

# Emergence of Quantum Phases in Novel Materials

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# More is different

“The ability to reduce everything to simple fundamental laws does not imply the ability to start from those laws and reconstruct the universe.”

“The behavior of large and complex aggregates of elementary particles, it turns out, is not to be understood in terms of a simple extrapolation of the properties of a few particles. Instead, at each level of complexity entirely new properties appear.”

1972, Anderson



**Emergence**

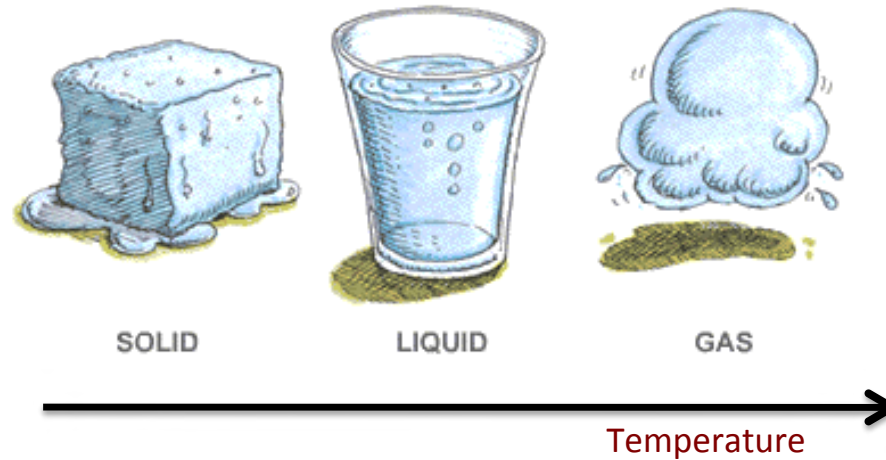
# Emergence

The arising of novel and coherent structures, patterns and properties during the process of self-organization in complex systems

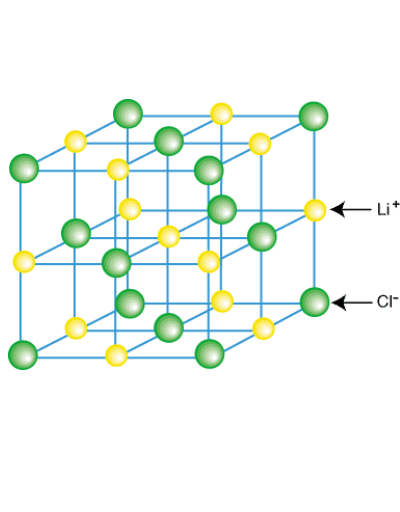
Goldstein, Economist (1999)



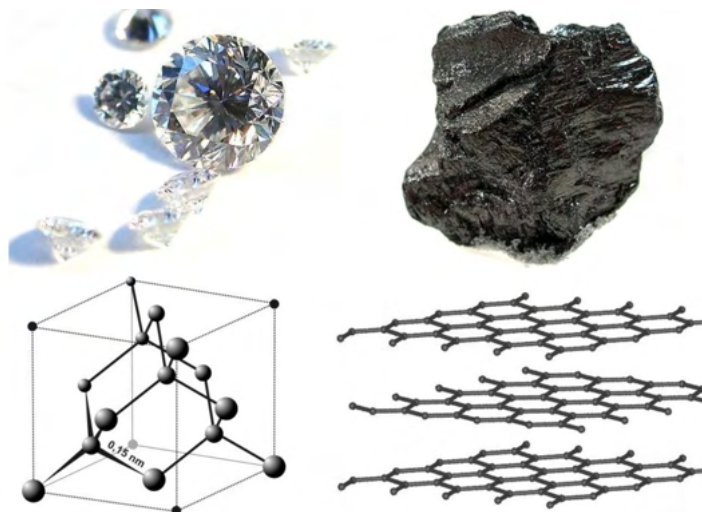
# Emergence in condensed matter physics



Solids: broken translational symmetry



©askitians



©Itub

Nematic liquid crystal:  
Broken rotational symmetry



©kebes

# Emergence in condensed matter

Electrons interact with each other and with the environment



Collective many-body behavior  
(strongly correlated materials & mesoscopic systems)



To understand the complex behavior  
Isolate the fundamental processes



More than 35 years of intensive research effort and  
continuously new surprises appear

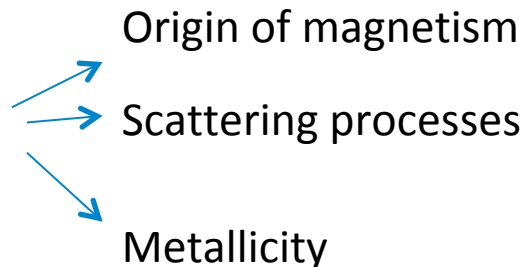
# Emergence in condensed matter

## Pauli exclusion principle

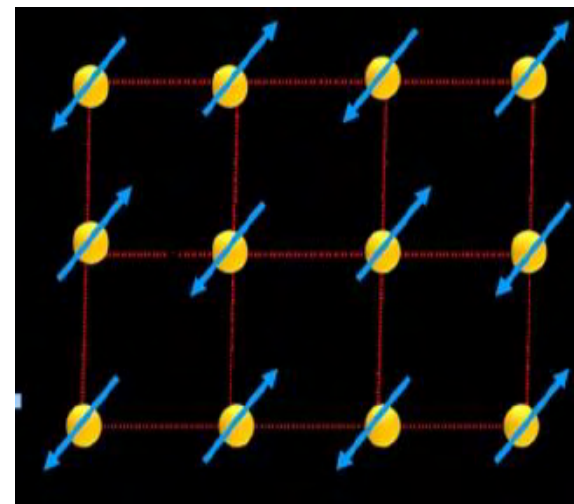
**Quantum states:** Magnetism: Ferromagnetism, Antiferromagnetism  
Charge density waves, Superconductivity, Nematicity, and other

## Electrons:

itinerant or localized



**Lattice:** Symmetries, Frustrated, Bipartite ...

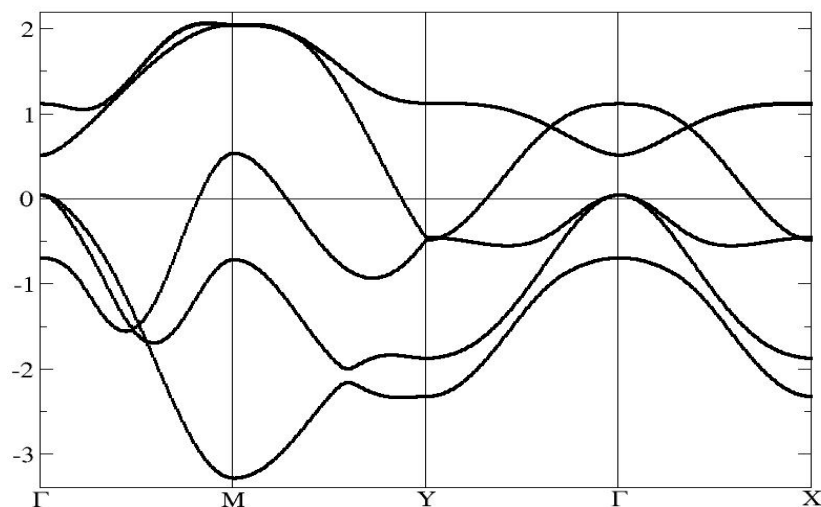


**Dimension:** Influence in ordered states but also in “normal state”

**Topology:** A new way to classify condensed matter systems with novel effects

And many other issues: interplay with disorder ...

# Band theory & DFT: Our basic description of solids



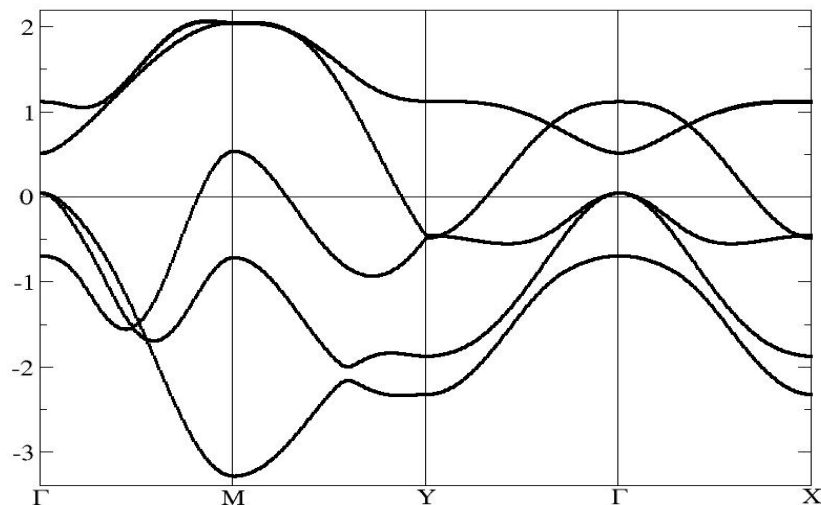
Bloch states: electronic bands

The electron moves in the average periodic potential of the solid

**Band theory:** Basis of our understanding of solids

- Metals and insulators
- Dependence on temperature of measurable quantities ( $C_v$ ,  $\chi$ , ..)
- Density Functional Theory: Ability to calculate the bands

# Emergence in condensed matter



Bands generally calculated using DFT

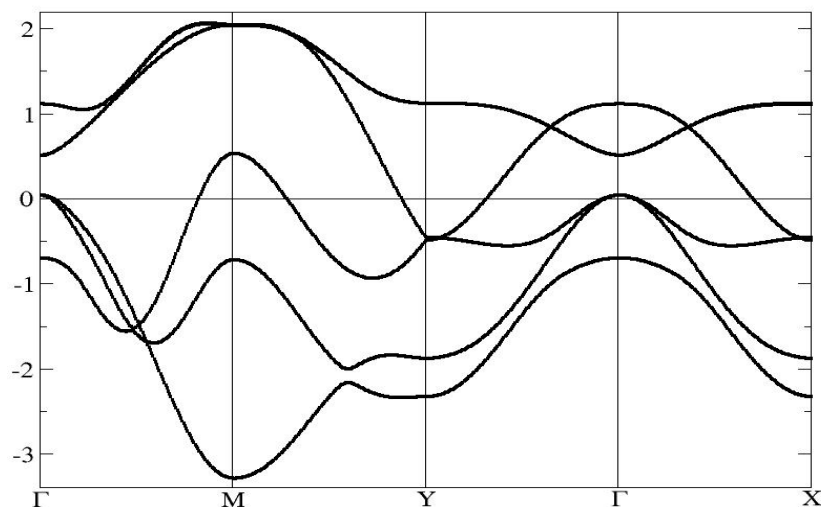
Band theory is basically a description based on single particle states

Interactions are not small and the electrons should react to the presence of other electrons

**Why does band theory work?**



# Emergence in condensed matter



Bands generally calculated using DFT

Band theory is basically a description based on single particle states

↓  
Fermi liquid theory

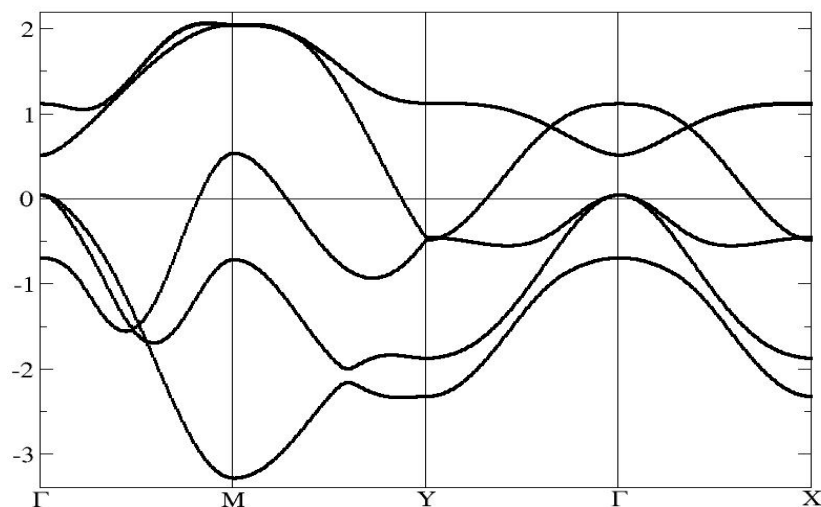
Perturbative versus non-perturbative effect of interactions

↓  
Same behavior but with renormalized parameters

{ Metals and insulators

{ Dependence on temperature of measurable quantities ( $C_v$ ,  $\chi$ , ..)

# Emergence in condensed matter



Bands generally calculated using DFT

Band theory is basically a description  
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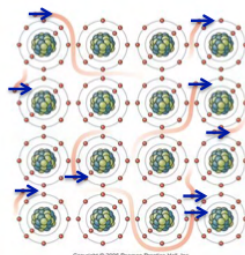
Perturbative versus non-perturbative effect of interactions

↙  
Phase transitions &  
symmetry breaking

# Examples of electronic ordered phases

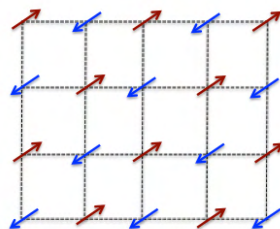
## Spin order

The symmetry of the atomic lattice is preserved



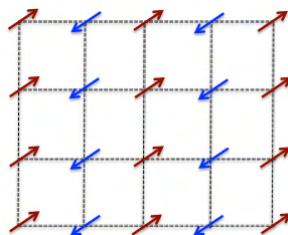
## Neel antiferromagnet

Lattice translational symmetry broken



## Stripe antiferromagnet

Lattice translational and rotational symmetry broken

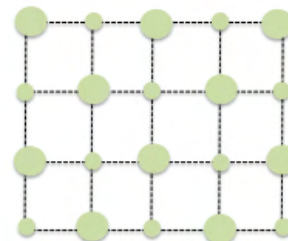


## Spin nematic

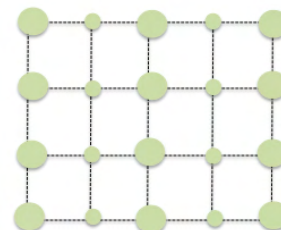
Lattice rotational symmetry broken

## Charge order

## Charge density wave

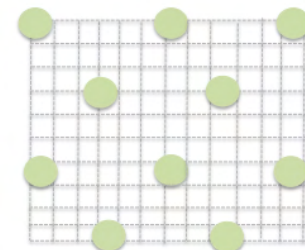


## Charge stripes

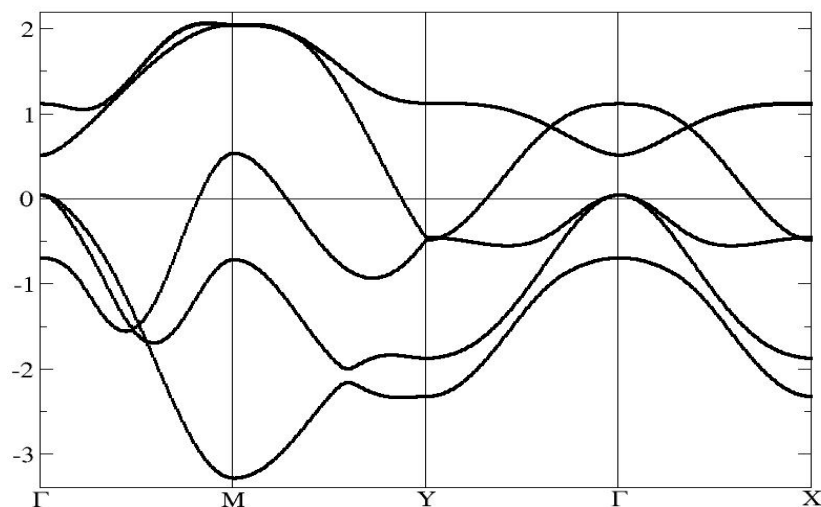


## Charge nematic

## Wigner crystal



# Emergence in condensed matter



Bands generally calculated using DFT

Band theory is basically a description based on single particle states

↓  
Fermi liquid theory

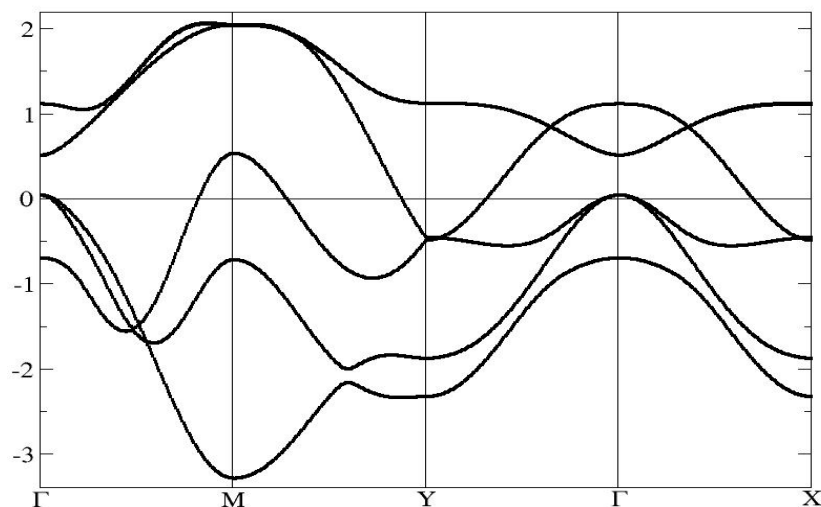
Perturbative versus non-perturbative effect of interactions

Phase transitions & symmetry breaking



- ←
- Fermi surface instabilities (itinerant electrons)
  - Localization (electronic bands are lost)
  - Itinerant + local electrons

# Emergence in condensed matter



Bands generally calculated using DFT

Band theory is basically a description based on single particle states

↓  
Fermi liquid theory

Perturbative versus non-perturbative effect of interactions

**Given a particular system,  
should we expect that band theory works?**

**What kind of instabilities may the system show?**

# Interactions: localization and superconductivity

## **Mott transition:**

a material predicted by band theory to be metallic becomes **an insulator**  
**due to electronic interactions**  
even without symmetry breaking

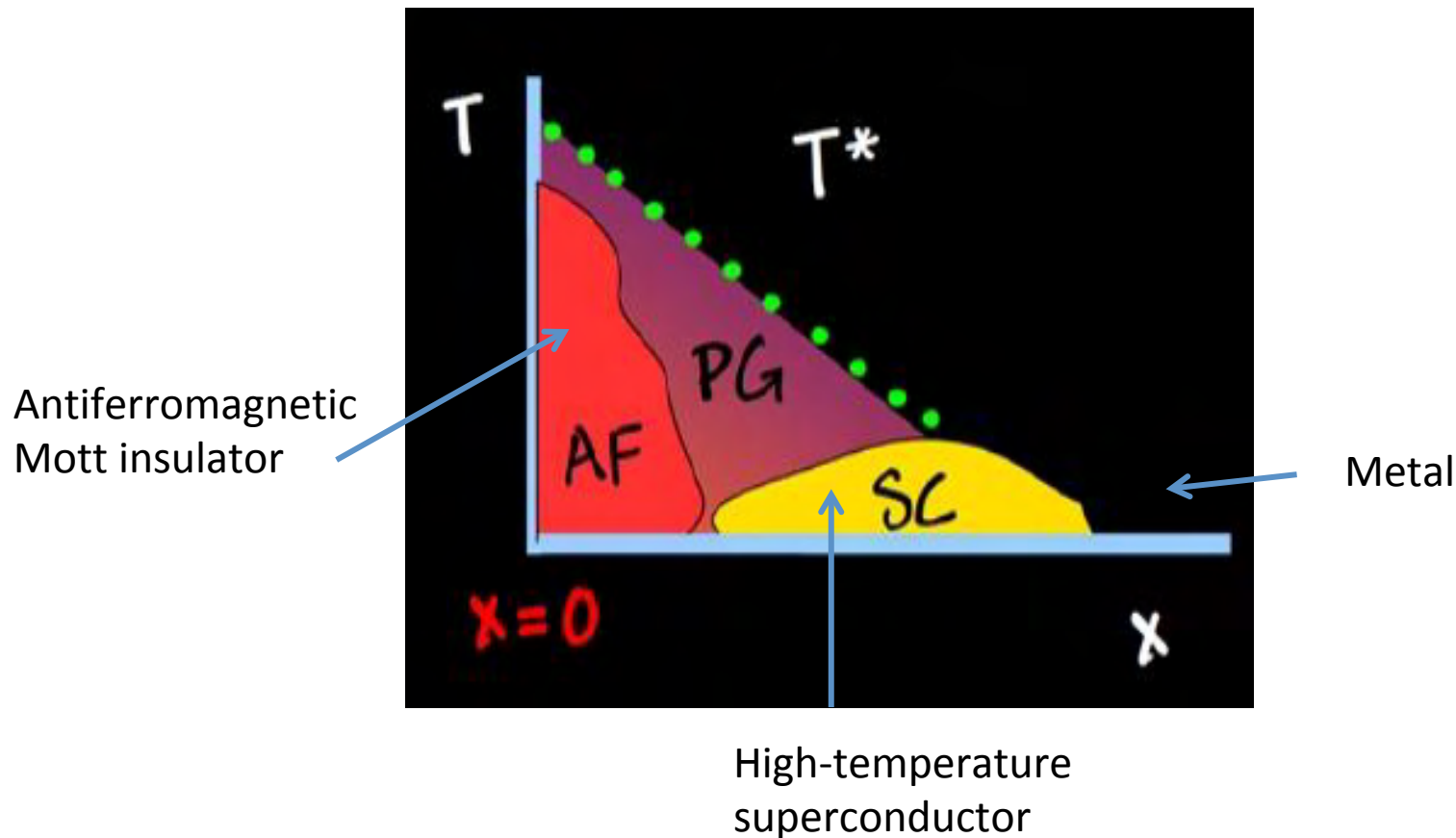
## **Superconductivity:**

Below a critical temperature **resistivity goes to zero**.  
(due to phonons we know, but probably also  
due to magnetic fluctuations or Mott physics)

# Interactions: localization and superconductivity

## Cuprates: high temperature superconductors

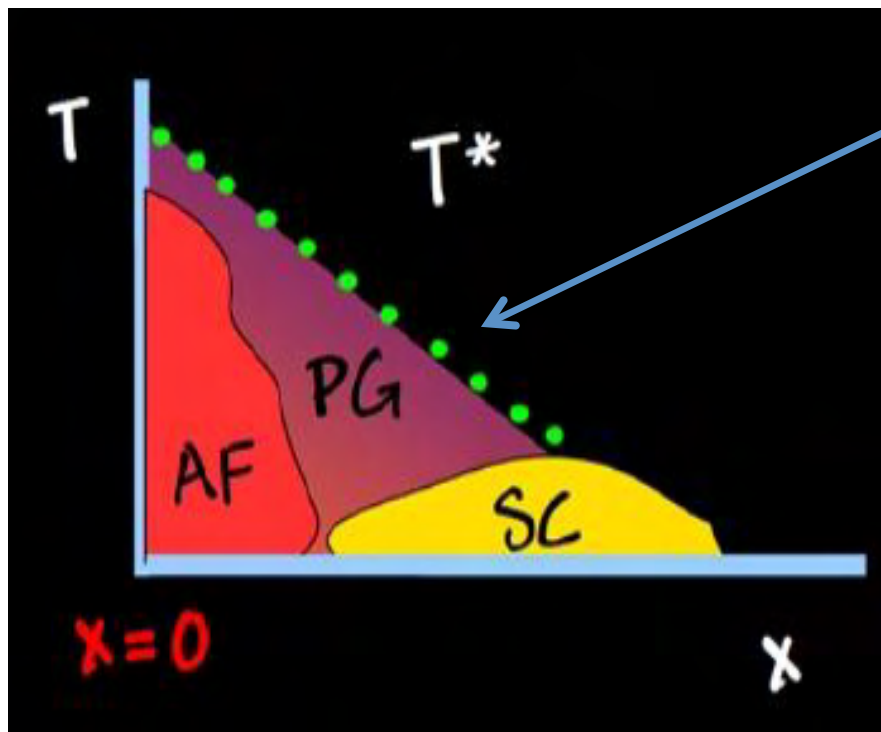
From an antiferromagnetic Mott insulator to a superconductor and then a metal



# Interactions: localization and superconductivity

## Cuprates: high temperature superconductors

From an antiferromagnetic Mott insulator to a superconductor and then a metal



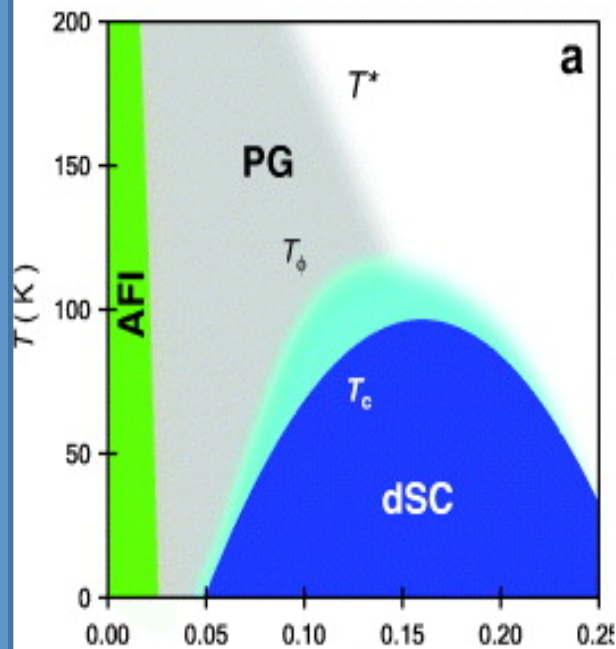
Pseudogap: Is it a new state of matter? A remanent of the Mott insulator or another broken symmetry phase?



# Interactions: localization and superconductivity

## Hole doped cuprates: high temperature superconductors

Huge developments in ideas and in theoretical and experimental techniques



Schmidt et al, NJP 13,  
065014 (2011)

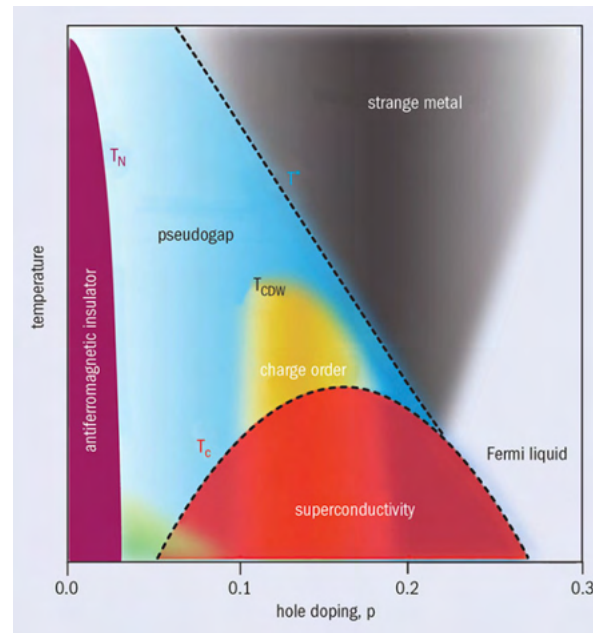
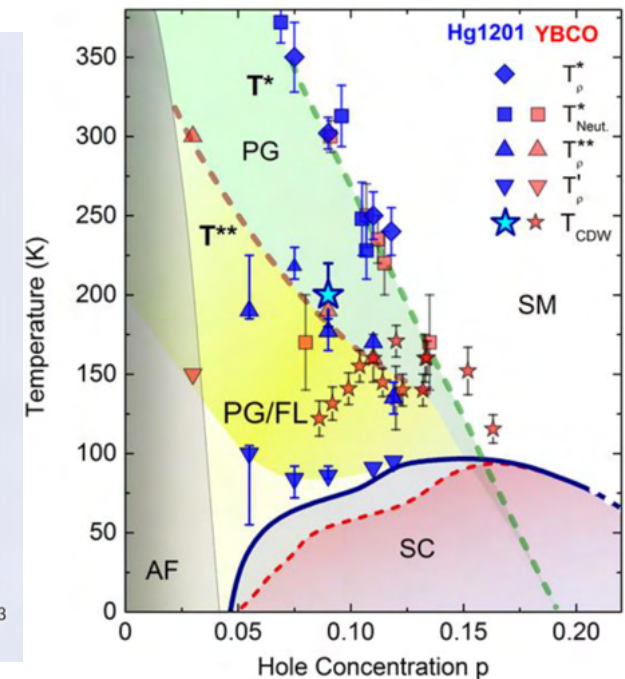
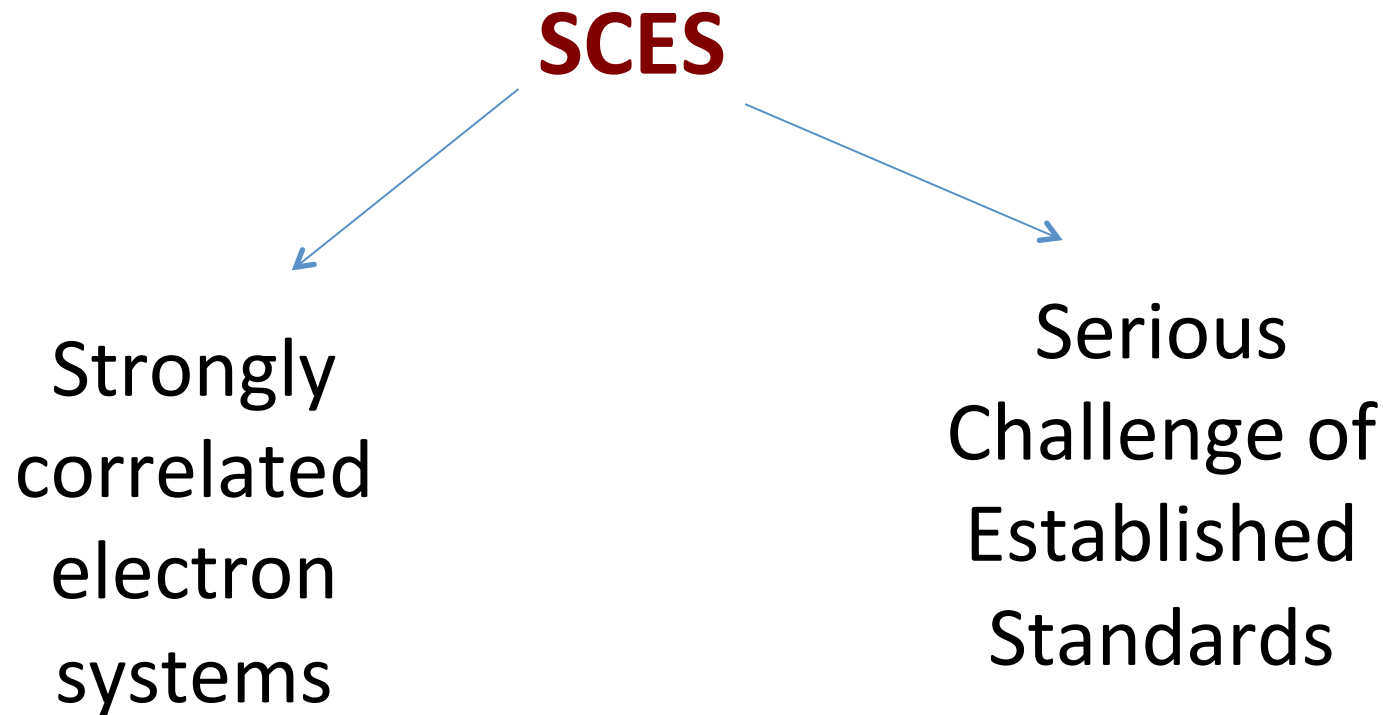


Fig: Inna Vishik



Nature Comms 5,  
5875 (2014)

# Emergence in condensed matter



# Emergence in condensed matter

**SCES**

```
graph TD; SCES --> SCES1[Strongly correlated electron systems]; SCES --> SCES2[Difficulty to unveil the fundamental properties both theoretically & experimentally (away from controlled theoretical limits, competing states, not always possible to do many experiments...)]
```

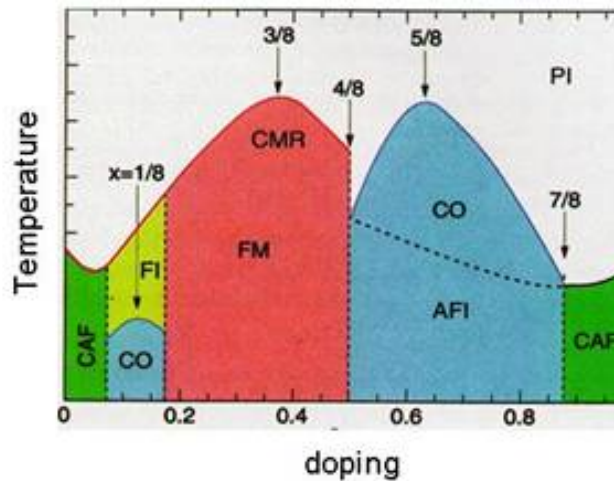
Strongly  
correlated  
electron  
systems

Difficulty to unveil the fundamental properties both theoretically & experimentally (away from controlled theoretical limits, competing states, not always possible to do many experiments...)

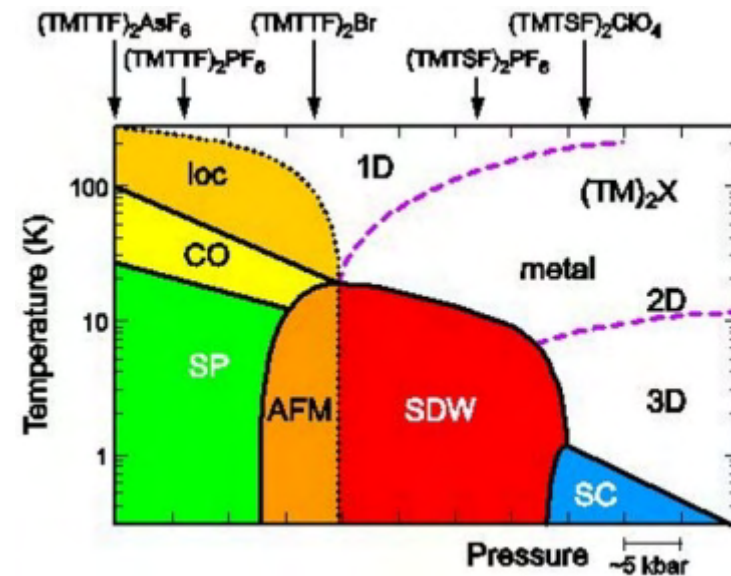
# Emergence in condensed matter from electronic interactions

## Strongly correlated electron systems:

very sensitive to changes(Pressure, Magnetic Field, doping...)



Typical phase diagram of manganites

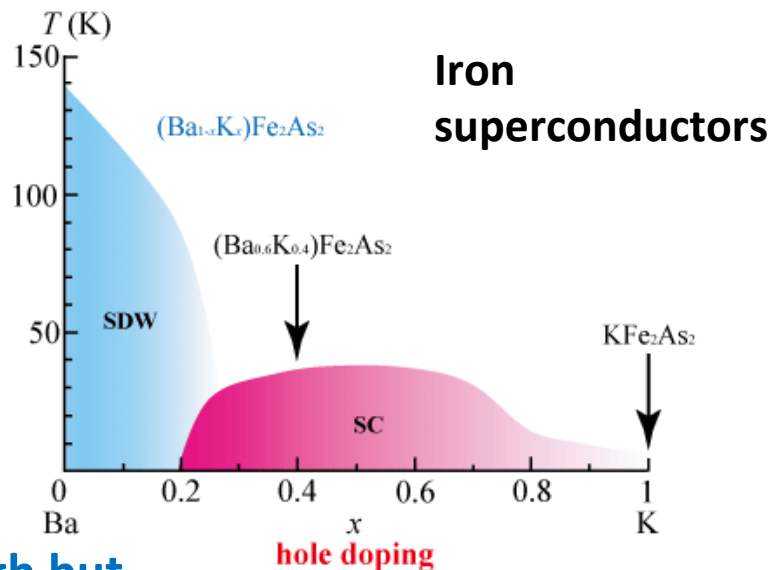
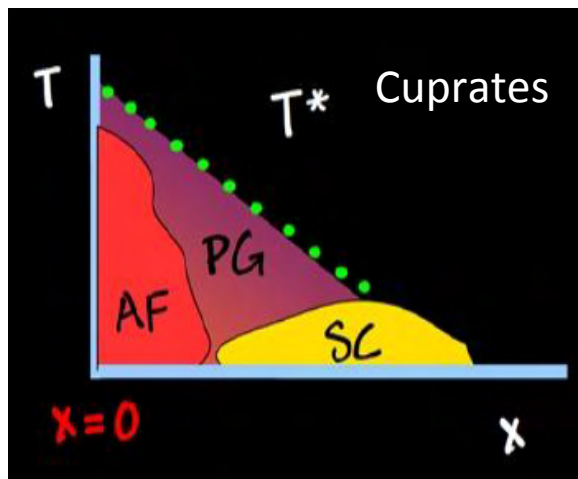


Organic material

Fig: [www.physics.berkeley.edu](http://www.physics.berkeley.edu)

# Magnetism and superconductivity often appear close to each other

## High temperature superconductors



Their critical temperatures do not look high but

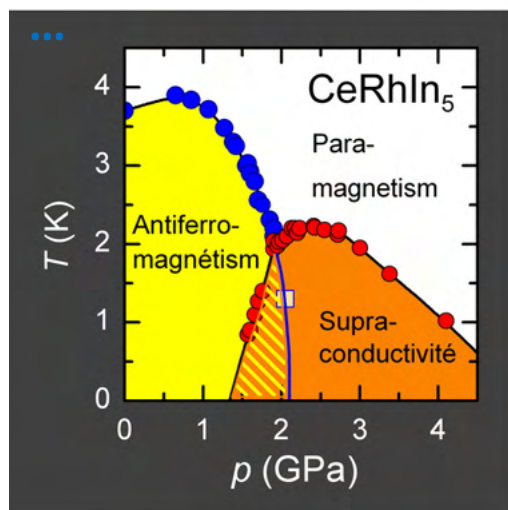
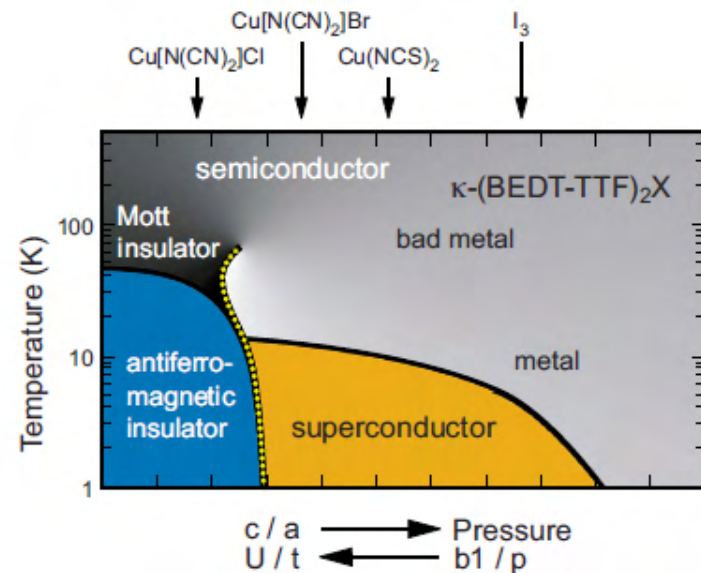


Fig: [www.supraconductivite.fr](http://www.supraconductivite.fr)

**Organic salt**

Fig: Faltelmeier, PRB (2007)



# Do other phases compete or cooperate with superconductivity?

## Description in terms of local or itinerant spins?

Parent compound:  
Insulator

Hole doped cuprates  
(charge order)

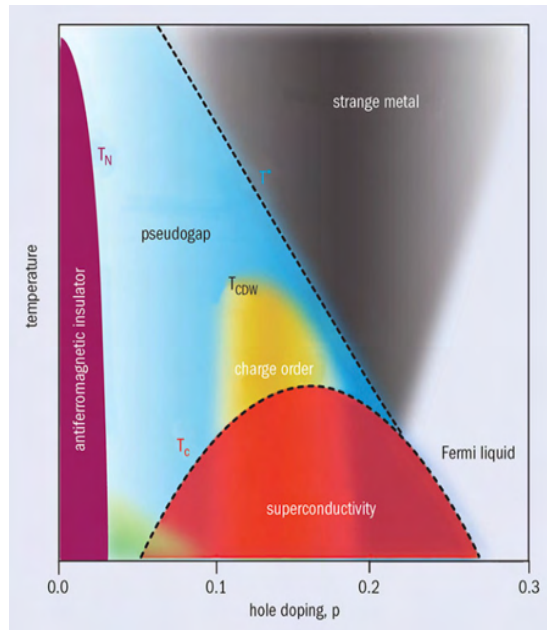
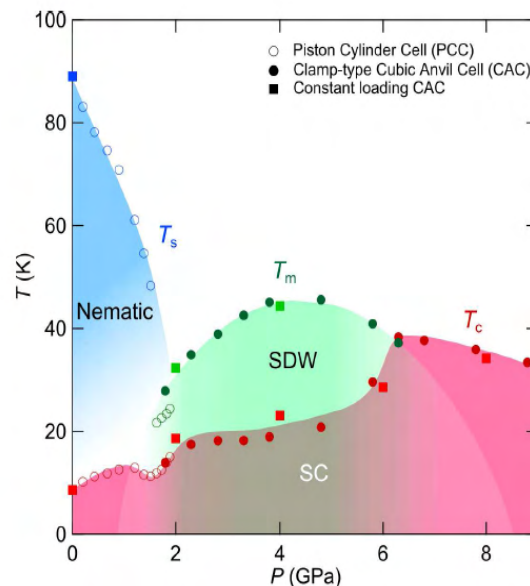


Fig: Inna Vishik

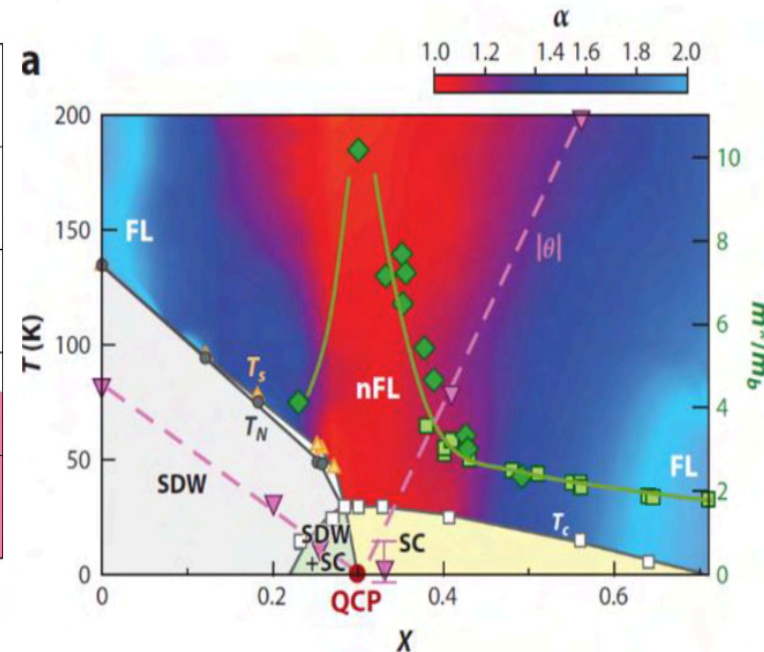
Parent compound: Metal

Iron superconductor FeSe  
(nematic state)



Sun et al, Nat. Comm.  
12146 (2016)

Iron superconductor Ba-122  
(quantum criticality)





# Emergence in condensed matter

## Kondo effect:

A minimum in the resistivity of metals with magnetic impurities with a lot of physics behind

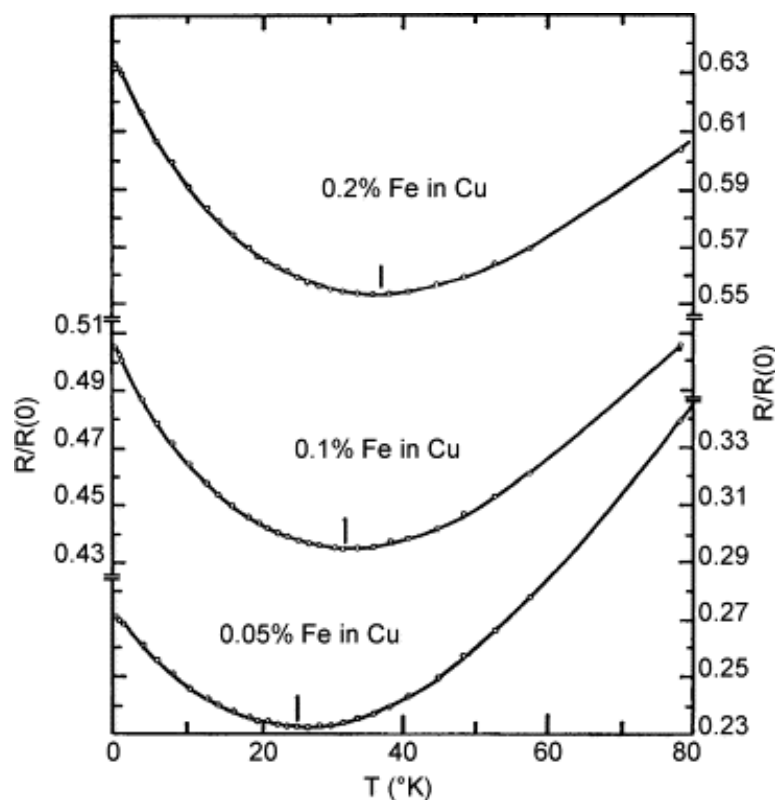
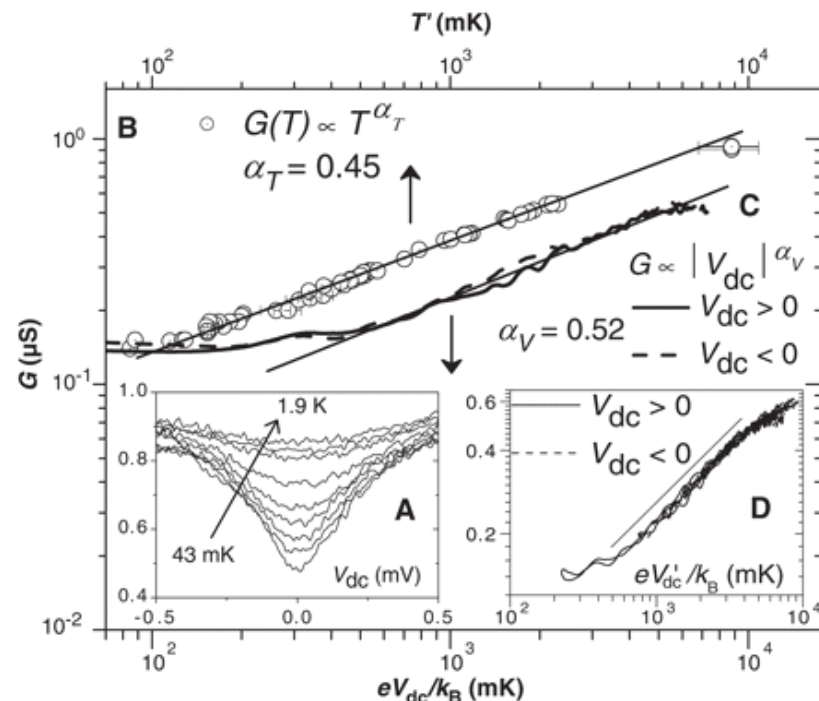


Fig: Kasai et al, (2001)

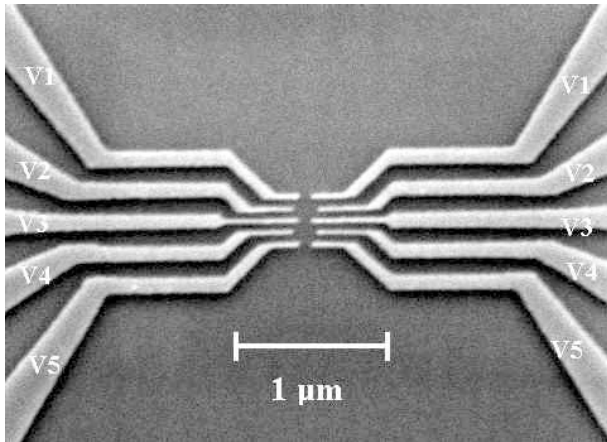


## One dimension:

Dramatic effect of interactions:  
Luttinger liquids

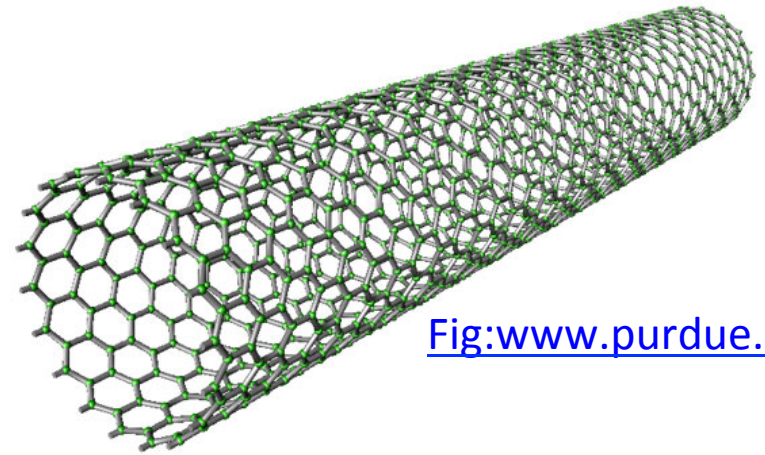
Fig: Jonpol et al, Science (2009)

# Emergence in mesoscopic systems



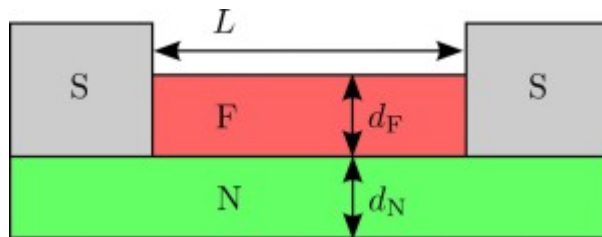
Kondo effect in  
Quantum Dots

[Fig: www.gaia3d.co.uk](http://www.gaia3d.co.uk)



[Fig:www.purdue.edu](http://www.purdue.edu)

Luttinger liquid behavior  
in carbon nanotubes



[Fig:iopscience.iop.org](http://iopscience.iop.org)

Different phases put in contact  
(superconducting & ferromagnetic )



# Topological and 2D systems

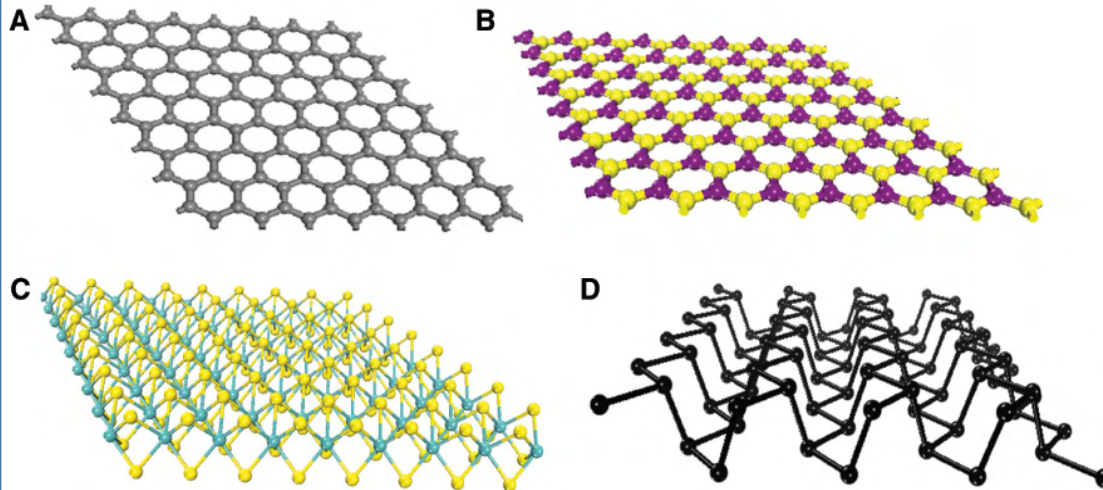
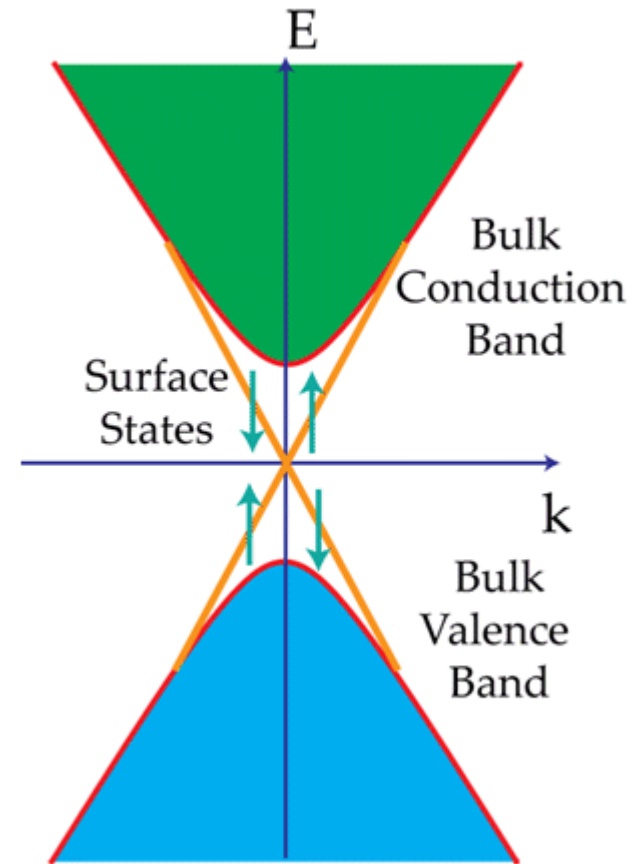


Fig: Nanophotonics 4, 128 (2015)

New properties in atomic layers.  
Even at the single particle level!



Topological insulators,  
Weyl semimetals

Fig: Hoffman's lab

# Engineering new materials and heterostructures

## 2D LEGO

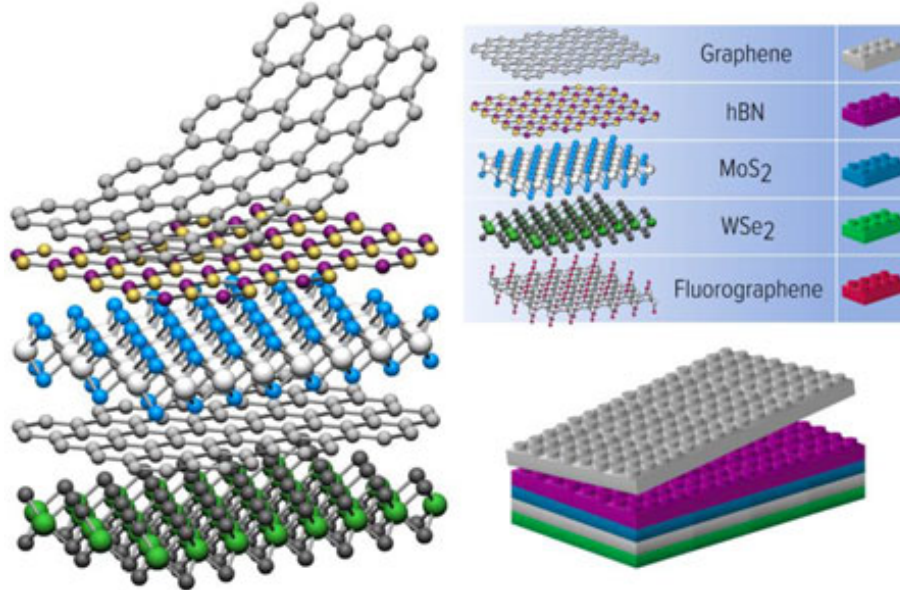
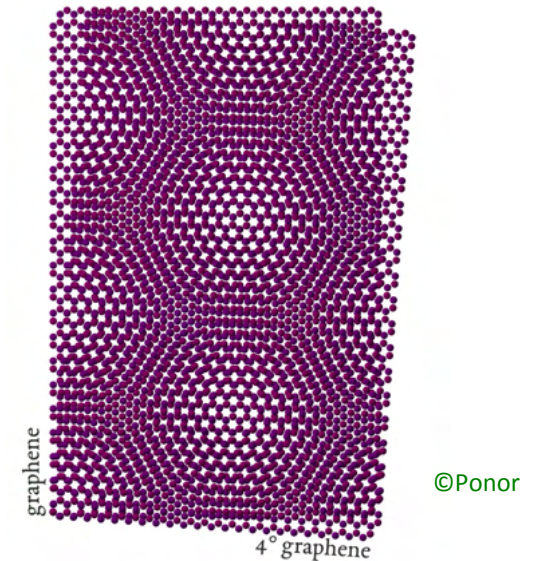


Fig: Geim & Grigorieva,  
Nature 499, 419 (2013)

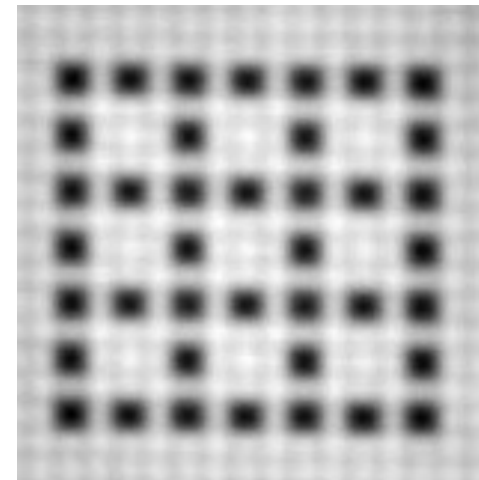


Moiré heterostructures  
(huge unit cells)

Possibility to engineer band structures or alternate materials with different functionalities (ferromagnetic, superconductor ...)

Atomic lattices on surfaces

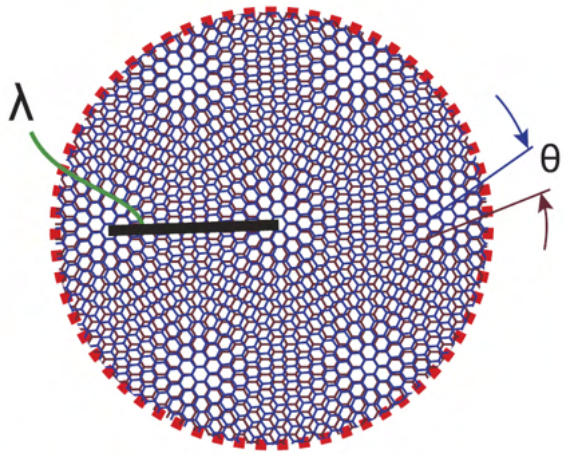
Yan & Liljeroth,  
Advances in Physics X, 4, 2019



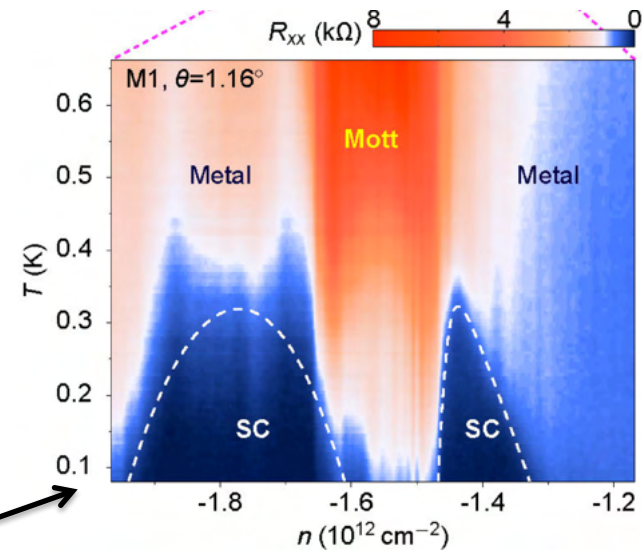
# Moiré flat bands: a new platform to study the effects of correlations

March 2018

## Magic angle twisted bilayer graphene (1.1°)

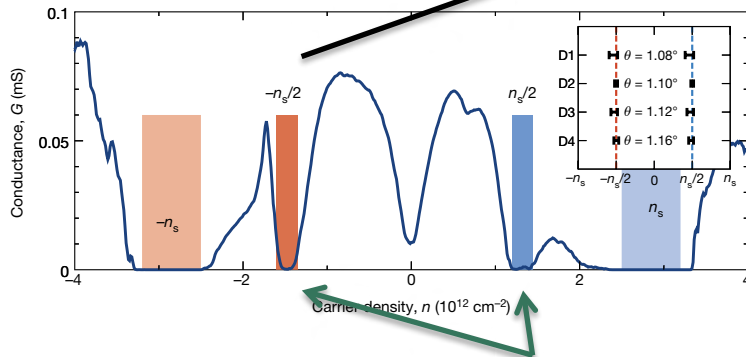


Moiré unit cell > 10.000 atoms  
Highly tunable system (doping, angle ...)



Cao et al, Nature  
556, 43 (2018)

Correlated  
insulating state



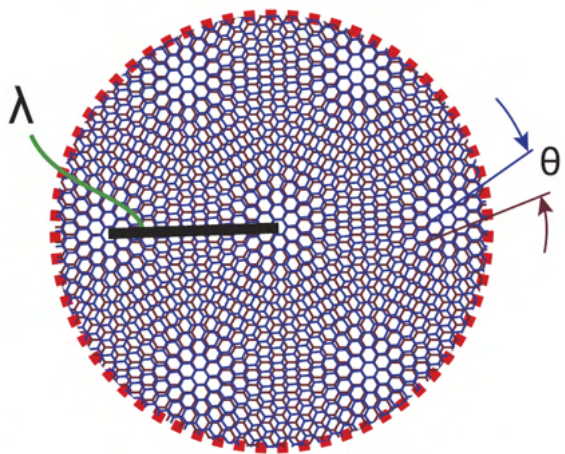
Two correlated insulating states  
(half-filling electron & hole bands)

Cao et al, Nature 556, 80 (2018), Nature 556, 43 (2018)

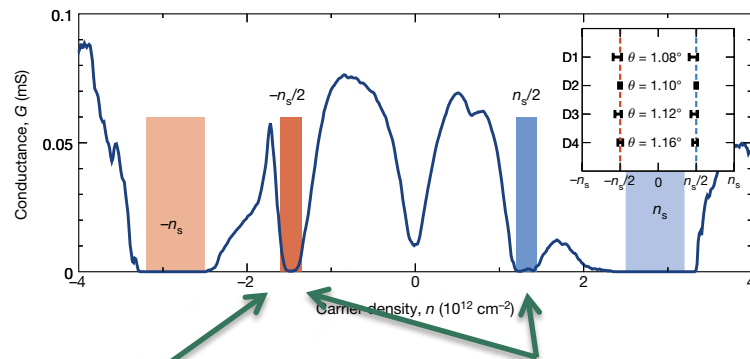


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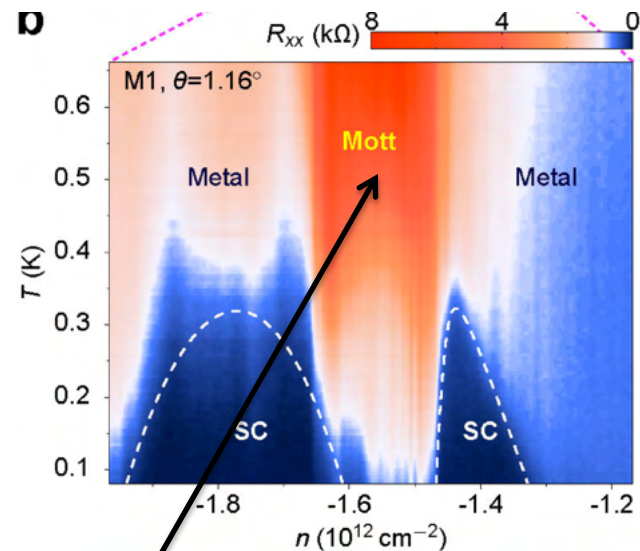


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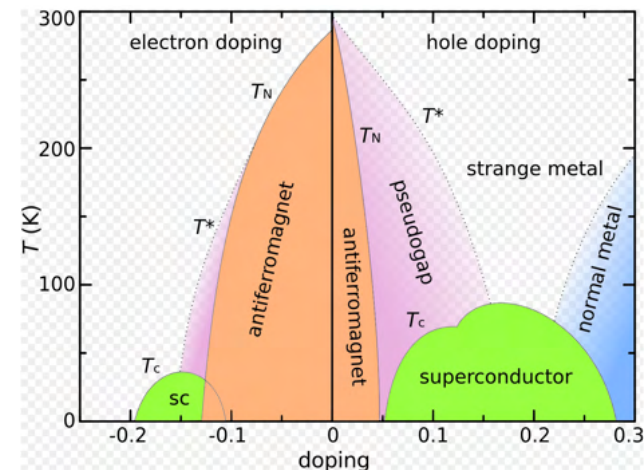
Superconductivity  
Two correlated insulating states (half-filling electron & hole bands)

Cao et al, Nature 556, 80 (2018), Nature 556, 43 (2018)



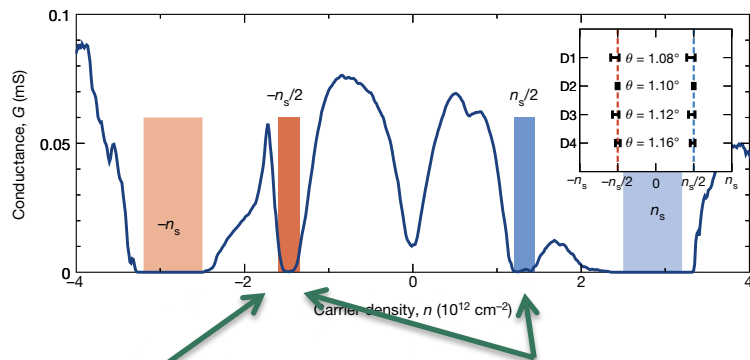
Correlated  
insulating state

Cao et al, Nature  
556, 43 (2018)



# Moiré flat bands where 2D materials, correlations and topology meet

March 2018

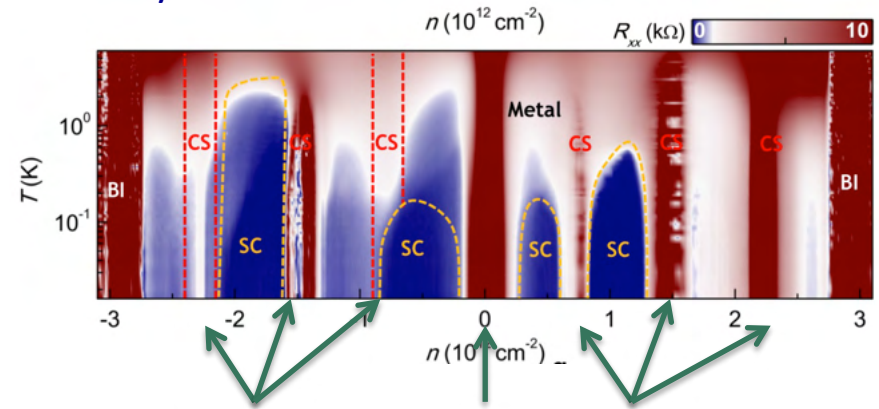


Two correlated insulating states  
(half-filling electron & hole bands)

Superconductivity

Cao et al, Nature 556, 80 (2018), Nature 556, 43 (2018)

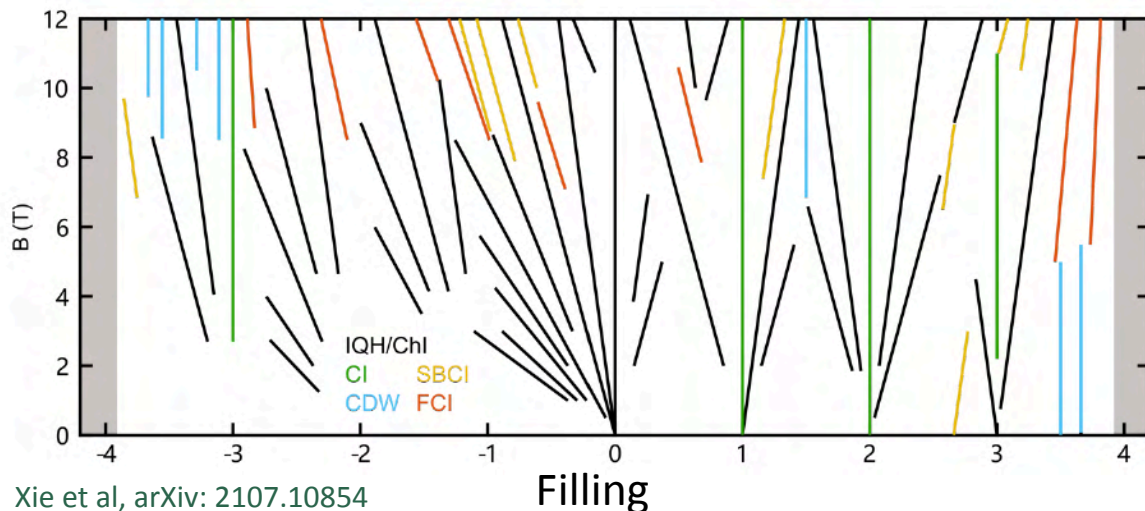
January 2019



Correlated states at all integer fillings

Lu et al Nature 574, 653 (2019)

July 2021 (compressibility measurements)



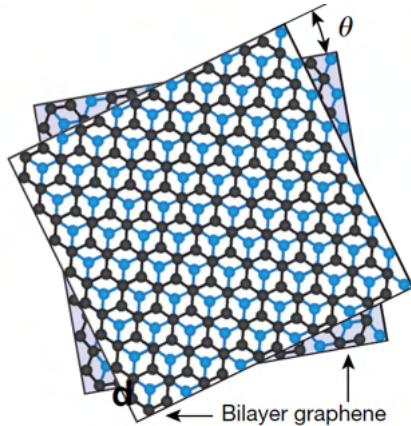
Xie et al, arXiv: 2107.10854

- Correlated insulators (integer filling)
- Charge Density Wave
- Chern Insulators/IQH
- Symmetry broken Chern insulators
- Fractional Chern insulators

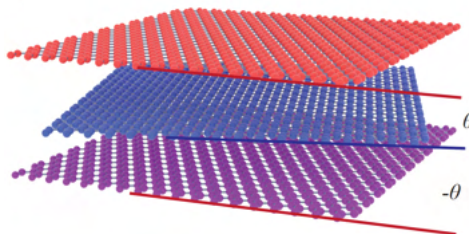
# Moiré flat bands where 2D materials, correlations and topology meet

Other graphene based  
twisted heterostructures

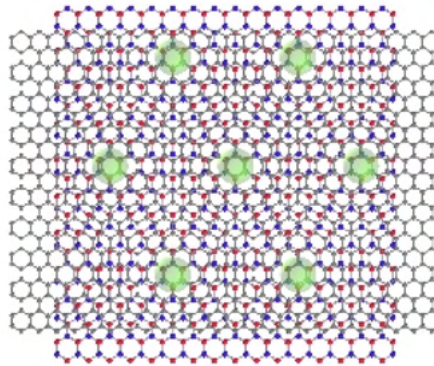
Twisted double bilayer graphene



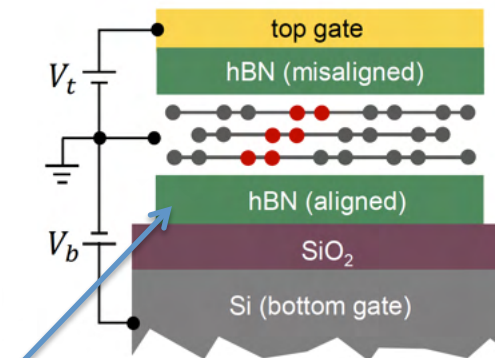
Twisted graphene trilayer  
(Moiré 3.0)



Play with the substrate  
also in twisted heterostructures

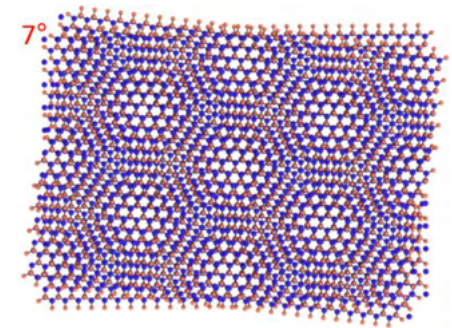


Trilayer ABC graphene/hBN

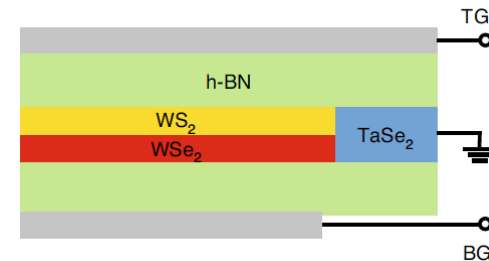


Twisting other 2D materials  
(semiconductors, magnetic ...)

Twisted bilayer WSe<sub>2</sub>



Twisted bilayer WSe<sub>2</sub>/WS<sub>2</sub>



Liu et al, Nature 583, 221 (2020), Park et al, Nature 590, 249 (2021), Chen et al, Nature 572, 215 (2019), An et al, Nanoscale Horizons 9,( 2020), Jin et al Nature Materials 20, 940 (2021)

# Quantum Phases in Novel Materials

## Basic ideas & generic concepts

Different kinds of phenomena & why they happen

## Theoretical description

Many different analytical & numerical methods and approaches

Experimental signatures of the quantum states

Materials and platforms where these quantum phases appear



# Emergence of Quantum Phases in Novel States: Outline

- ❑ Introduction: Emergence and Basic Concepts (L. Bascones)
- ❑ Fermi liquid theory (L. Bascones)
- ❑ Electronic correlations: Mott, Hund and Luttinger Physics (L. Bascones)
- ❑ Magnetism (M.J. Calderón)
- ❑ Superconductivity (M.J. Calderón)
- ❑ Dirac Materials (A. Cortijo)
- ❑ Topological Insulators and topological semimetals (A. Cortijo)
- ❑ Kondo effect in metals and nanostructures (R. Aguado)
- ❑ Topological superconductivity (R. Aguado)



# Basic concepts: the Fermi gas

- Focus on electrons. Work at fixed  $\mu$
- Electrons are fermions: **Fermi-Dirac Statistics**

$$f(\varepsilon) = \frac{1}{e^{(\varepsilon - \mu)/k_B T} + 1}$$

energy

chemical potential

## Zero temperature

Step function

States filled up to the Fermi Energy  $\varepsilon_F$  which defines a **Fermi surface**

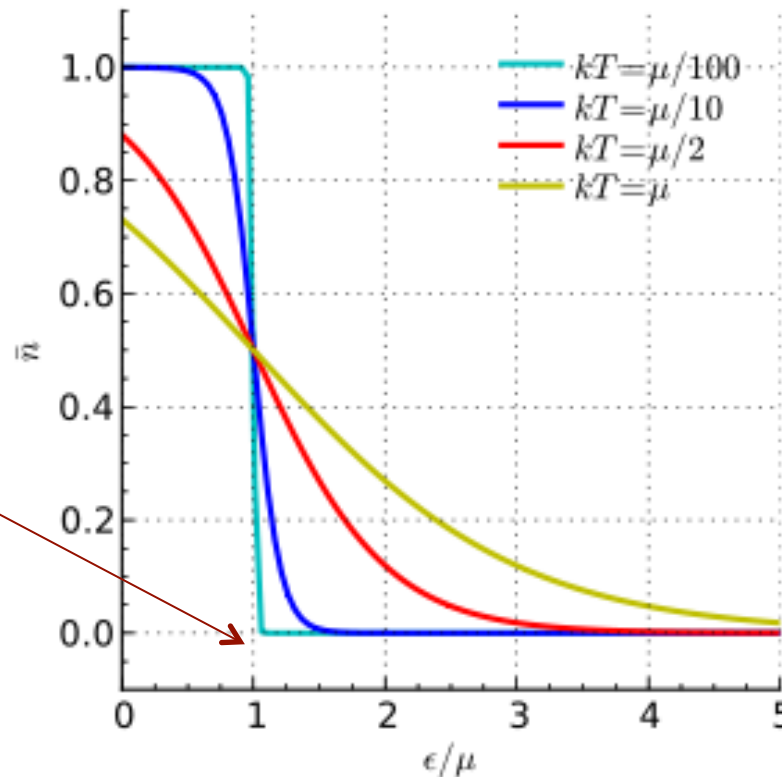


Fig: Wikipedia

**High temperatures**  
(classical gas)

$$k_B T \gg \mu$$

$$f(\varepsilon) \propto e^{-\varepsilon/k_B T}$$

Maxwell-Boltzmann distribution function

# Basic concepts: the Fermi gas

- **Low temperatures**

(quantum gas, Fermi-Dirac)

$$K_B T \ll \mu$$

- **Specific heat**

$$C_v = \left. \frac{\partial F}{\partial T} \right|_{\mu}$$

Free energy

$$C_v = \gamma T$$

Linear in temperature

- **Spin susceptibility**

$$\chi_s = \frac{\partial M}{\partial H}$$

Magnetization

Magnetic field

$$\chi_s = \mu_B^2 N(\epsilon_F)$$

independent of T

Bohr magneton

Density of states at Fermi level

**Pauli susceptibility**

- **High temperatures**

(classical gas, Maxwell-Boltzmann)

$$K_B T \gg \mu$$

- **Specific heat**

$$C_v = \text{independent of } T$$

- **Spin susceptibility**

$$\chi_s \propto \frac{1}{T}$$

**Curie law**

# Basic concepts: the Fermi gas

Different temperature dependence of measurable quantities  
in the degenerate (quantum) and classical limits

- **Low temperatures**  
(quantum gas)  $k_B T \ll \mu$

- **High temperatures**  
(classical gas)  $k_B T \gg \mu$

○ **Specific heat**

$$C_V = \gamma T \quad \text{Linear in temperature}$$

$$C_V = \text{independent of } T$$

○ **Spin susceptibility**

$$\chi_s = \mu_B^2 N(\epsilon_F)$$

independent of  $T$

$$\chi_s \propto \frac{1}{T} \quad \text{Curie law}$$

**Pauli susceptibility**

Consequence of Pauli exclusion principle

**Non-interacting fermions are correlated due to Fermi statistics & Pauli principle**

# Basic concepts: the Fermi gas

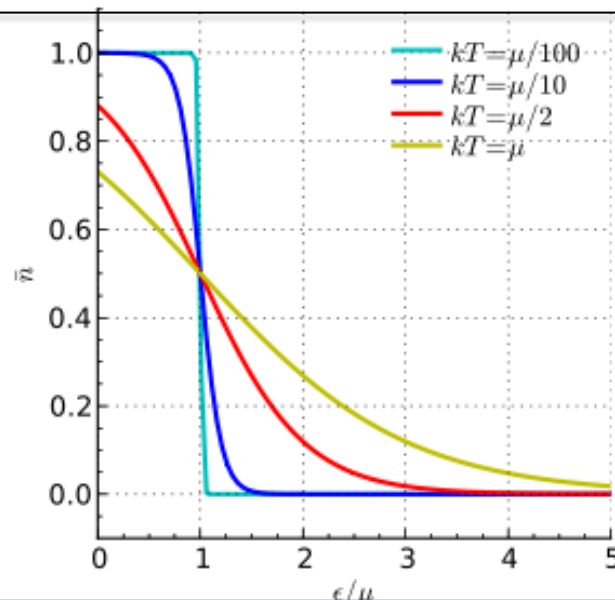
Different temperature dependence  
of measurable quantities  
in the degenerate (quantum)  
and classical limits

• **Low temperatures**  
(quantum gas)  $k_B T \ll \mu$

• **High temperatures**  
(classical gas)  $k_B T \gg \mu$

Fermi temperature  $T_F = \epsilon_F / k_B$

Temperature below which quantum effects are important



# Basic concepts: the Fermi gas

Different temperature dependence  
of measurable quantities  
in the degenerate (quantum)  
and classical limits

- **Low temperatures**  
(quantum gas)  $k_B T \ll \mu$
- **High temperatures**  
(classical gas)  $k_B T \gg \mu$

$$\text{Fermi temperature } T_F = \epsilon_F / k_B$$

Temperature below which quantum effects are important

**In metals**

$$\epsilon_F \sim 3 \text{ eV}$$

$$T_F \sim 2400 \text{ K}$$

**Metals generically have  
to be treated  
as degenerate gases**

**In TBG & doped  
semiconductors**

$$\epsilon_F \sim \text{few meV}$$

$$T_F \sim 50 \text{ K}$$

**TBG & SMC behave as  
degenerate gases ONLY  
at very low T**

# Basic concepts: lattice and energy bands vs the continuum

**In free space:** Parabolic band

- Isotropic
- No length scale
- Momentum conserved

$$\text{Kinetic energy} = \frac{k^2}{2m}$$

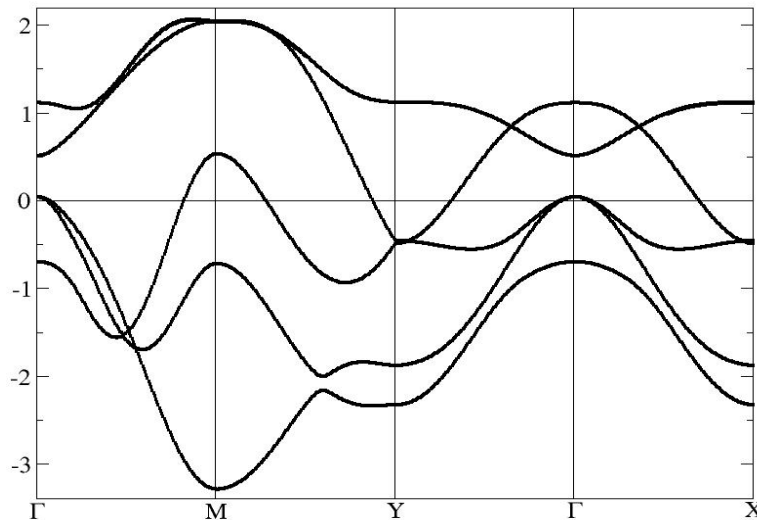
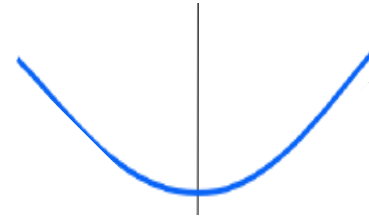


Fig: Calderón et al,  
PRB, 80, 094531 (2009)

**In a solid:**

- periodic potential of the ionic lattice
- Length scale: the lattice constant **a**
- Momentum conserved modulus  **$2\pi/a$**
- In general, anisotropic potential
- Energy bands filled up to  $\epsilon_F$ . **Fermi surface**
- Effective mass (band mass)

$$m^{-1} = \left| \partial^2 \epsilon / \partial k^2 \right|$$



# Basic concepts: lattice and energy bands vs the continuum

**In free space:** Parabolic band

$$\text{Kinetic energy} = \frac{k^2}{2m}$$

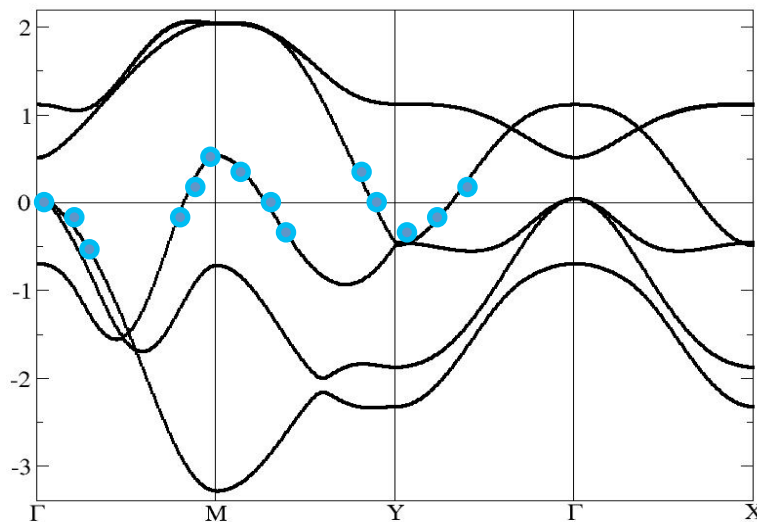
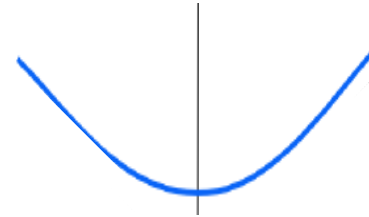


Fig: Calderón et al, PRB, 80, 094531 (2009)

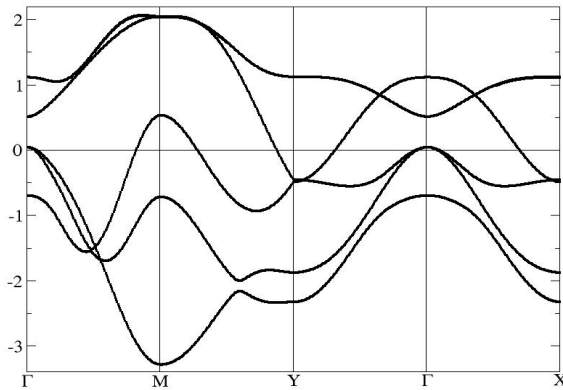
Some phenomena can be described in terms of **parabolic bands** which substitute the energy bands close to the Fermi surface



**Careful!**

This is not always possible  
Some effects are intrinsic to the lattice

# Basic concepts: massless fermions in graphene



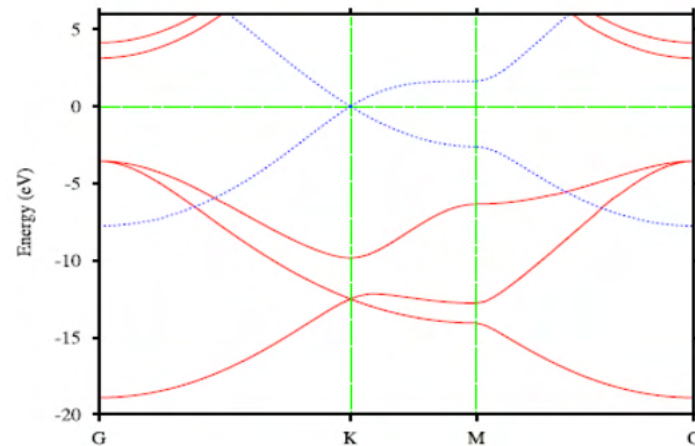
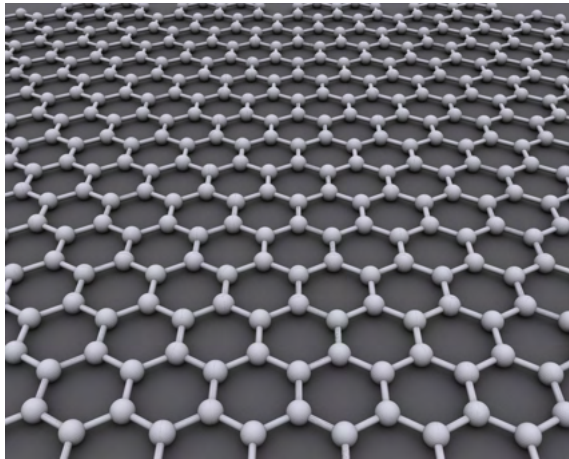
## Parabolic bands:

Continuum approximation  $\frac{k^2}{2m}$

Effective mass (band mass)  $m^{-1} = |\partial^2 \epsilon / \partial k^2|$

Fig: Calderón et al, PRB, 80, 094531 (2009)

## Graphene:



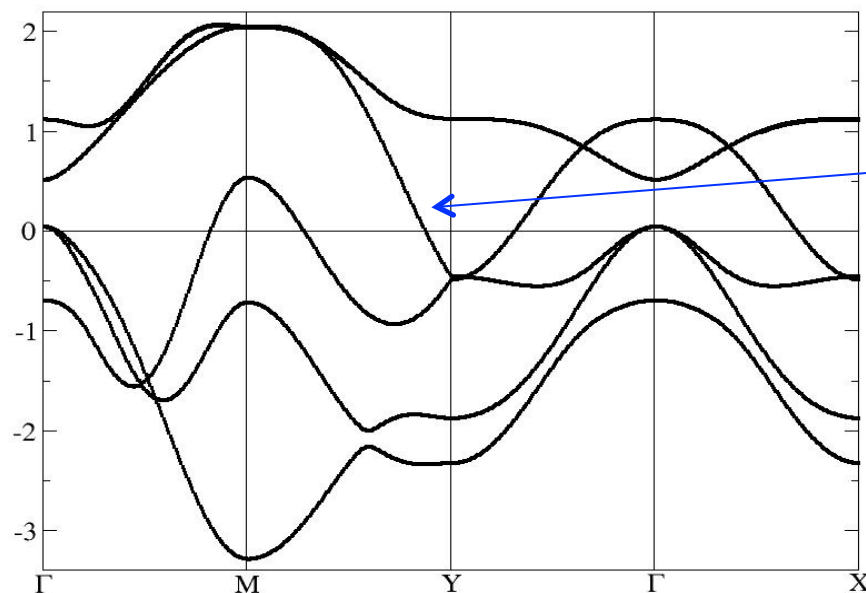
## Linear bands close to Fermi level

Continuum approximation

$$E \sim v_F k$$

Effective mass (band mass) is zero!

# Basic concepts: metals and insulators



**Metallicity**  
in clean systems  
Bands crossing  
the Fermi level  
(finite DOS)

Fig: Calderón et al, PRB, 80, 094531 (2009)

**Insulating behaviour**  
in clean systems  
Bands below  
Fermi level filled

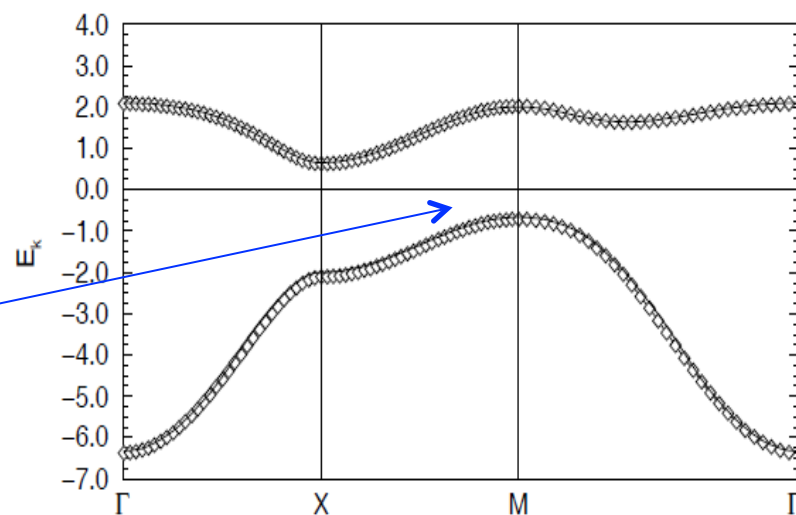
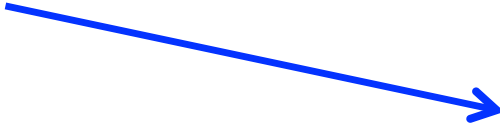


Fig: Hess & Serene, PRB 59, 15167 (1999)

# Basic concepts: metals and insulators

Spin degeneracy (no symmetry breaking):  
Each band can hold 2 electrons per unit cell

Odd number  
of electrons  
per unit cell  Metallic (or semimetal)

Even number  
of electrons  
per unit cell  Insulating  
 Metallic (in case  
of band overlap)

# Basic concepts: metals and insulators

Spin degeneracy:  
Each band can hold 2 electrons per unit cell

Odd number  
of electrons  
per unit cell

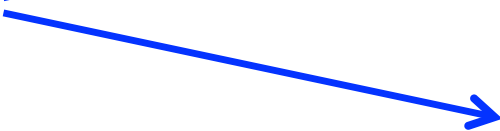


Metallic

Even number  
of electrons  
per unit cell



Insulating



Metallic (in case  
of band overlap)

**Stops being valid in a Mott insulator!**

# Basic concepts: strength of interactions

**Strength of interactions:**  $U$

$$U/W$$

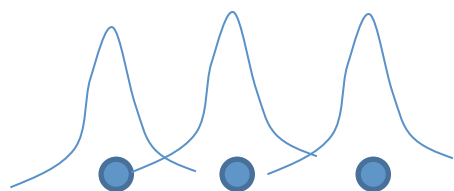
Narrow bands  
more sensitive to interactions

**Kinetic energy:**  $W$  bandwidth

Interactions are not small compared to kinetic energy

- Focus on electrons close to the Fermi surface.
- Core electrons + nucleus form the ion

**Kinetic energy:** tight binding model using atomic orbitals as a basis



Larger overlap between orbitals  
in neighbouring sites  
(larger kinetic energy)

Larger spread of wave function (less localized orbitals)



Two electrons are  
less likely to be found  
very close  
(smaller effective interaction)

# Basic concepts: strength of interactions

3d: competition between kinetic energy & interaction

Interaction strength decreases in 4d & overall in 5d due to larger extension of the orbital

Legend:

- Alcalinos
- Alcalinotérreos
- Metales de transición
- Lantánidos
- Actínidos
- Metales del bloque p
- No metales
- Gases nobles
- C Solid
- L Liquid
- H Gas
- Tc Synthetic

Atomic masses in parentheses are those of the most stable or common isotope.

s & p electrons  
kinetic energy  
more important

4f overall and 5f orbitals are quite localized on a site.  
Very small kinetic energy. Interactions win



# Basic concepts: strength of interactions

Periodic table showing elements categorized by groups and properties. The table includes atomic numbers, element symbols, names, and atomic masses. A blue arrow points from the text 'p-orbitals, extended wave functions (interactions in graphene not expected to be very relevant)' to the p-block elements (groups 13-18).

| Group | 1                     | 2                   | 3                       | 4                  | 5                    | 6                   | 7                     | 8                  | 9                     | 10                  | 11                    | 12                  | 13                   | 14                  | 15                    | 16                  | 17                   | 18                  |
|-------|-----------------------|---------------------|-------------------------|--------------------|----------------------|---------------------|-----------------------|--------------------|-----------------------|---------------------|-----------------------|---------------------|----------------------|---------------------|-----------------------|---------------------|----------------------|---------------------|
| IA    | 1<br>H<br>1.00794     | 2<br>He<br>4.002602 |                         |                    |                      |                     |                       |                    |                       |                     |                       |                     |                      |                     |                       |                     |                      |                     |
| IIA   | 3<br>Li<br>6.941      | 4<br>Be<br>9.012182 |                         |                    |                      |                     |                       |                    |                       |                     |                       |                     |                      |                     |                       |                     |                      |                     |
| IIIB  | 11<br>Na<br>22.989769 | 12<br>Mg<br>24.3050 | 21<br>Sc<br>44.955910   | 22<br>Ti<br>47.887 | 23<br>V<br>50.9415   | 24<br>Cr<br>51.9961 | 25<br>Mn<br>54.938045 | 26<br>Fe<br>55.845 | 27<br>Co<br>58.933200 | 28<br>Ni<br>58.6934 | 29<br>Cu<br>63.546    | 30<br>Zn<br>65.409  | 31<br>Ga<br>69.723   | 32<br>Ge<br>72.64   | 33<br>As<br>74.92160  | 34<br>Se<br>78.96   | 35<br>Br<br>79.904   | 36<br>Kr<br>83.798  |
| IVB   | 37<br>Rb<br>85.4678   | 38<br>Sr<br>87.62   | 39<br>Y<br>88.90585     | 40<br>Zr<br>91.224 | 41<br>Nb<br>92.90638 | 42<br>Mo<br>95.94   | 43<br>Tc<br>[98]      | 44<br>Ru<br>101.07 | 45<br>Rh<br>102.90550 | 46<br>Pd<br>106.42  | 47<br>Ag<br>107.8682  | 48<br>Cd<br>112.411 | 49<br>In<br>114.818  | 50<br>Sn<br>118.710 | 51<br>Sb<br>121.760   | 52<br>Te<br>127.60  | 53<br>I<br>126.90447 | 54<br>Xe<br>131.293 |
| VB    | 55<br>Cs<br>132.90545 | 56<br>Ba<br>137.327 | 57 to 71<br>Lanthanides | 72<br>Hf<br>178.49 | 73<br>Ta<br>180.9479 | 74<br>W<br>183.84   | 75<br>Re<br>186.207   | 76<br>Os<br>190.23 | 77<br>Ir<br>192.227   | 78<br>Pt<br>195.078 | 79<br>Au<br>196.96655 | 80<br>Hg<br>200.59  | 81<br>Tl<br>204.3833 | 82<br>Pb<br>207.2   | 83<br>Bi<br>208.98038 | 84<br>Po<br>(209)   | 85<br>At<br>(210)    | 86<br>Rn<br>(222)   |
| VIB   | 87<br>Fr<br>(223)     | 88<br>Ra<br>(226)   | 89 to 103<br>Actinides  | 104<br>Rf<br>(261) | 105<br>Db<br>(262)   | 106<br>Sg<br>(266)  | 107<br>Bh<br>(264)    | 108<br>Hs<br>(269) | 109<br>Mt<br>(268)    | 110<br>Ds<br>(271)  | 111<br>Rg<br>(272)    | 112<br>Uub<br>(285) | 113<br>Uut<br>(284)  | 114<br>Uuq<br>(289) | 115<br>Uup<br>(288)   | 116<br>Uuh<br>(292) | 117<br>Uus<br>(293)  | 118<br>Uuo<br>(294) |
| VIIA  |                       |                     |                         |                    |                      |                     |                       |                    |                       |                     |                       |                     |                      |                     |                       |                     |                      |                     |
| VIIIA |                       |                     |                         |                    |                      |                     |                       |                    |                       |                     |                       |                     |                      |                     |                       |                     |                      |                     |

Atomic masses in parentheses are those of the most stable or common isotope.

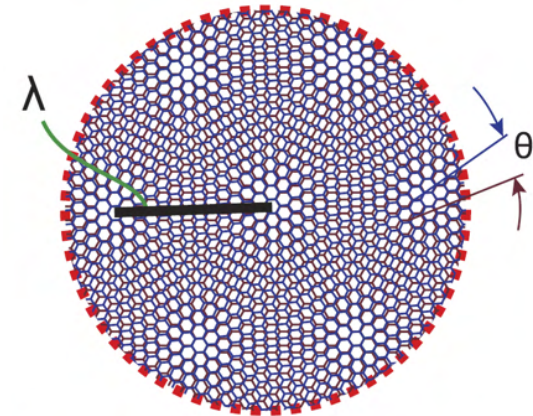
p-orbitals,  
extended wave functions  
(interactions in graphene  
not expected to be very  
relevant)

# Basic concepts: strength of interactions

|                            |                     |                       |                     |                      |                     |                       |                    |                       |                     |                         |                     |                        |                     |                         |                     |                      |                     |
|----------------------------|---------------------|-----------------------|---------------------|----------------------|---------------------|-----------------------|--------------------|-----------------------|---------------------|-------------------------|---------------------|------------------------|---------------------|-------------------------|---------------------|----------------------|---------------------|
| 1<br>IA<br>New<br>Original | 2<br>IIA            | 3<br>IIIB             | 4<br>IVB            | 5<br>VB              | 6<br>VIB            | 7<br>VIIB             | 8<br>VIII          | 9<br>VIII             | 10<br>VIII          | 11<br>IB                | 12<br>IIB           | 13<br>IIIA             | 14<br>IVA           | 15<br>VA                | 16<br>VIA           | 17<br>VIIA           | 18<br>VIIIA         |
| 1<br>H<br>1.00794          | 2<br>He<br>4.002602 | 3<br>Li<br>6.941      | 4<br>Be<br>9.012182 | 5<br>B<br>10.811     | 6<br>C<br>12.011    | 7<br>N<br>14.00643    | 8<br>O<br>15.9994  | 9<br>F<br>18.9984032  | 10<br>Ne<br>20.1797 | 11<br>Na<br>22.98976928 | 12<br>Mg<br>24.304  | 13<br>Al<br>26.9815385 | 14<br>Si<br>28.0855 | 15<br>P<br>30.973761998 | 16<br>S<br>32.06    | 17<br>Cl<br>35.453   | 18<br>Ar<br>39.948  |
| 19<br>K<br>39.0983         | 20<br>Ca<br>40.078  | 21<br>Sc<br>44.955912 | 22<br>Ti<br>47.88   | 23<br>V<br>50.9415   | 24<br>Cr<br>51.9961 | 25<br>Mn<br>54.938045 | 26<br>Fe<br>55.845 | 27<br>Co<br>58.933200 | 28<br>Ni<br>58.6934 | 29<br>Cu<br>63.546      | 30<br>Zn<br>65.409  | 31<br>Ga<br>69.723     | 32<br>Ge<br>72.64   | 33<br>As<br>74.921595   | 34<br>Se<br>78.96   | 35<br>Br<br>79.904   | 36<br>Kr<br>83.798  |
| 37<br>Rb<br>85.4678        | 38<br>Sr<br>87.62   | 39<br>Y<br>88.90584   | 40<br>Zr<br>91.224  | 41<br>Nb<br>92.90638 | 42<br>Mo<br>95.94   | 43<br>Tc<br>98        | 44<br>Ru<br>101.07 | 45<br>Rh<br>102.90550 | 46<br>Pd<br>106.42  | 47<br>Ag<br>107.8682    | 48<br>Cd<br>112.411 | 49<br>In<br>114.818    | 50<br>Sn<br>118.710 | 51<br>Sb<br>121.757     | 52<br>Te<br>127.60  | 53<br>I<br>126.90447 | 54<br>Xe<br>131.29  |
| 55<br>Cs<br>132.90545      | 56<br>Ba<br>137.327 | 57-71<br>Lanthanides  | 72<br>Hf<br>178.49  | 73<br>Ta<br>180.9479 | 74<br>W<br>183.84   | 75<br>Re<br>186.207   | 76<br>Os<br>190.23 | 77<br>Ir<br>192.222   | 78<br>Pt<br>195.078 | 79<br>Au<br>196.96655   | 80<br>Hg<br>200.59  | 81<br>Tl<br>204.3833   | 82<br>Pb<br>207.2   | 83<br>Bi<br>208.98038   | 84<br>Po<br>(209)   | 85<br>At<br>(210)    | 86<br>Rn<br>(222)   |
| 87<br>Fr<br>(223)          | 88<br>Ra<br>(226)   | 89-103<br>Actinides   | 104<br>Rf<br>(261)  | 105<br>Db<br>(262)   | 106<br>Sg<br>(266)  | 107<br>Bh<br>(264)    | 108<br>Hs<br>(265) | 109<br>Mt<br>(268)    | 110<br>Ds<br>(271)  | 111<br>Rg<br>(272)      | 112<br>Uub<br>(285) | 113<br>Uut<br>(284)    | 114<br>Uuq<br>(289) | 115<br>Uup<br>(288)     | 116<br>Uuh<br>(289) | 117<br>Uus<br>(289)  | 118<br>Uuo<br>(294) |

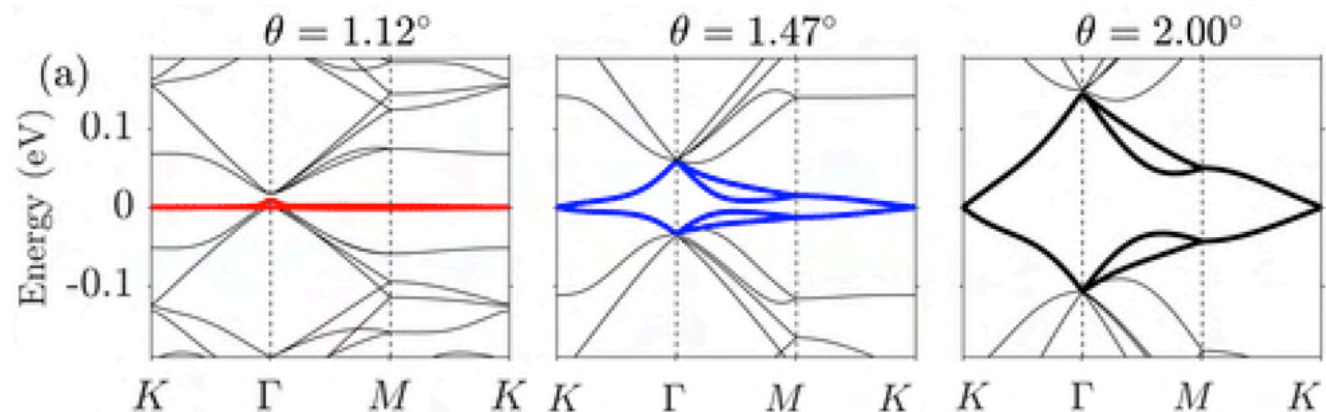
Atomic masses in parentheses are those of the most stable or common isotope.

**p-orbitals,**  
extended wave functions  
(interactions in graphene  
not expected to be very  
relevant)



**Flat bands close to  
the magic angle  $\sim 1.1^\circ$**

Very small  $W$



# Basic concepts: strength of interactions

|           |              |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |          |
|-----------|--------------|--|--|--|--|--|--|--|--|--|--|--|--|--|--|--|--|----------|
| 1         | 2            |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 18       |
| 1A        | New Original |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 8A       |
| 1         | 2            |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 2        |
| 1         | H            |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | He       |
| 1.00794   |              |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 4.002602 |
| 3         | 4            |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 10       |
| Li        | Be           |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | Ne       |
| 6.941     | 9.012182     |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 20.1797  |
| 11        | 12           |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 18       |
| Na        | Mg           |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | Ar       |
| 22.989769 | 24.3050      |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 39.948   |
| 19        | 20           |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 36       |
| K         | Ca           |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | Kr       |
| 39.0983   | 40.078       |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 83.796   |
| 37        | 38           |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 54       |
| Rb        | Sr           |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | Xe       |
| 85.4678   | 87.62        |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 131.29   |
| 55        | 56           |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 86       |
| Cs        | Ba           |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | Rn       |
| 132.90545 | 137.327      |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 222      |
| 7         | 8            |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 118      |
| Fr        | Ra           |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | Uuo      |
| (223)     | (226)        |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | (294)    |

Alcalinos

Alcalinotérreos

Metales de transición

Lantánidos

Actínidos

Metales del bloque p

No metales

Gases nobles

Cr Solid

B Liquid

H Gas

Tc Synthetic

|           |          |          |         |           |         |           |           |          |          |         |           |           |       |           |        |
|-----------|----------|----------|---------|-----------|---------|-----------|-----------|----------|----------|---------|-----------|-----------|-------|-----------|--------|
| 3         | 4        | 5        | 6       | 7         | 8       | 9         | 10        | 11       | 12       | 13      | 14        | 15        | 16    | 17        | 18     |
| IIIB      | IVB      | VB       | VIB     | VIIB      | VIII    | VIII      | IB        | IIB      |          | IIIA    | IVA       | VA        | VIA   | VIIA      | 8A     |
| 21        | 22       | 23       | 24      | 25        | 26      | 27        | 28        | 29       | 30       | 31      | 32        | 33        | 34    | 35        | 36     |
| Sc        | Ti       | V        | Cr      | Mn        | Fe      | Co        | Ni        | Cu       | Zn       | Ga      | Ge        | As        | Se    | Br        | Kr     |
| 44.955912 | 47.867   | 50.9415  | 51.9961 | 54.938045 | 55.845  | 58.933195 | 58.6934   | 63.546   | 65.409   | 69.723  | 72.64     | 74.921595 | 78.96 | 79.904    | 83.796 |
| 39        | 40       | 41       | 42      | 43        | 44      | 45        | 46        | 47       | 48       | 49      | 50        | 51        | 52    | 53        | 54     |
| Y         | Zr       | Nb       | Mo      | Tc        | Ru      | Rh        | Pd        | Ag       | Cd       | In      | Sn        | Sb        | Te    | I         | Xe     |
| 88.905848 | 91.224   | 92.90638 | 95.94   | (98)      | 101.07  | 102.90550 | 106.42    | 107.8682 | 112.411  | 114.818 | 118.710   | 121.757   | 127.6 | 126.90547 | 131.29 |
| 72        | 73       | 74       | 75      | 76        | 77      | 78        | 79        | 80       | 81       | 82      | 83        | 84        | 85    | 86        | 87     |
| Hf        | Ta       | W        | Re      | Os        | Ir      | Pt        | Au        | Hg       | Tl       | Pb      | Bi        | Po        | At    | Rn        |        |
| 178.49    | 180.9479 | 183.84   | 186.207 | 190.23    | 192.222 | 195.078   | 196.96655 | 200.59   | 204.3833 | 207.2   | 208.98038 | (209)     | (210) | (222)     | (223)  |
| 104       | 105      | 106      | 107     | 108       | 109     | 110       | 111       | 112      | 113      | 114     | 115       | 116       | 117   | 118       | 119    |
| Rf        | Db       | Sg       | Bh      | Hs        | Mt      | Ds        | Rg        | Uub      | Uut      | Uuq     | Uup       | Uuh       | Uus   | Uuo       |        |
| (261)     | (262)    | (266)    | (264)   | (277)     | (268)   | (271)     | (272)     | (285)    | (284)    | (289)   | (288)     | (292)     | (294) | (294)     | (294)  |

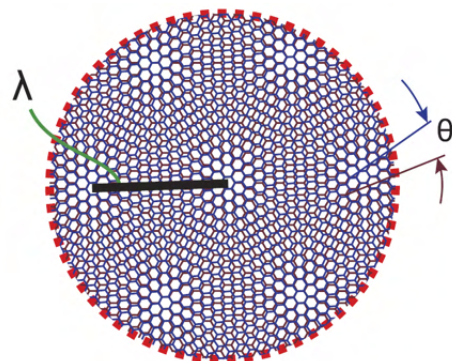
Atomic masses in parentheses are those of the most stable or common isotope.

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|           |          |             |           |          |          |          |          |           |            |            |         |            |         |           |       |
|-----------|----------|-------------|-----------|----------|----------|----------|----------|-----------|------------|------------|---------|------------|---------|-----------|-------|
| 57        | 58       | 59          | 60        | 61       | 62       | 63       | 64       | 65        | 66         | 67         | 68      | 69         | 70      | 71        | 72    |
| La        | Ce       | Pr          | Nd        | Pm       | Sm       | Eu       | Gd       | Tb        | Dy         | Ho         | Er      | Tm         | Yb      | Lu        |       |
| Lantano   | Cerio    | Praseodimio | Niobeo    | Prometio | Samario  | Európio  | Gadolino | Terbio    | Dispro     | Holmio     | Eritio  | Tulio      | Yterbio | Lutecio   |       |
| 138.90547 | 140.116  | 140.90768   | 144.242   | (145)    | 150.36   | 151.964  | 157.25   | 158.92534 | 162.500    | 164.93032  | 167.259 | 168.93421  | 173.047 | 174.967   | (175) |
| 89        | 90       | 91          | 92        | 93       | 94       | 95       | 96       | 97        | 98         | 99         | 100     | 101        | 102     | 103       | 104   |
| Ac        | Th       | Pa          | U         | Np       | Pu       | Am       | Cm       | Bk        | Cf         | Es         | Fm      | Md         | No      | Lr        |       |
| Actinio   | Torio    | Protactinio | Uranio    | Neptunio | Plutonio | Americio | Curcio   | Berkelio  | Californio | Einsteinio | Fermio  | Mendelevio | Nobelio | Lawrencio | (105) |
| (227)     | 232.0381 | 231.03688   | 238.02891 | (237)    | (244)    | (243)    | (247)    | (247)     | (251)      | (252)      | (257)   | (258)      | (259)   | (262)     | (261) |

Cuprates, manganites,  
iron superconductors

$U, W \sim 2-3 \text{ eV}$



Twisted bilayer graphene and other moiré heterostructures

$U, W \sim 1-50 \text{ meV}$

# Basic concepts: strength of interactions

Assume 3D, free space (continuum), let  $n = N_e / V$  ( $n$  **electronic density**)

$N_e$ : Number of electrons

$V$ : Volume

**Kinetic energy**  $\int_{-\infty}^{\epsilon_F} \epsilon g(\epsilon) d\epsilon \propto n^{2/3}$

$g(\epsilon)$ : density of states

**Interaction energy**  $\propto \langle 1/r \rangle \cong n^{1/3}$

Coulomb interaction:  $\frac{e^2}{r}$

Valid for  $1/r$  interaction

**Interaction energy**

---

**Kinetic energy**  $\propto n^{-1/3}$

Important in semiconductors

Careful in metals !

Due to Pauli principle the importance of interactions decreases with increasing density

# Basic concepts: Screening and Hubbard model

Coulomb interaction:  $\frac{e^2}{r}$

Interaction is larger when electrons are closer

Long range character

**Hamiltonian on the lattice** (kinetic energy + interactions)

$$\sum_{ij\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.} + U \sum_j n_{j\uparrow} n_{j\downarrow} + \sum_{i \neq j \sigma \sigma'} U_{ij} n_{i\sigma} n_{j\sigma'}$$

$i, j$  lattice sites  
 $\sigma$  spin

Kinetic Energy  
(Tight binding)

Interaction (repulsion  
between electrons in  
the same site, only  
different spin)

Interaction (repulsion  
between electrons in  
different sites)

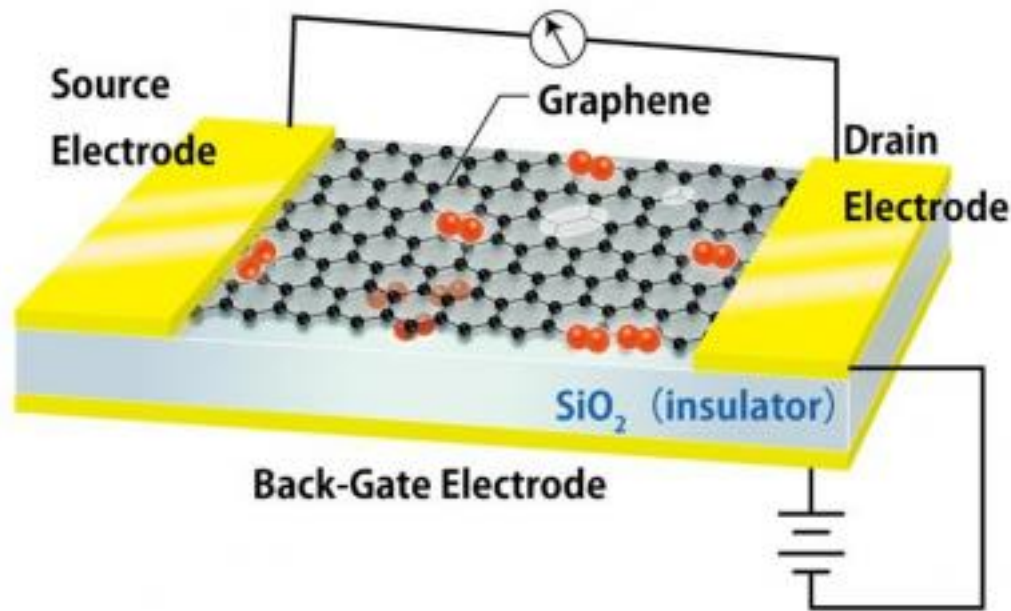
# Basic concepts: Screening and Hubbard model

Coulomb interaction:  $\frac{e^2}{\epsilon r}$

Interaction is larger when electrons are closer

Long range character

Other electrons in the solid (metal) or gate screen the Coulomb interaction.  
The interaction decays faster than  $1/r$

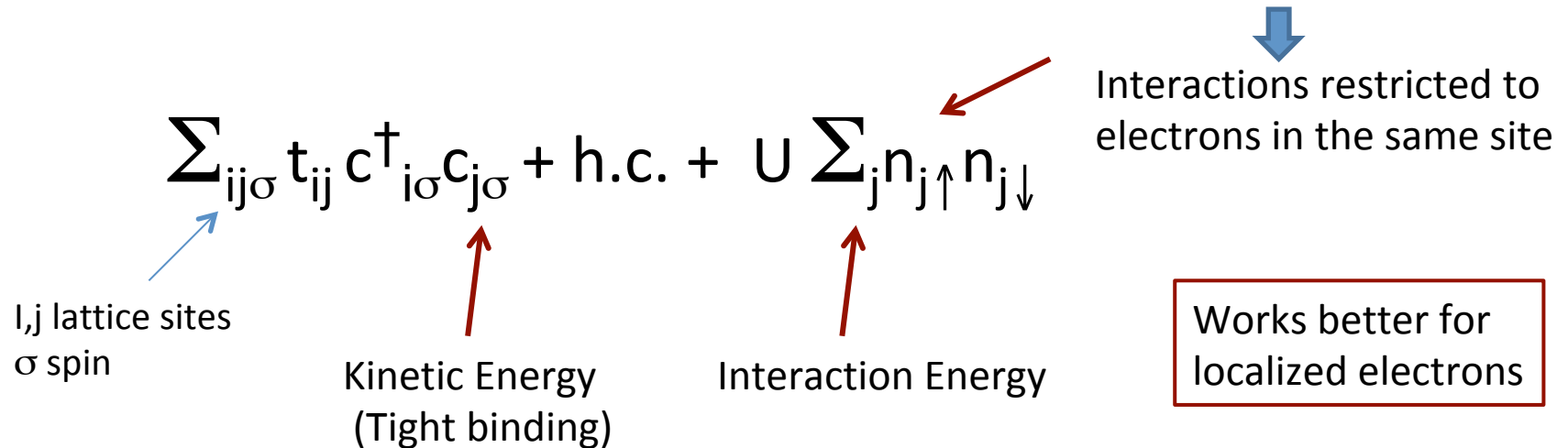


Screening also enters  
increases  $\epsilon$

# Basic concepts: Screening and Hubbard model

**Hubbard model** : lattice model, 1 orbital per site . Approximation

$$\sum_{ij\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.} + U \sum_j n_{j\uparrow} n_{j\downarrow}$$



$i, j$  lattice sites  
 $\sigma$  spin

Kinetic Energy  
(Tight binding)

Interaction Energy

Interactions restricted to  
electrons in the same site

Works better for  
localized electrons

It looks simple but it is not well understood. Basic in the study of correlated electrons



# Basic concepts: Summary

❑ Electrons in a solid follow Fermi-Dirac statistics. In a typical metal the degeneracy temperature is much higher than room temperature (in MATBG no).

❑  $C_v = \gamma T$  Linear in temperature  $\chi_s = \mu_B^2 N(\epsilon_F)$  independent of T

❑ Parabolic bands (continuum) versus lattice models. Linear bands (no mass)

❑ Band theory: metallic or insulating character on the basis of the number of electrons per unit cell.

❑  $U/W$  controls strength of interactions

❑ s and p orbitals less sensitive to interactions, f orbitals are the most correlated. d-electrons interplay between kinetic energy & interactions. In TBG & other correlated moirés interactions are important due to very small W

❑ In 3 D and with  $1/r$  in the continuum limit the importance of interactions decreases with increasing density

❑ Screening and Hubbard model