mechanics

Crystal Hamiltonian:

$$H_{\text{crys}} = T_{\text{ions}} + T_e + V_{e-\text{ions}} + V_{e-e} + V_{\text{ions-ions}} \quad \text{Many-body problem! } \text{☹️}$$

Approximations

- Born-Oppenheimer: ions fixe compared to electrons  
 $\langle T_{\text{ions}} \rangle \ll \langle T_e \rangle$ ,  $\langle V_{\text{ions-ions}} \rangle \approx \text{constant}$
- Independent electrons

$$H_{\text{crys}} = \sum_i H(\vec{r}_i), \quad H(\vec{r}) = \frac{p_i^2}{2m} + V(\vec{r}), \quad \text{one-body problem } \text{😊}$$

$V(\vec{r}) = V(\vec{r} + \vec{R})$  periodic potential

$$H(\vec{r}) = \frac{p_i^2}{2m} + V(\vec{r}) \text{ with } V(\vec{r}) = V(\vec{r} + \vec{R}) \quad \Rightarrow \quad H(\vec{r}) \text{ commute with } T_{\vec{R}} \text{ (translational operator)}$$

$T_{\vec{R}}$  is unitary  $\Rightarrow$  Eigenfunctions of the form  $e^{i\vec{k} \cdot \vec{R}}$ ,  $\vec{k}$  wave vector **Quiz 5: Prove it.**

$[T_{\vec{R}}, H(\vec{r})] = 0 \Rightarrow$  Eigenfunctions of  $H(\vec{r})$  the form  $\psi_{\vec{k}}(\vec{\rho}, \vec{R}) = f(\vec{\rho})e^{i\vec{k} \cdot \vec{R}}$

$\vec{\rho}$ : position of the electron in the unit cell

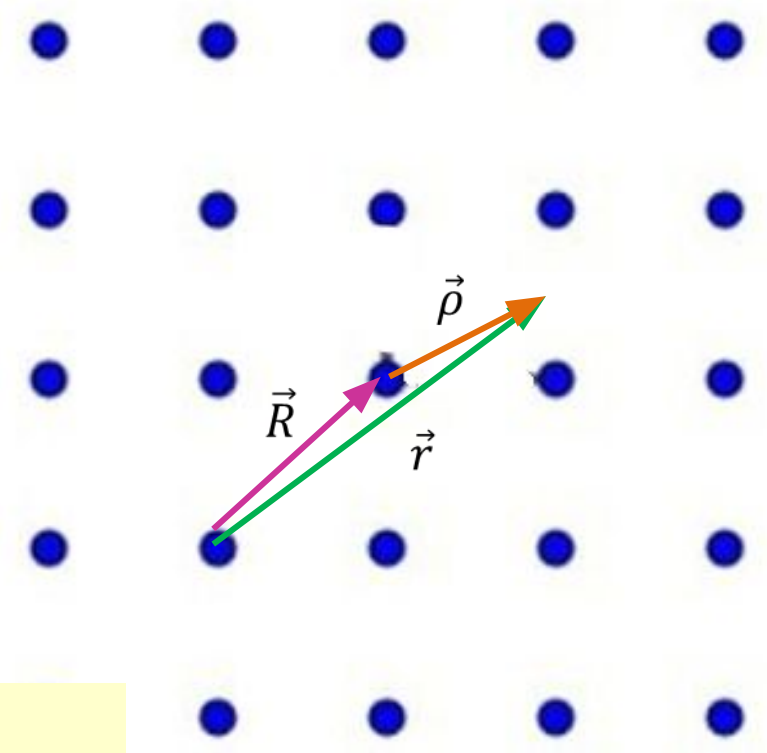
$f(\vec{\rho})$  defined in the unit cell

$\vec{r}$ : position of the electron in the crystal

$$\vec{r} = \vec{\rho} + \vec{R}$$

$$\psi_{\vec{k}}(\vec{r}) = u_{\vec{k}}(\vec{r})e^{i\vec{k} \cdot \vec{r}}$$

$$u_{\vec{k}}(\vec{r} + \vec{R}) = u_{\vec{k}}(\vec{r}) \text{ cellular function}$$



Felix  
Bloch

## Bloch Theorem

**Quiz 6: Prove the Bloch theorem.**



**Thank you for your attention**

**Any questions?**