

# Emergence of Quantum Phases in Novel Materials

VIII Edition ICMM School

## Introduction to Electronic Correlations

# Emergence



# 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...

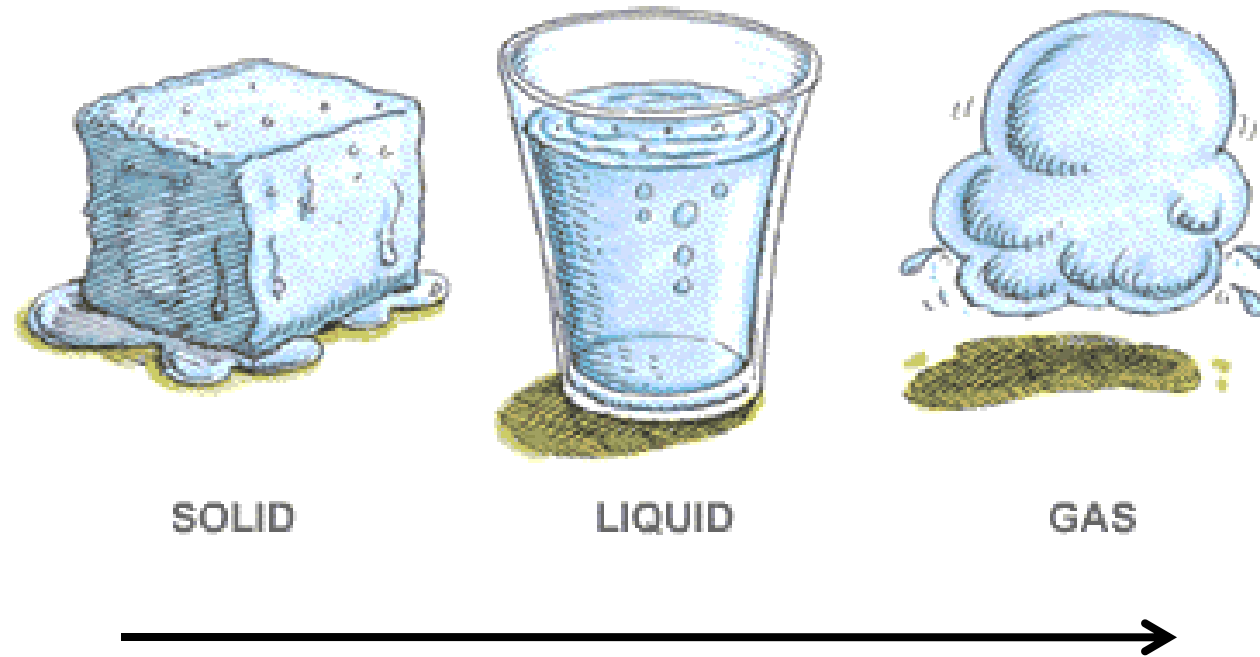
At each level of complexity, entirely new properties appear.>>

Anderson

Science 177, 4047 (1972)

New phenomena due to the interactions between particles

# Phase transitions



Temperature

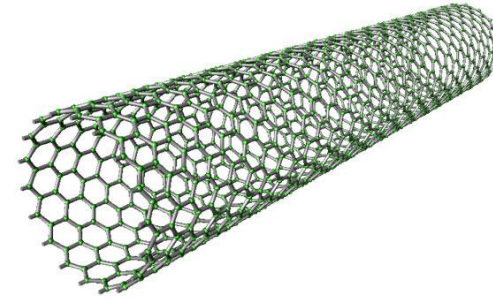
Changes also as a function of pressure ...

Posibility of detecting but also of controlling the state of the system

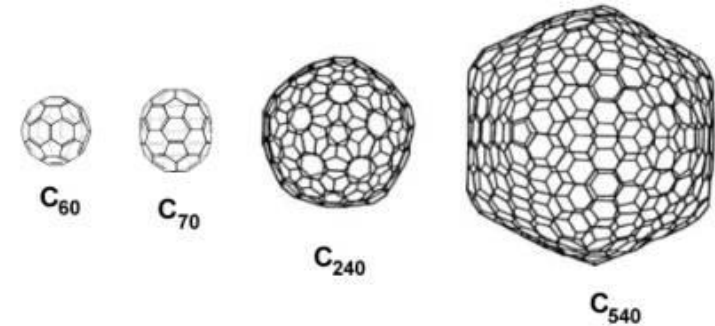
# Crystalline order in solids



©Itub



Molecules

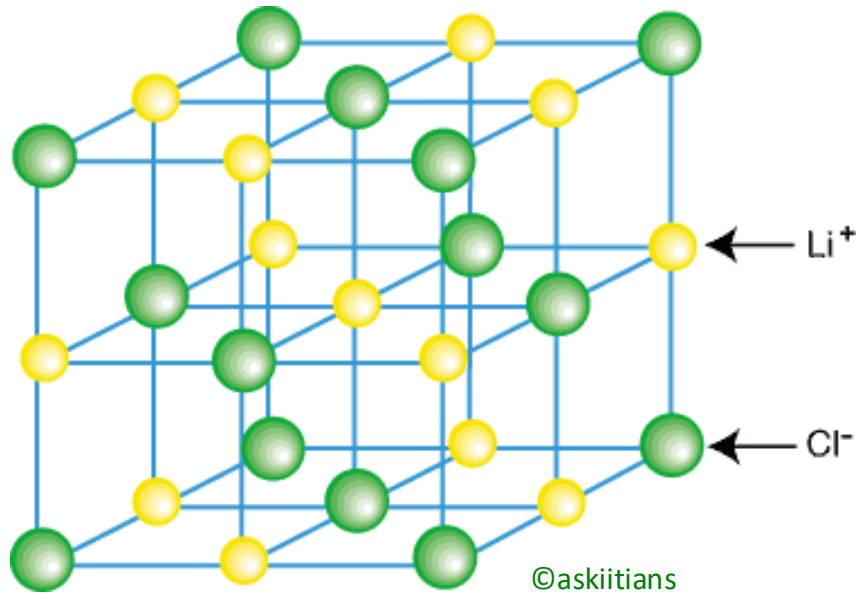


©Fig:web Belén Garrido

Symmetry breaking (translational symmetry), long-range order: ordered phases

# Ordered phases and symmetry breaking

Translational symmetry breaking  
(solid)

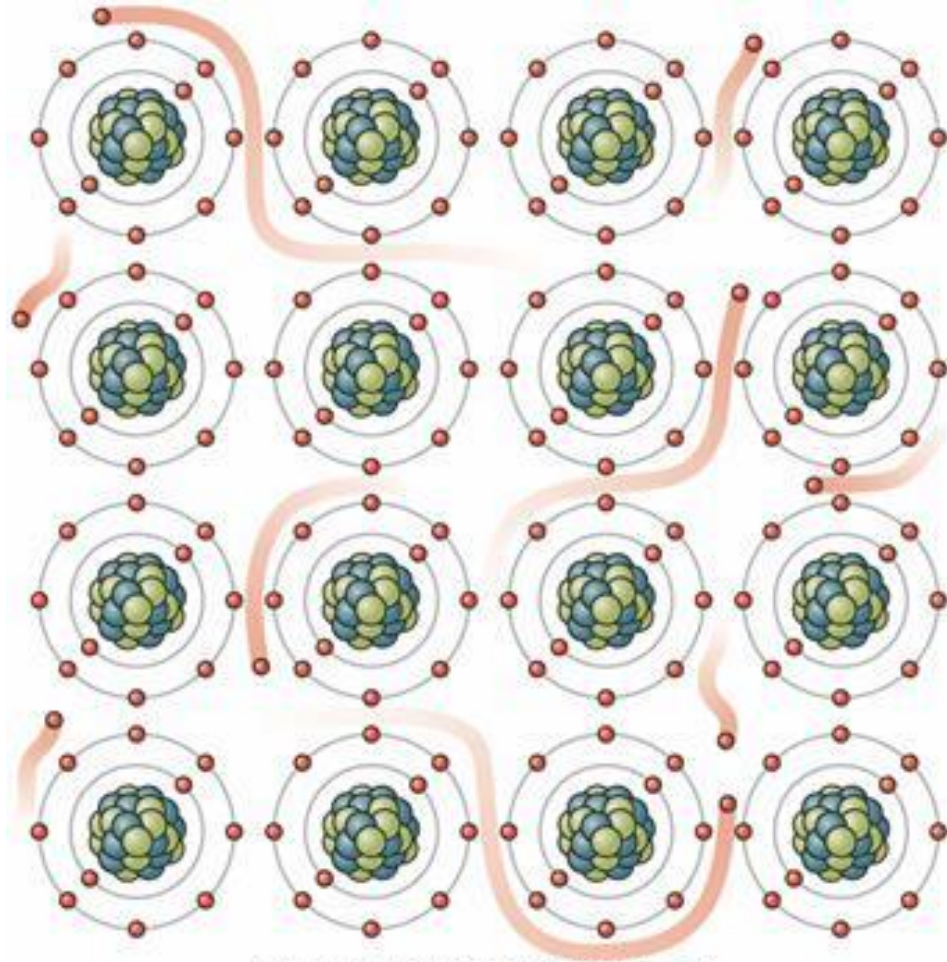


Rotational symmetry breaking  
(nematic liquid crystal)



Different symmetries that can be broken

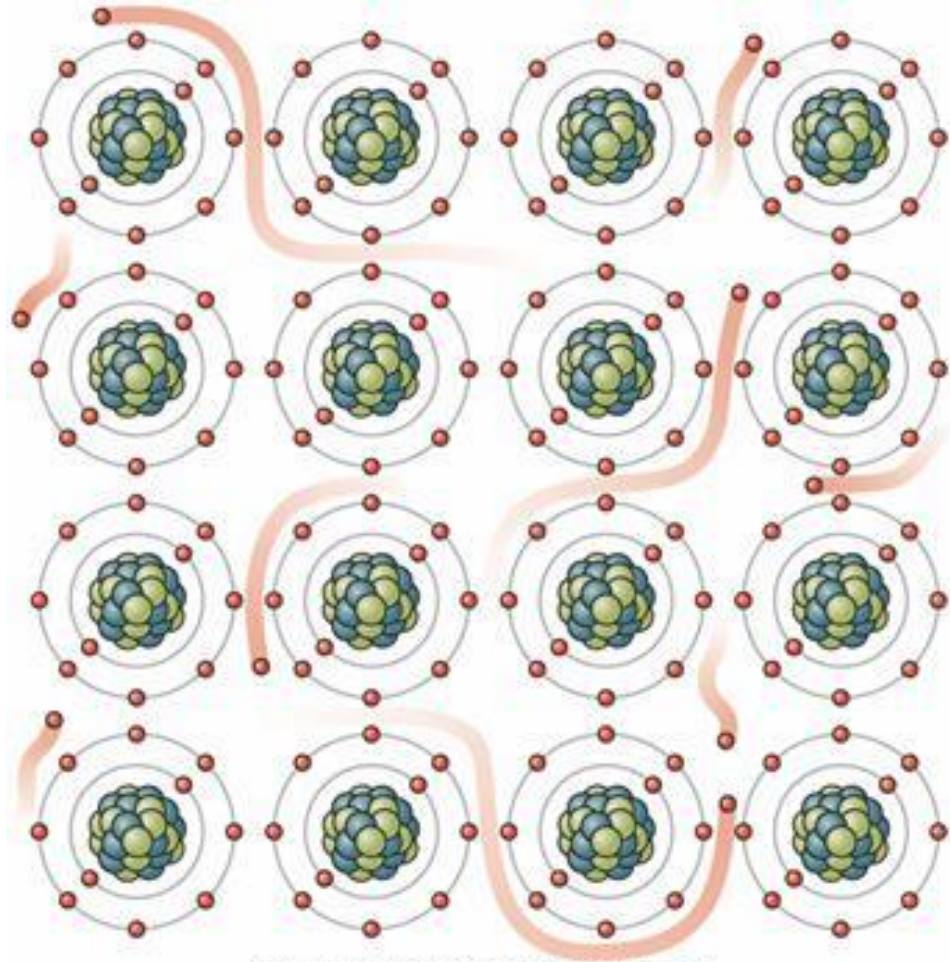
# Emergence of quantum phases in novel materials



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Electrons interact among them  
and with the environment

# Electronic correlations: The difficulty of the many body problem



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Electrons interact among them  
and with the environment

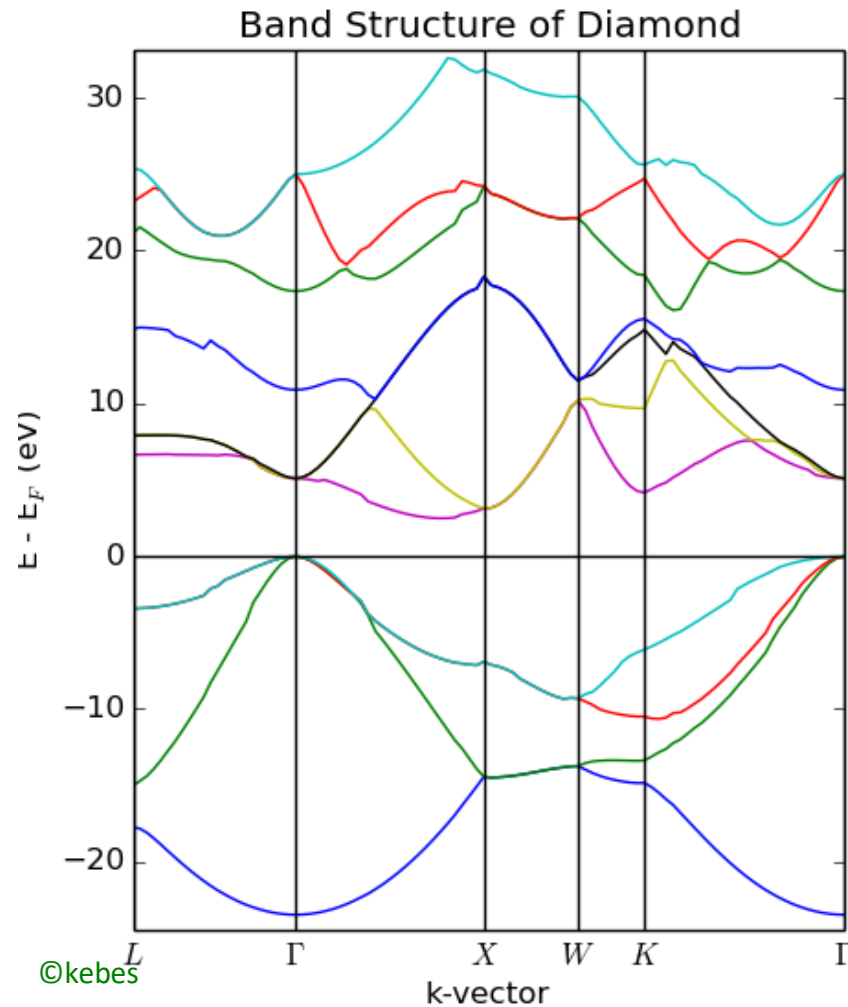
→  $\sim 10^{23}$  electrons/cm<sup>3</sup>

Very few problems involving interacting  
electrons, even starting from approximations,  
can be solved exactly, most of them in 1D



Effective descriptions, models, techniques  
and concepts to capture the essence

# Band theory: the basis of our understanding of solids



Bloch states: electronic bands

Band structure  $E(k)$

The electron moves in the average periodic potential of the solid

Density Functional Theory:  
Ability to calculate the bands

# Band theory: the basis of our understanding of solids

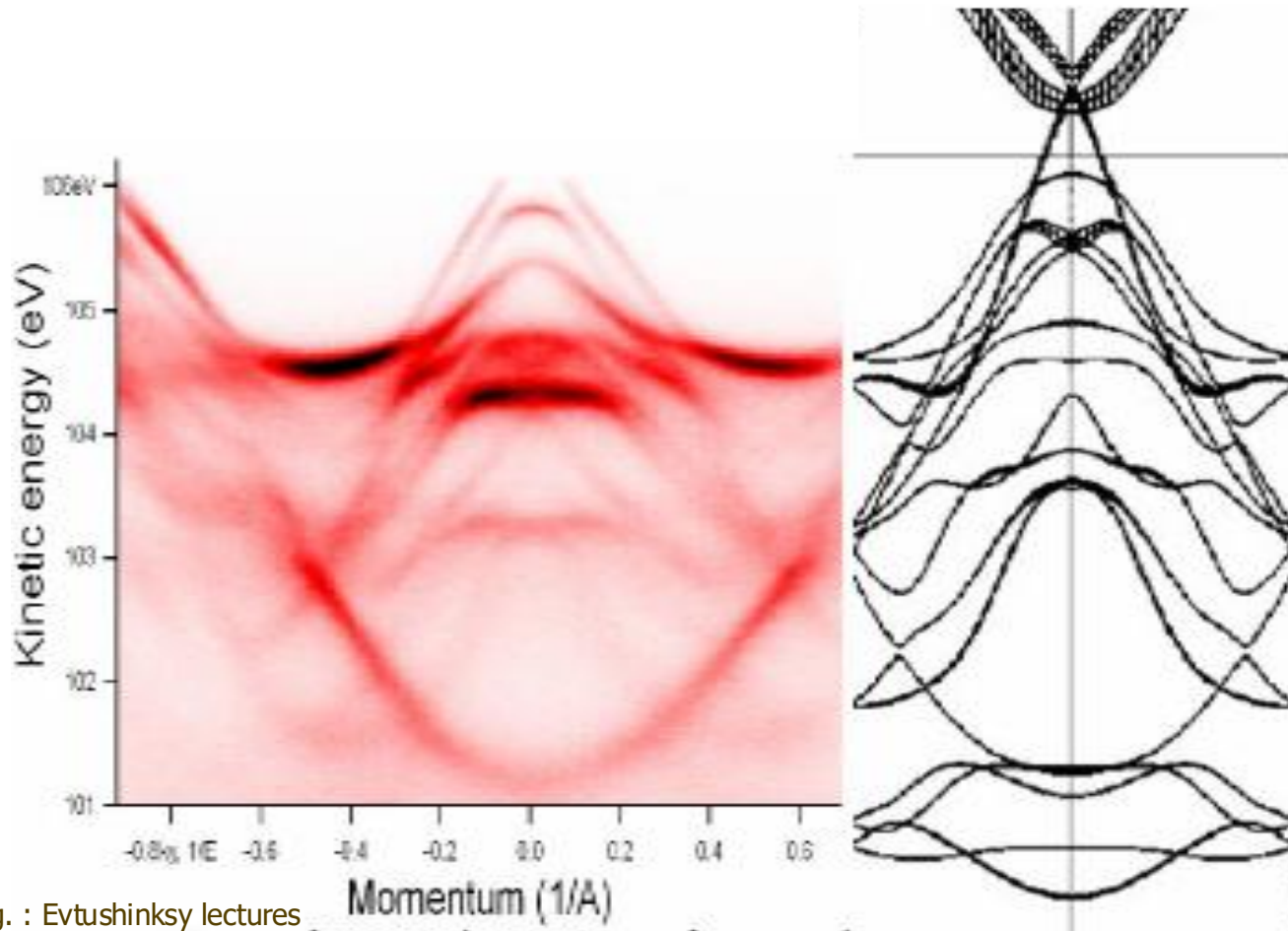
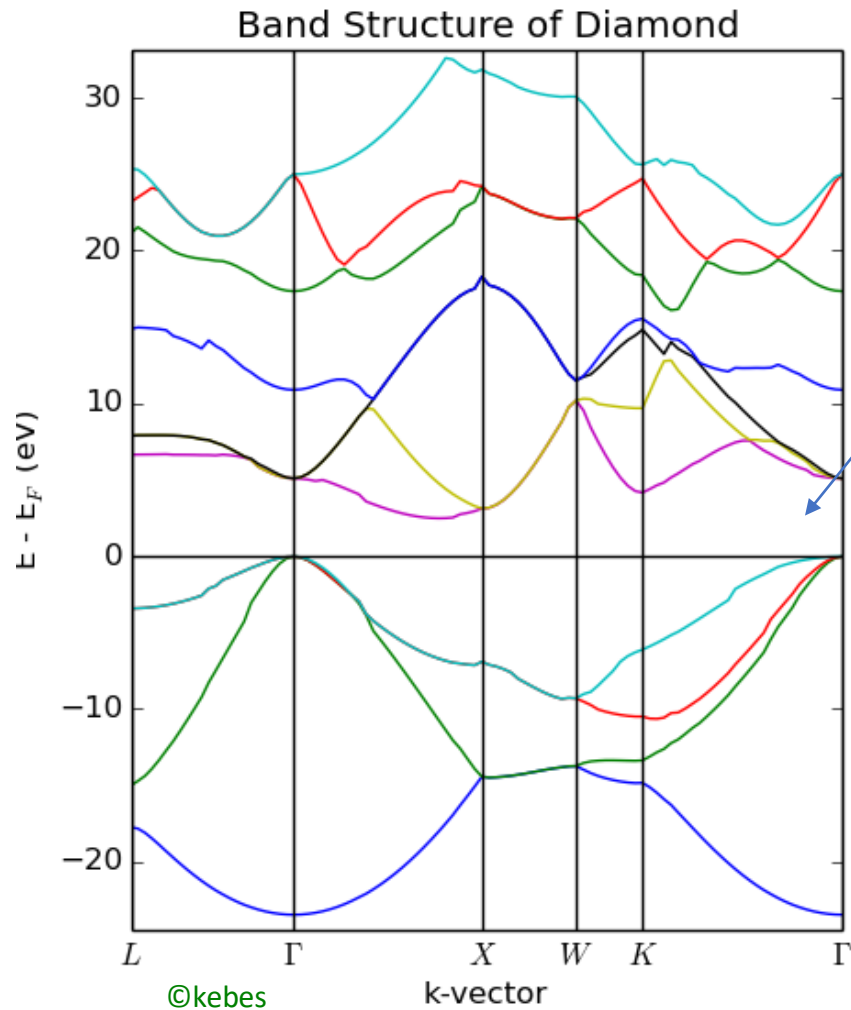


Fig. : Evtushinsky lectures

The bandstructure can be measured Experimentally with probes such as angle resolved photoemission (ARPES) and compared to theoretical predictions

# Band theory: the basis of our understanding of solids



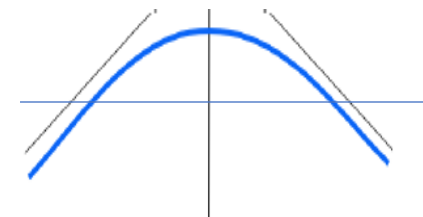
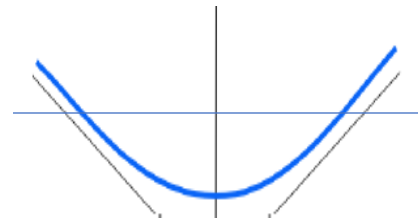
Metals and insulators

- Doping with electrons or holes (shift of chemical potential and filling)

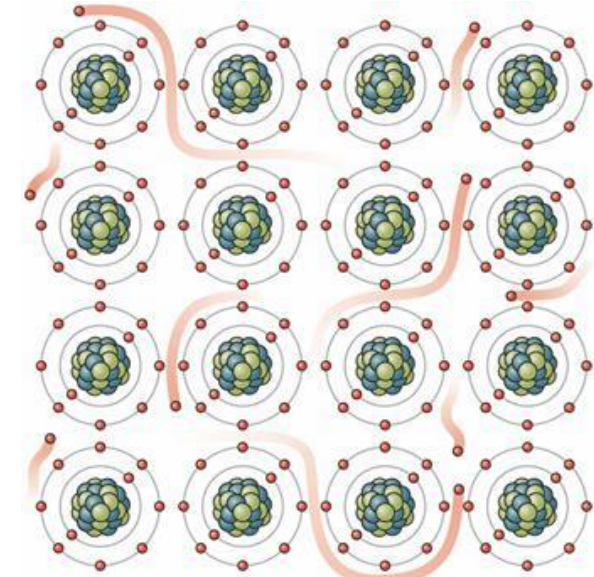
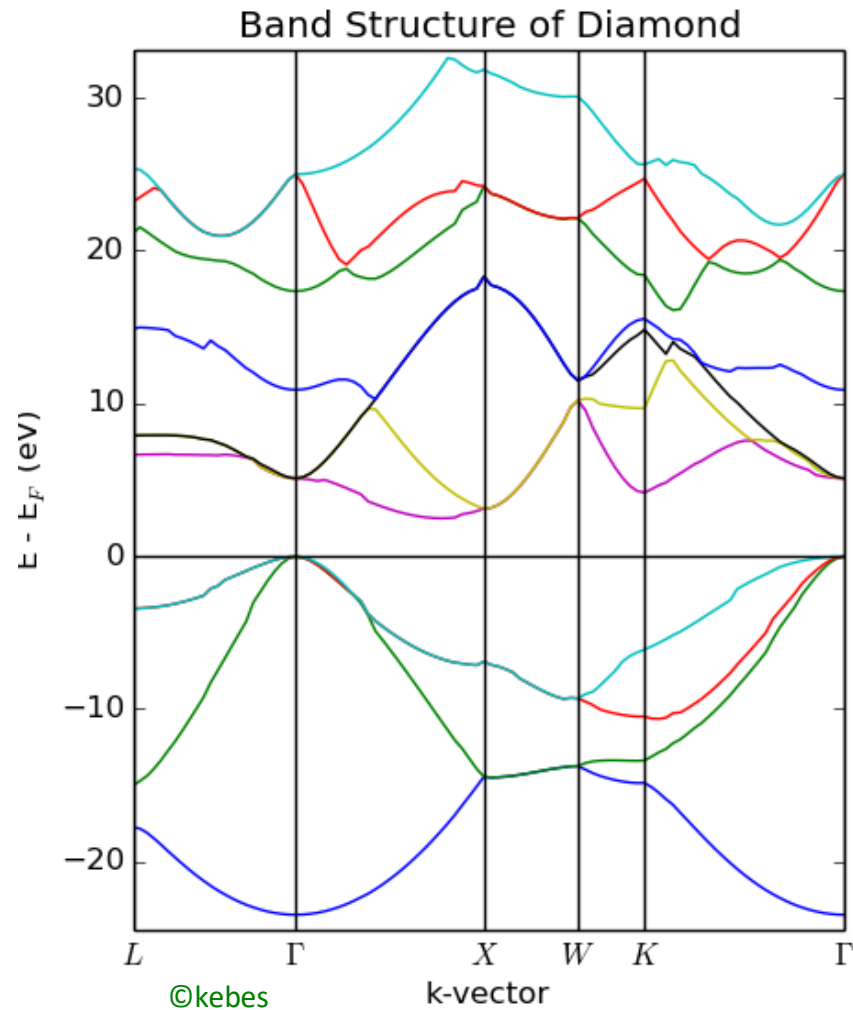
Conduction band

Valence band

- Electron or hole band



# Band theory: an “effective non-interacting” description

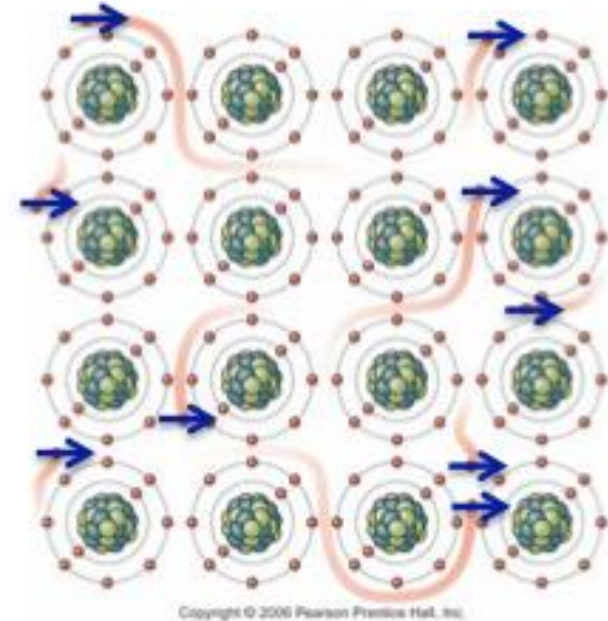
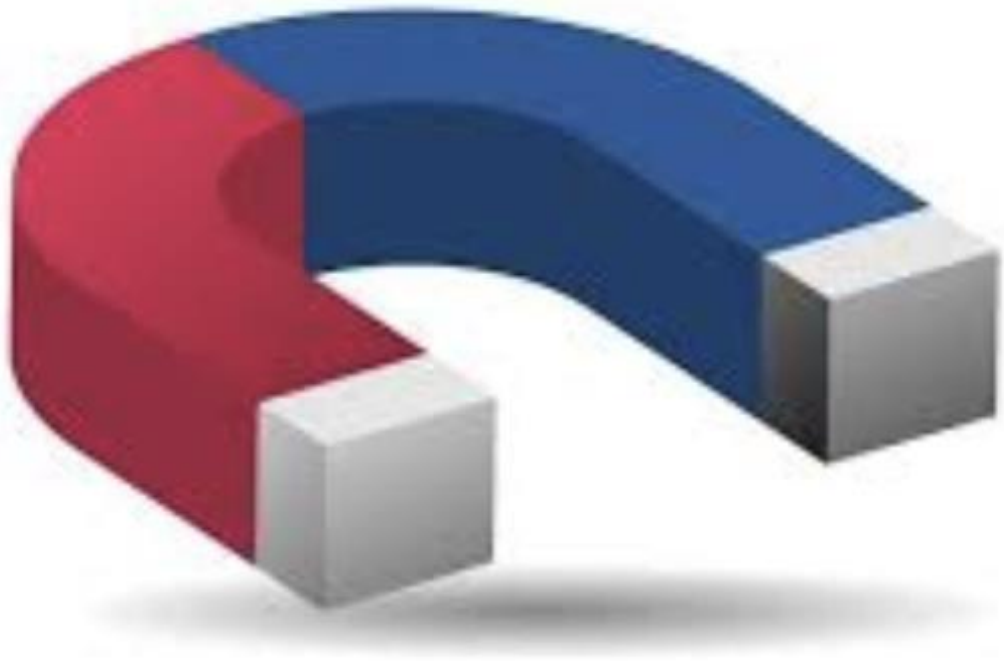


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## Bandstructure:

Effective “independent” electronic states including in an effective way the symmetry of the lattice and the interactions of the electron with the atomic lattice and with other electrons.

# Electronic phases: symmetry breaking



## Ferromagnetism:

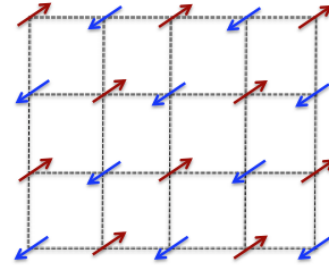
Spin order

It does not require lattice symmetry breaking

# Electronic phases which break lattice symmetry

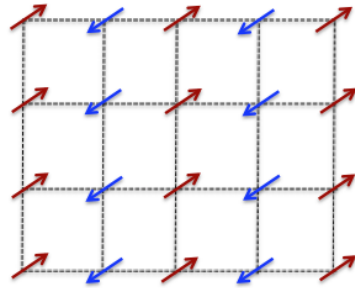
## Spin Order

Lattice translational symmetry broken  
(density waves)



Neel  
antiferromagnet

Lattice translational and rotational symmetry broken  
(stripe-like phases)

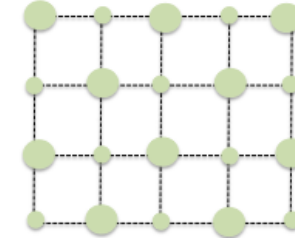


Stripe  
antiferromagnet

Lattice rotational symmetry broken  
(nematic states)

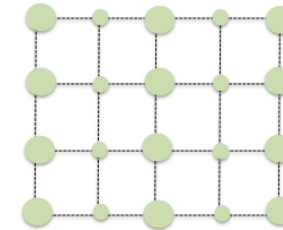
Spin nematic

## Charge Order

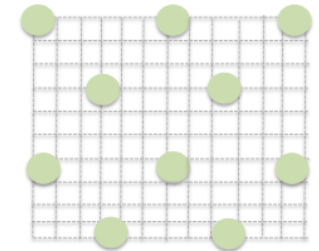


Charge  
density wave

Charge stripes

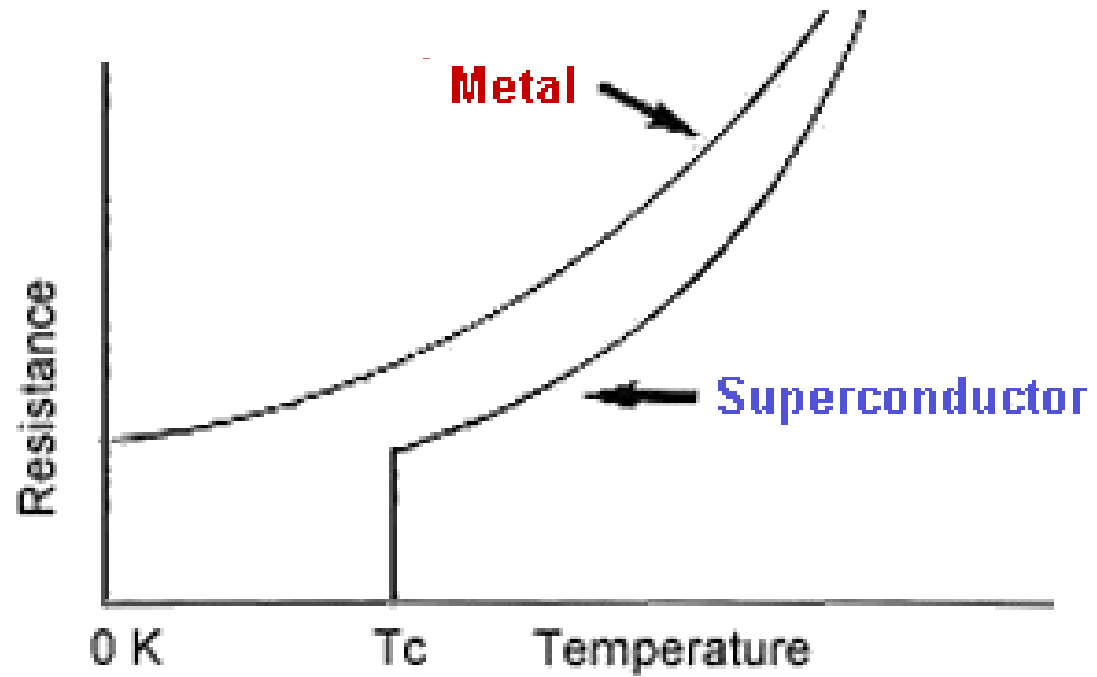


Wigner crystal



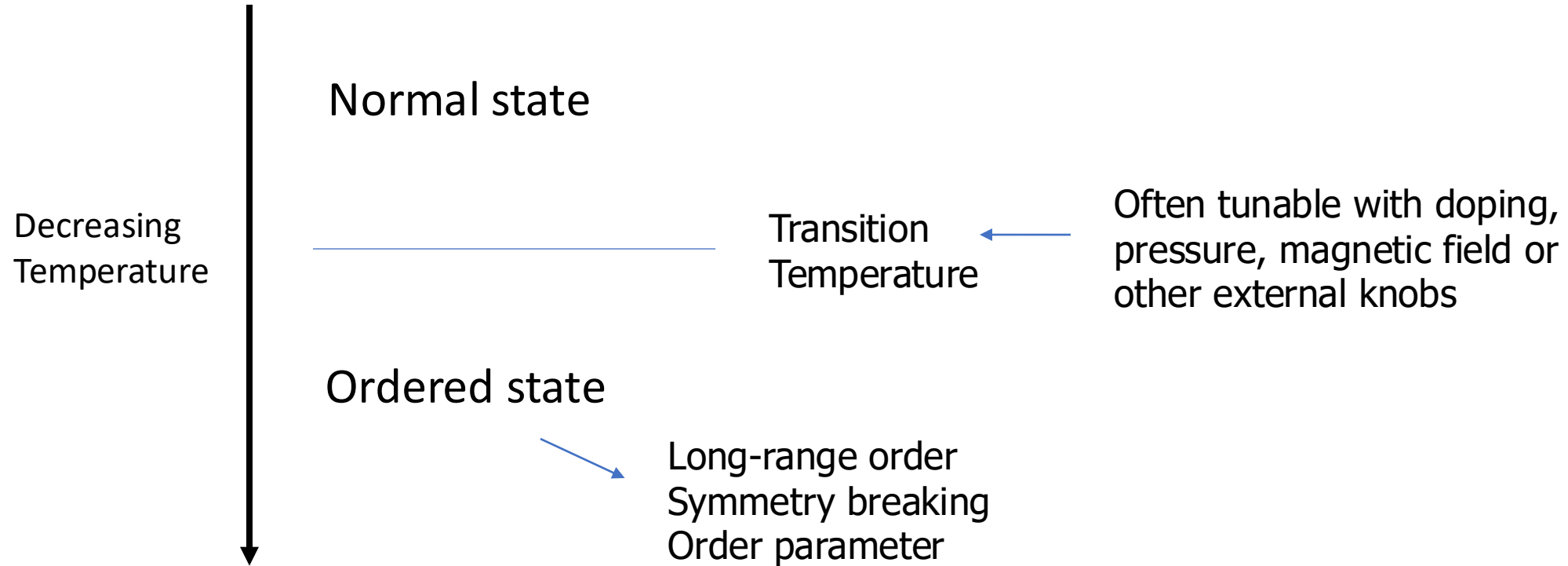
Charge nematic

# Superconductivity



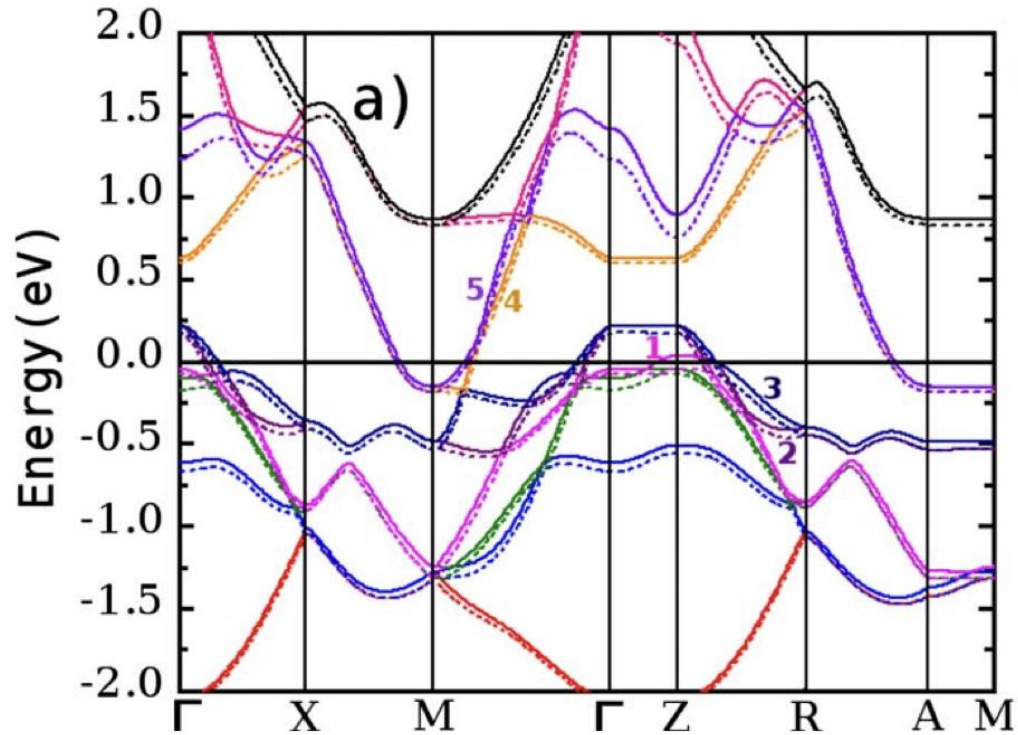
Breaking of gauge symmetry

# Normal vs ordered state

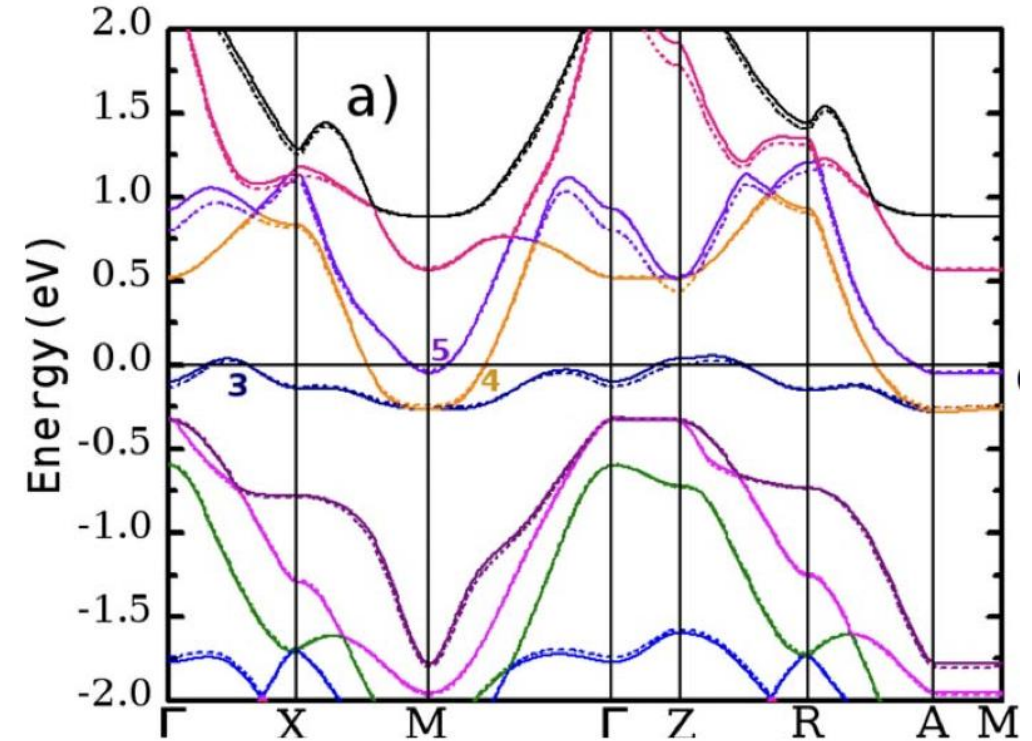


# Band structure in normal vs ordered state.

Non-ordered "normal" state



Symmetry breaking:  
ordered state at low temperature



Ma & Lu, PRB 78, 033111 (2008)

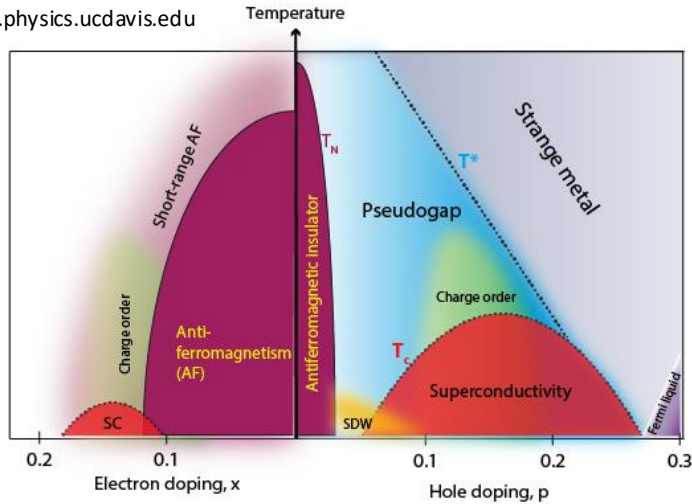
Band structure  $E(k)$

Is it  $E(k)$  always well defined? How good are DFT-like and static mean field descriptions?  
Why and when does band theory work?

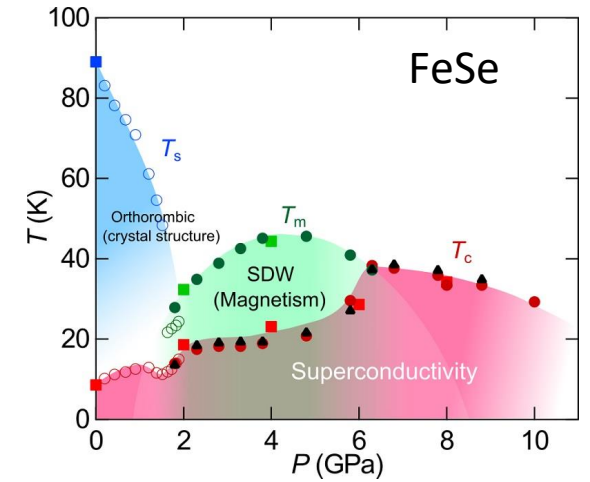
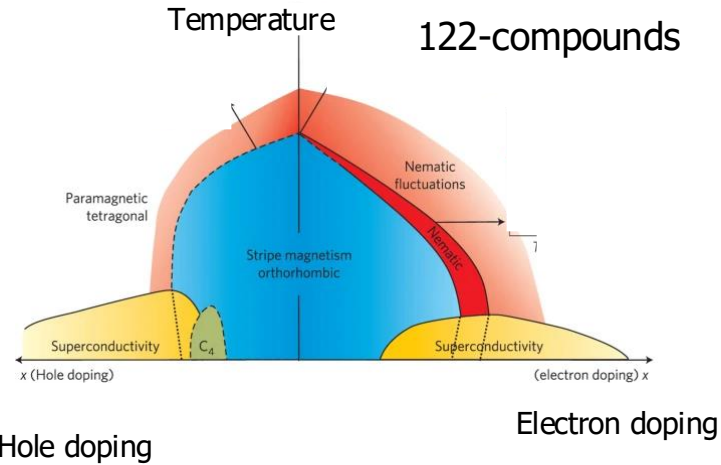
# Strongly correlated electron systems: complex phase diagrams

## High-Tc superconducting cuprates

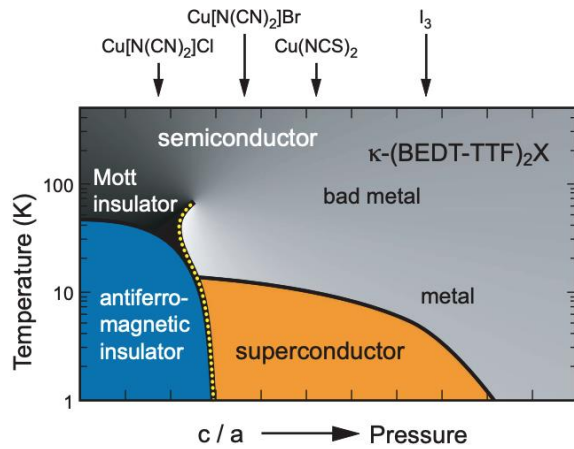
Fig: cme.physics.ucdavis.edu



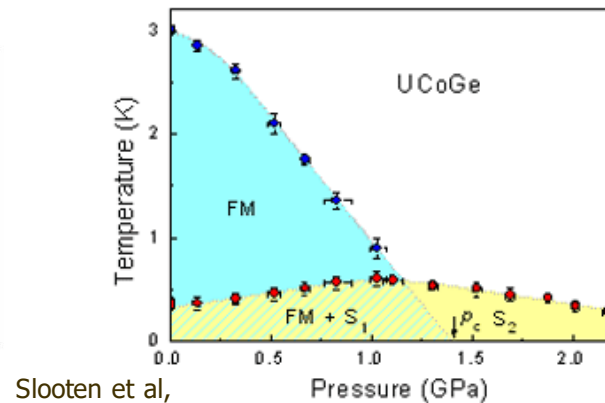
## Iron superconductors



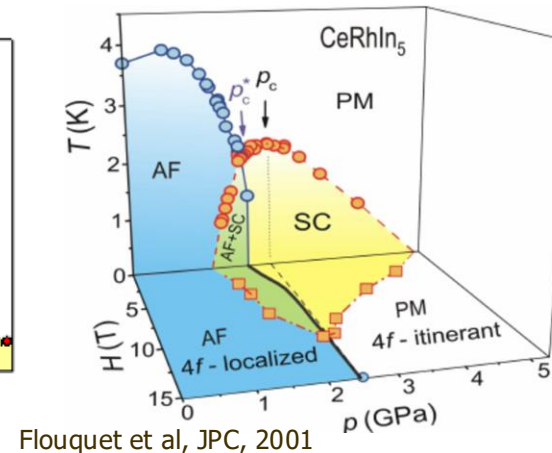
## Organic superconductors



## Heavy fermion compounds

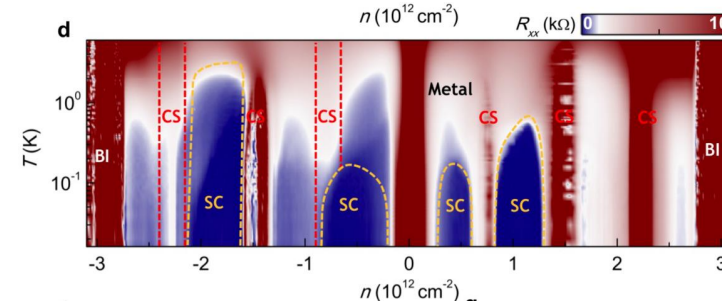


Slooten et al,  
PRL 103 , 097003(2009)



Flouquet et al, JPC, 2001

## Twisted bilayer graphene



# The “normal” state of strongly correlated systems

When the band picture does not work so well

## Weakly correlated system

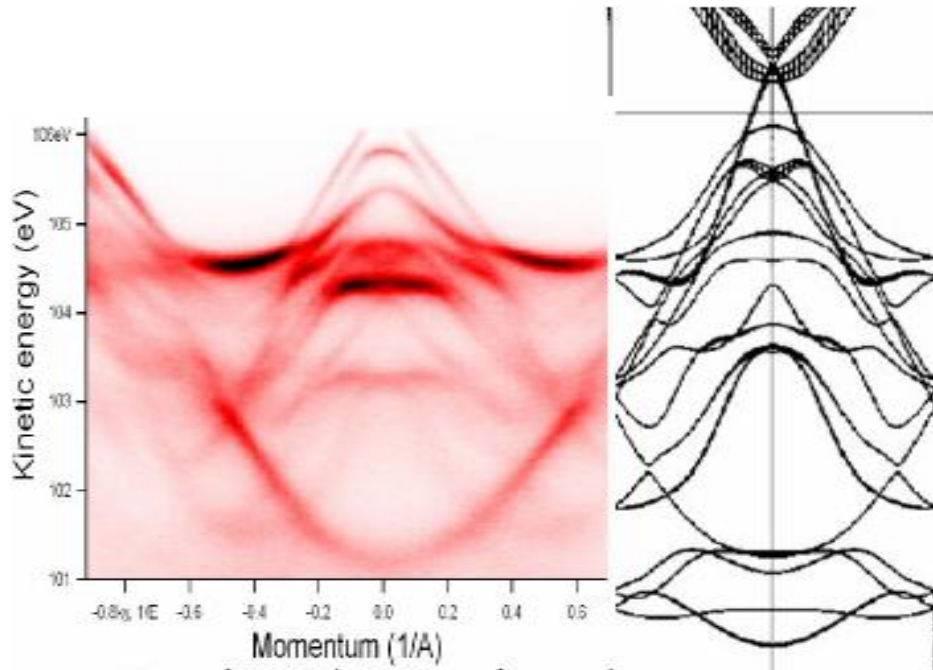


Fig. : Evtushinsky lectures

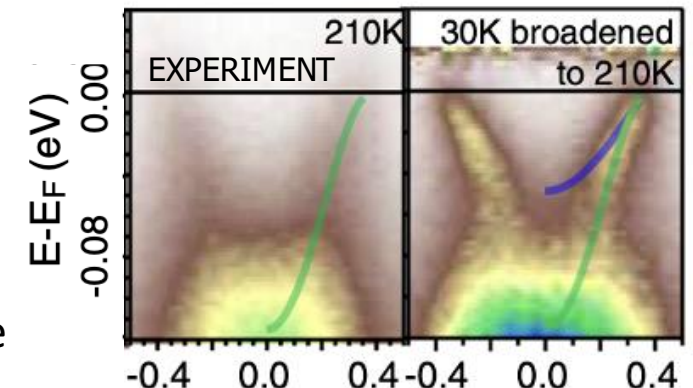
## Strongly correlated system

Not just ordered phases and symmetry breaking states

Correlated metals

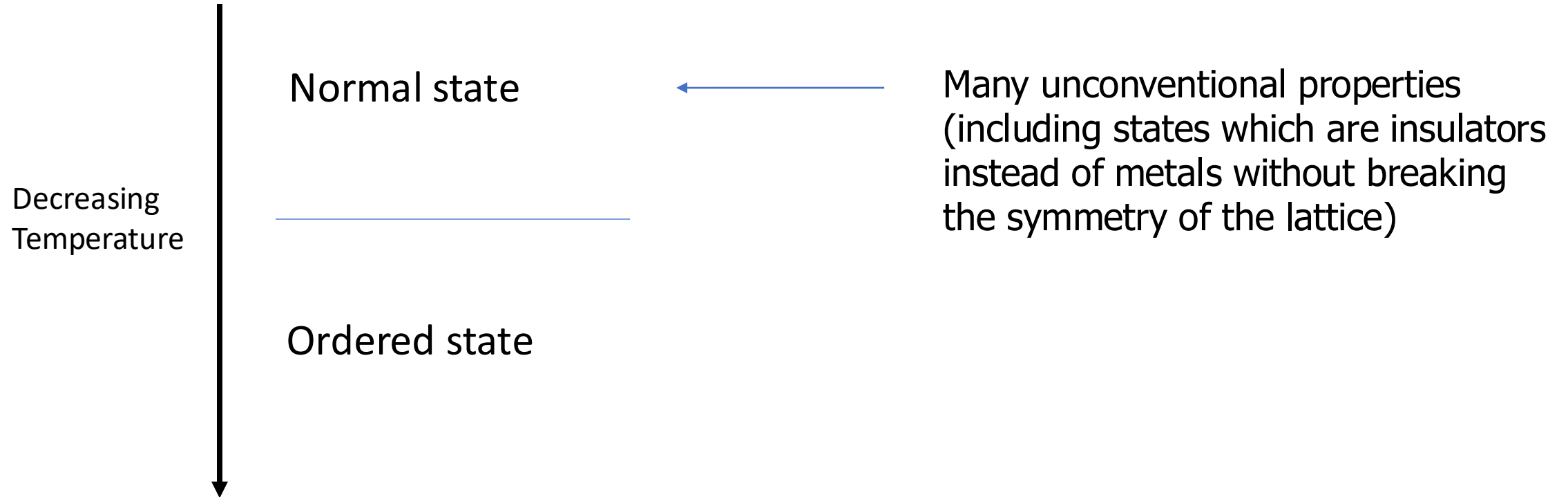
- ❑ Bandwidths which deviate from DFT predictions (larger mass, up to 1000 thousands times larger)
- ❑ Blurred spectrum and anomalous temperature behavior

Iron chalcogenide



PRL 110, 067003 (2013)

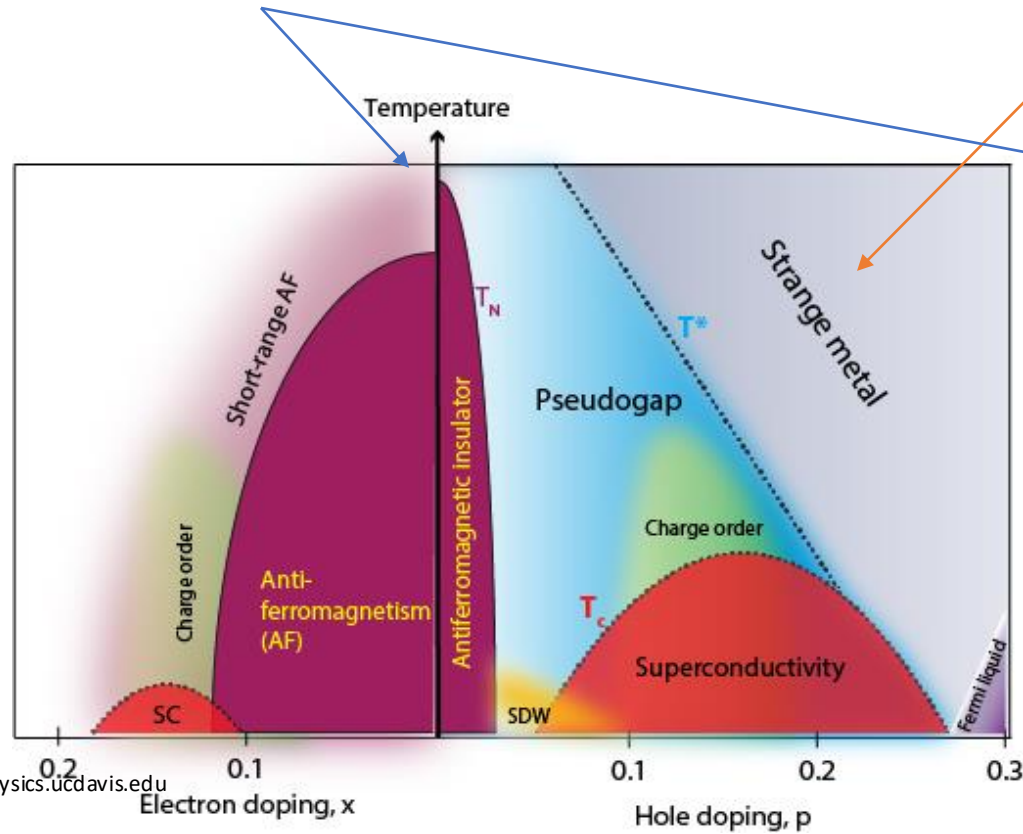
# Strongly correlated metals



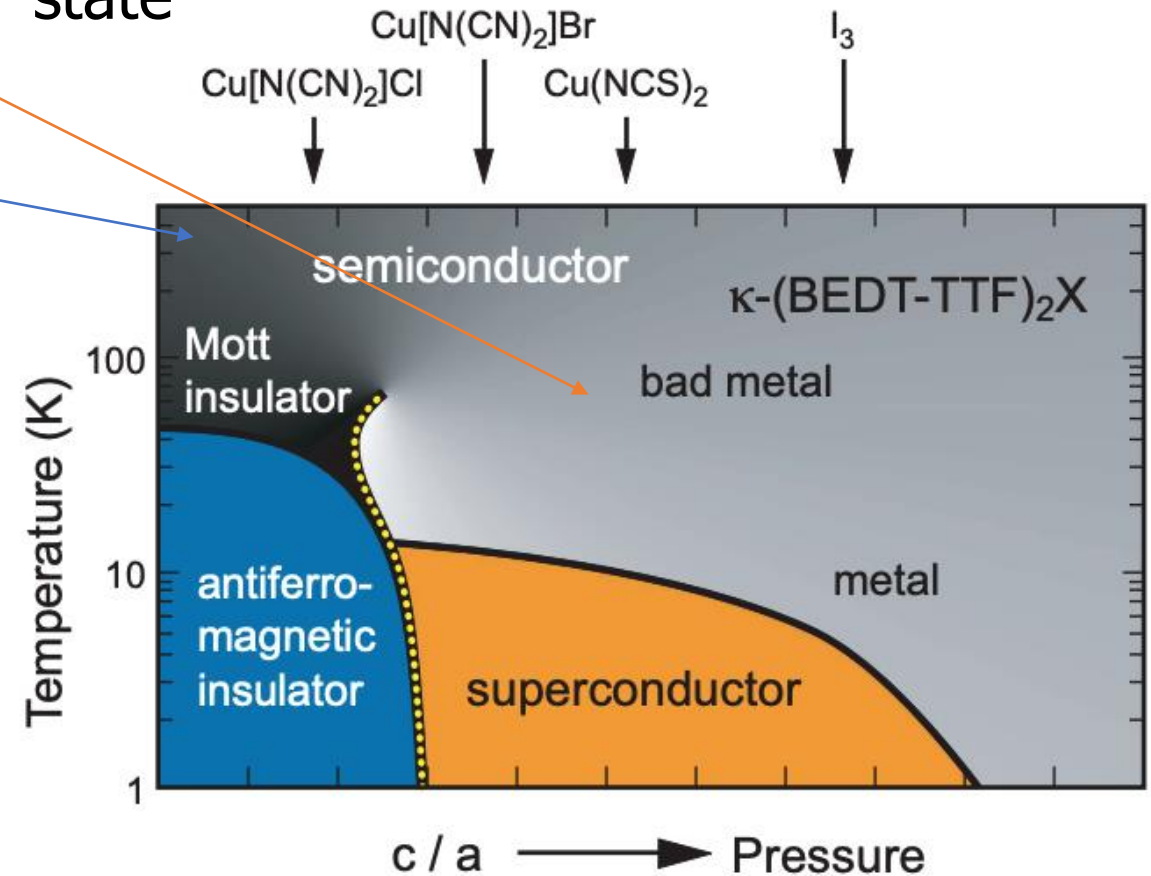
# Strongly correlated metals

Mott insulator

"Normal" state



High- $T_c$  superconducting cuprates

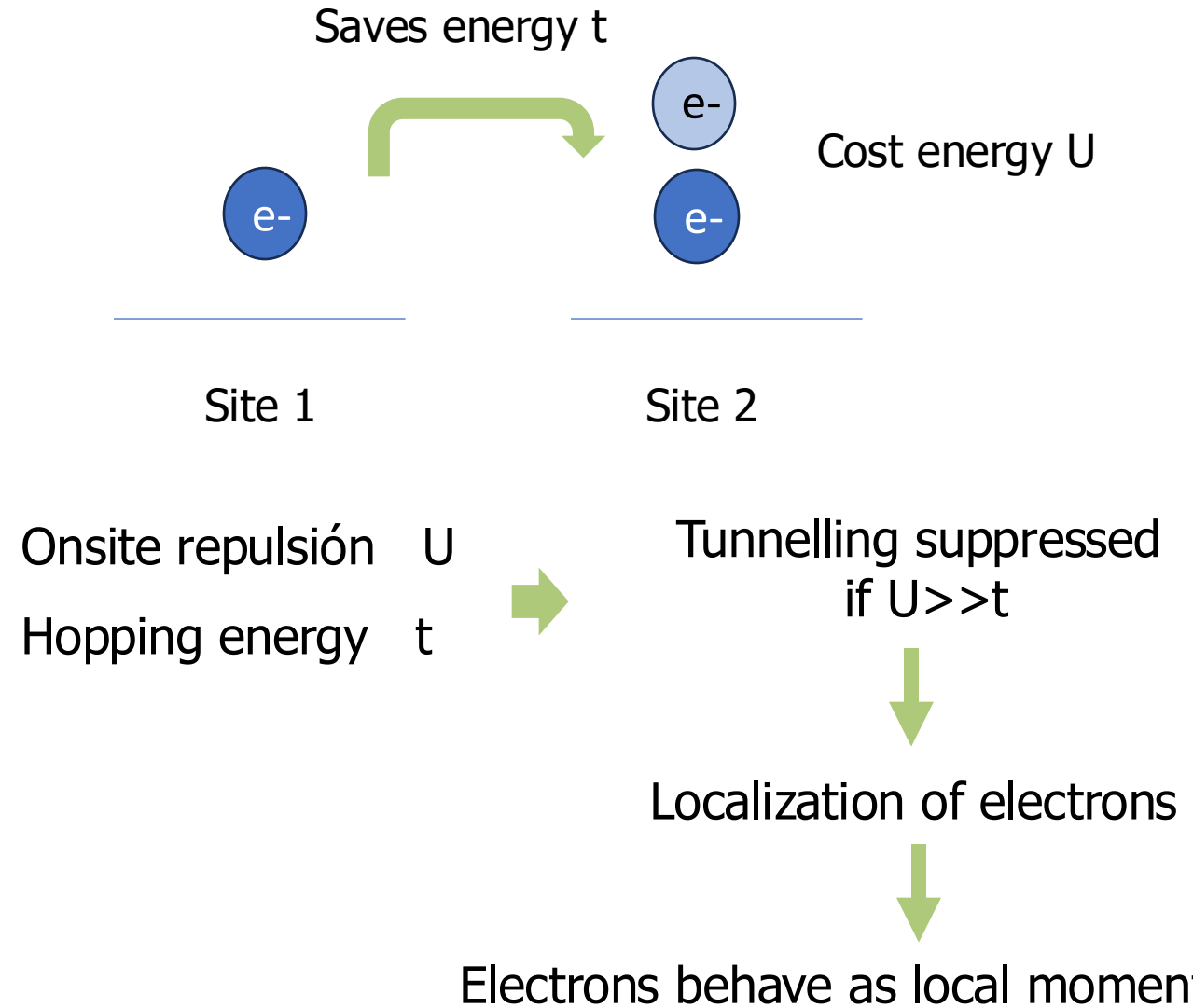
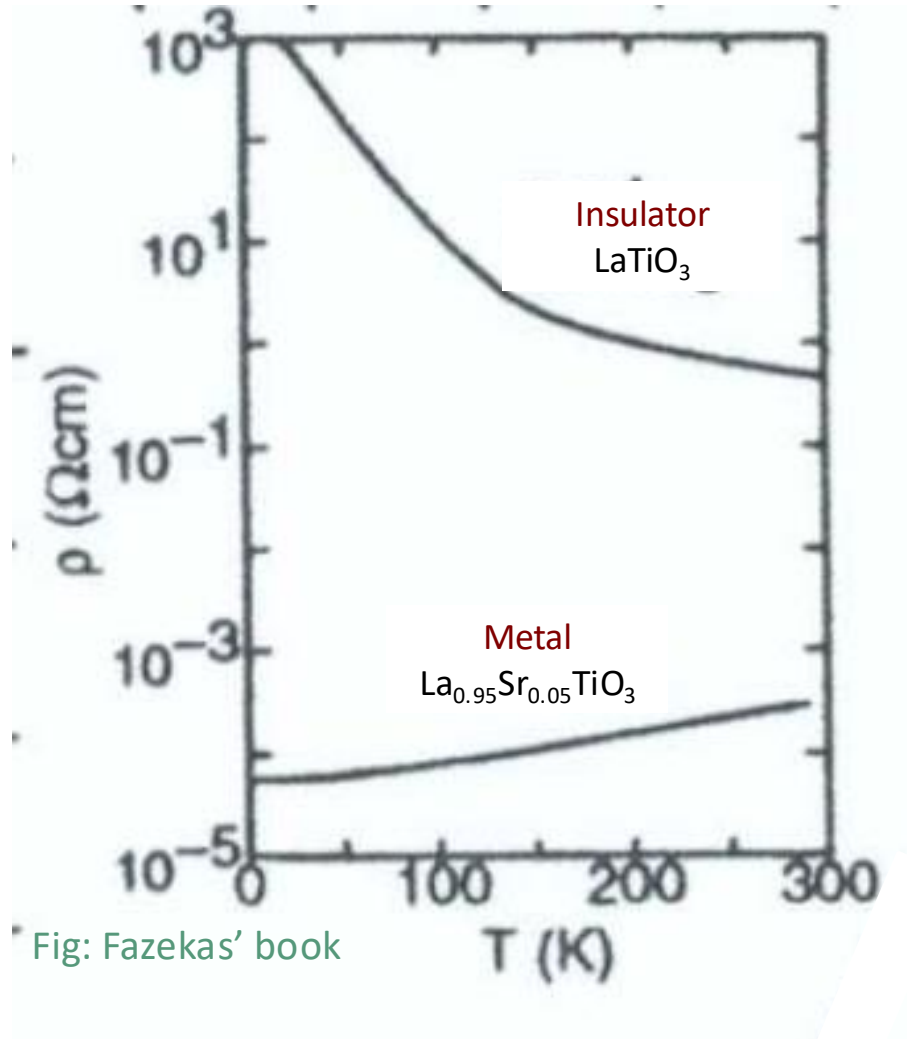


Organic superconductors

Many effects also in the Density of States measured by Scanning Tunnelling microscope (STM), transport, optical conductivity and in other probes

# Mott insulator and local moments

Having a metal when we expect an insulator (even without symmetry breaking)



# Local moments and itinerant electrons

## Weakly correlated system

Itinerant electrons

Momentum-space

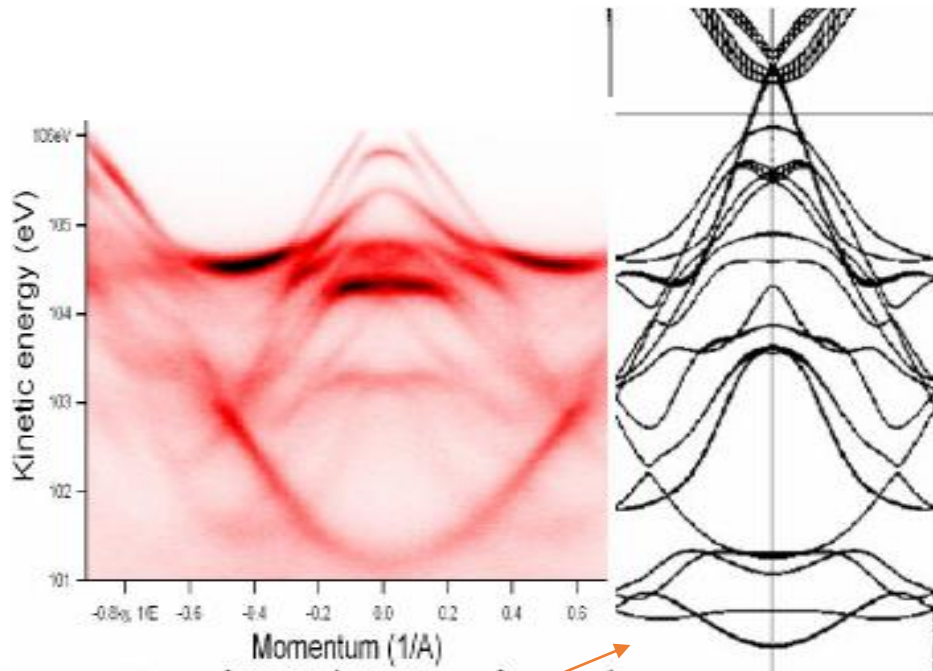


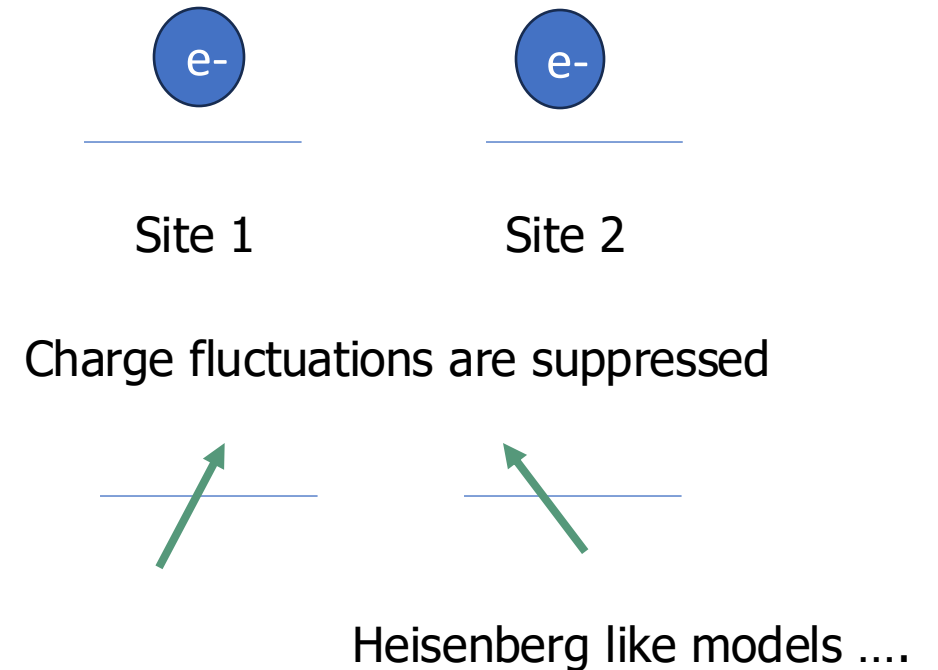
Fig. : Evtushinsky lectures

Band description

## Strongly correlated system

Local moments

Real-space



Strong modification of the spectrum & not always a binary choice:  
Strongly correlated (non-ordered) metals

# When different types of electrons play a role

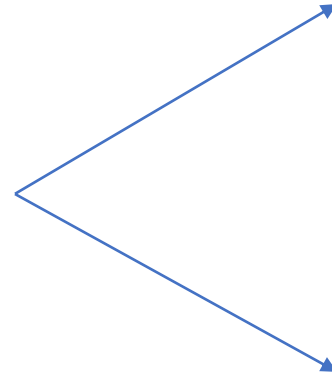
## Itinerant electrons

less correlated (larger kinetic energy  
or smaller interactions)



## Local electrons: local moments

More correlated (smaller kinetic energy  
or larger interactions)



## Kondo effect

Screening of a local moment  
by a bath of itinerant electrons  
(macroscopic measurable effects)

## Heavy fermions

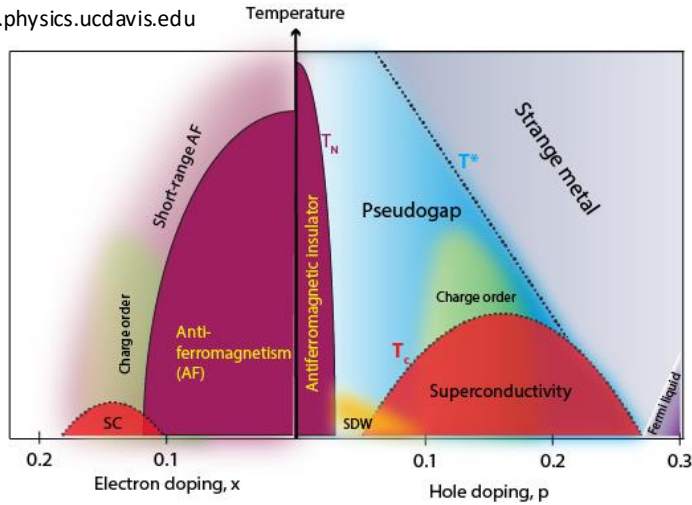
A lattice of local electrons  
coupled through tunneling to  
Itinerant electrons

Also: Hund's physics in multi-orbital systems ...

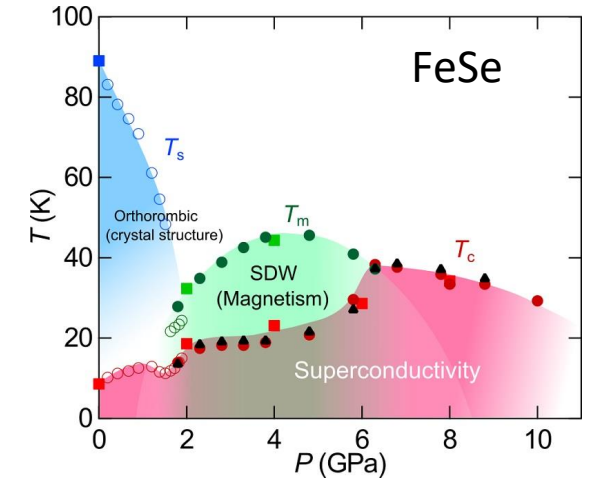
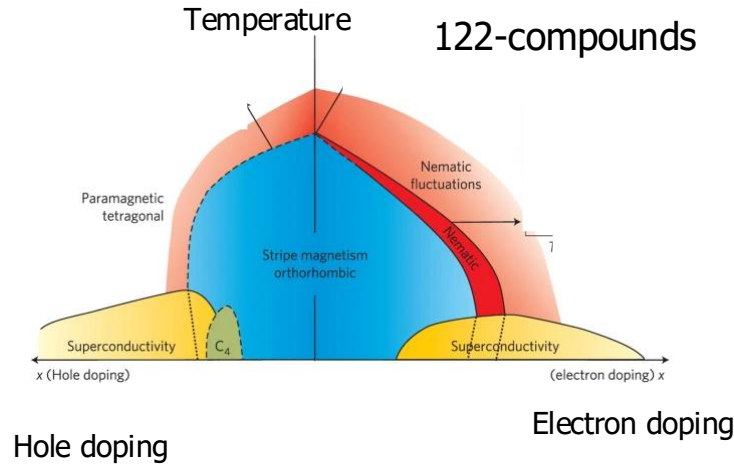
# Superconductivity in strongly correlated electron systems

## High-Tc superconducting cuprates

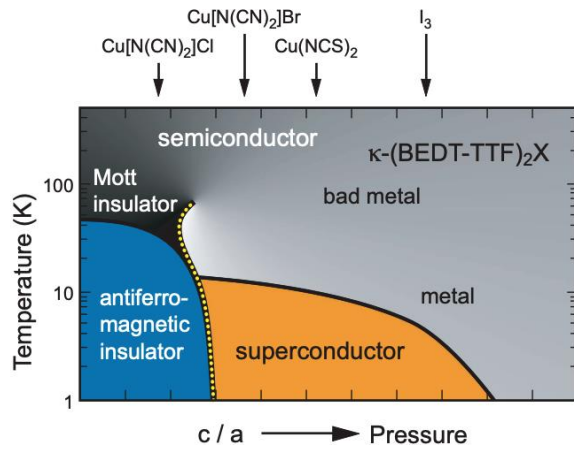
Fig: cme.physics.ucdavis.edu



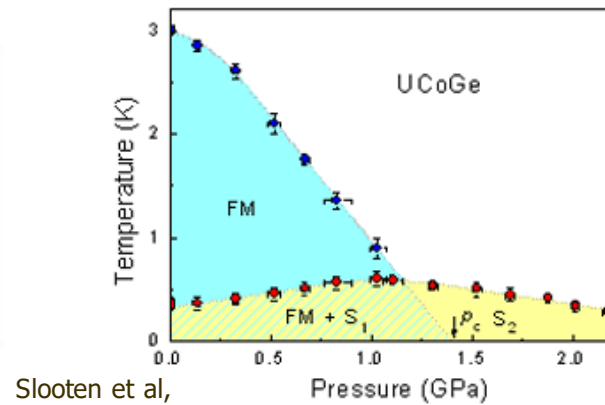
## Iron superconductors



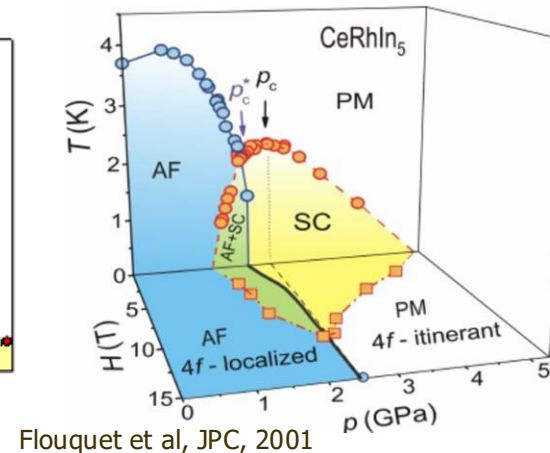
## Organic superconductors



## Heavy fermion compounds

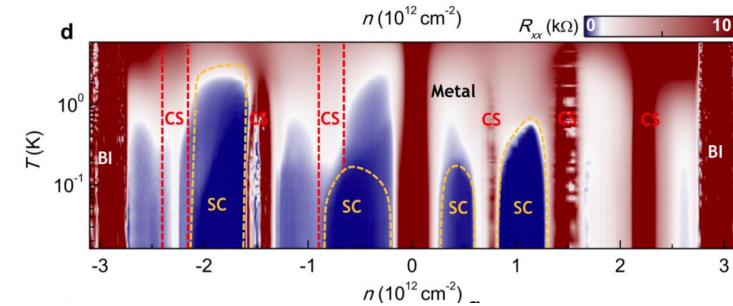


Slooten et al,  
PRL 103 , 097003(2009)



Flouquet et al, JPC, 2001

## Twisted bilayer graphene



Lu et al, Nature 574, 653 (2019)

# From a Mott insulator to high-temperature superconductivity

## High-T<sub>c</sub> superconducting cuprates

Which is the role of Mott (local) physics and strong correlations in high temperature superconductivity?

Which is the best way to describe the system? Local or itinerant?

Many degrees of freedom. Who is in the driver seat?

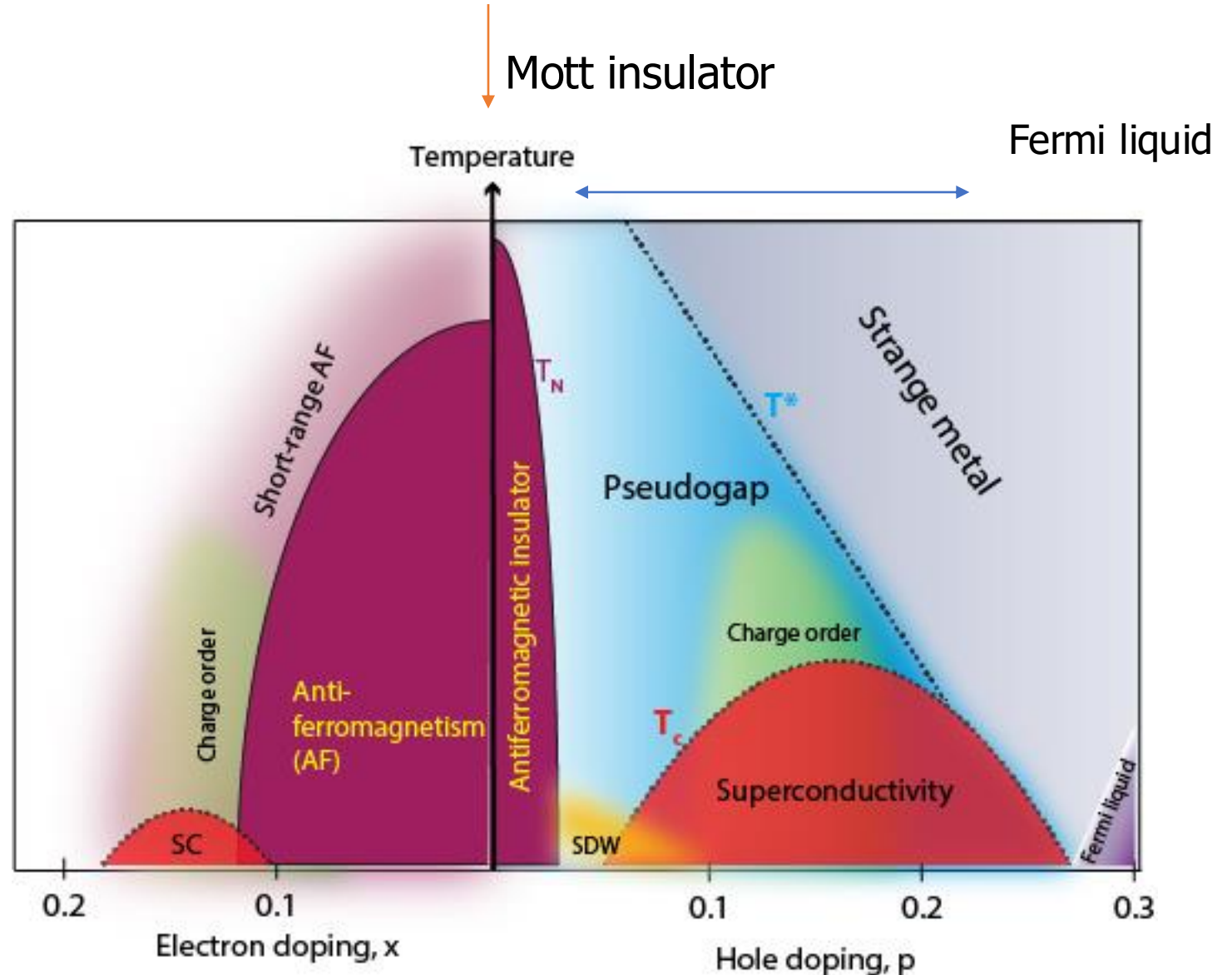
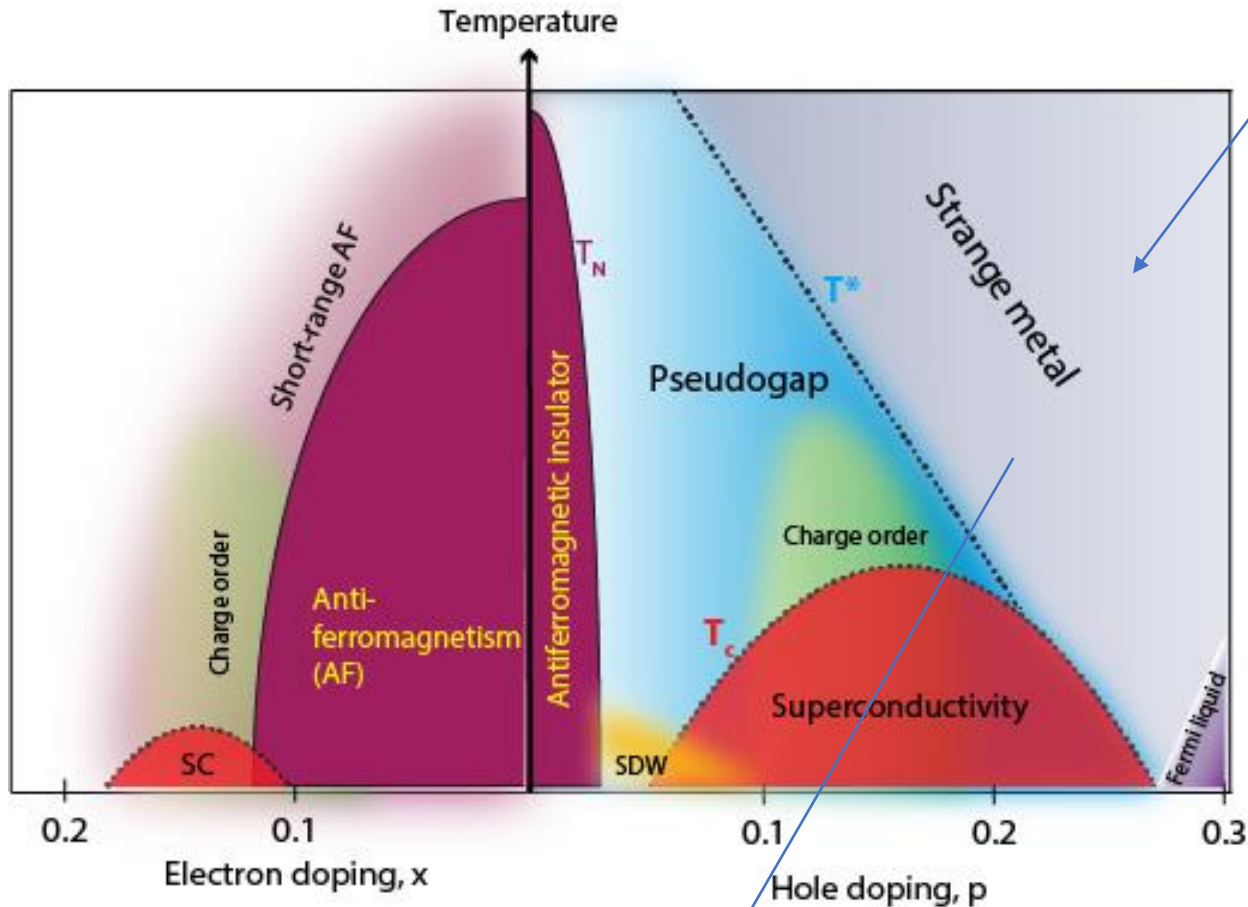


Fig: cme.physics.ucdavis.edu

# Anomalous electronic properties and the concept of quantum materials

## High-Tc superconducting cuprates



Strange metal, distinct from bad metal (high resistivity)

Linear in  $T$  resistivity  
(found in different correlated materials)

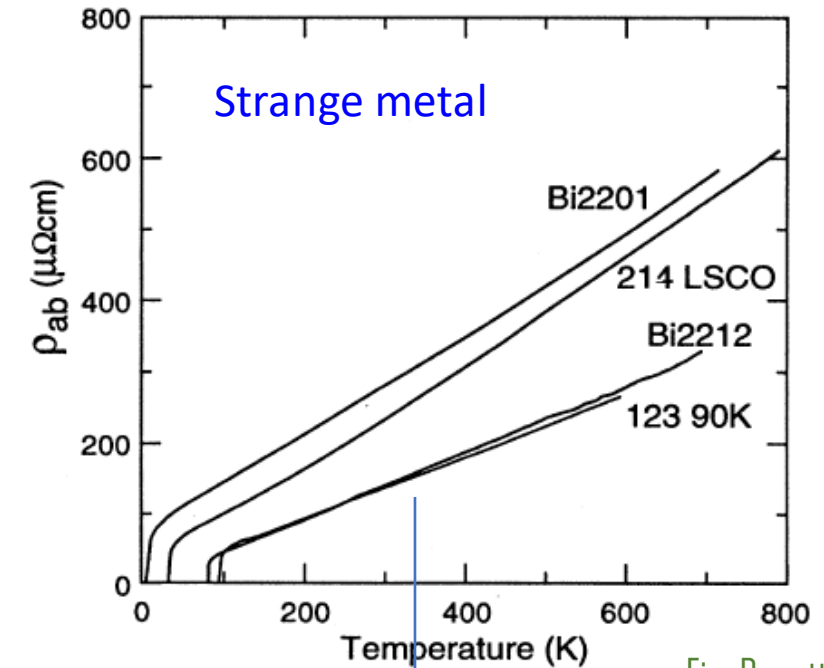


Fig: Dagotto,  
RMP 66, 763 (1993)

Non-Fermi liquid behavior.  
(non-conventional)  
No quasiparticles?  
Low  $T$  limit

# Tuning parameters for correlated states

Interaction energy vs Kinetic energy

ratio  $U/W$  large



Absolute values  
of  $U$ ,  $W$



Temperatures at which  
the correlated states are observed

$U$ : scale of interaction

$W$ : kinetic energy

# Tuning parameters for correlated states

Interaction energy vs Kinetic energy

- ❑ Filling of electronic bands
- ❑ Electronic bands details
- ❑ Dimensionality
- ❑ Crystalline lattice
- ❑ Screening
- ❑ External knobs (pressure, ...)
- ❑ Interaction with lattice
- ❑ Other (spin-orbit, ...)

# Quantum materials: lattice and dimensionality

3 dimensions



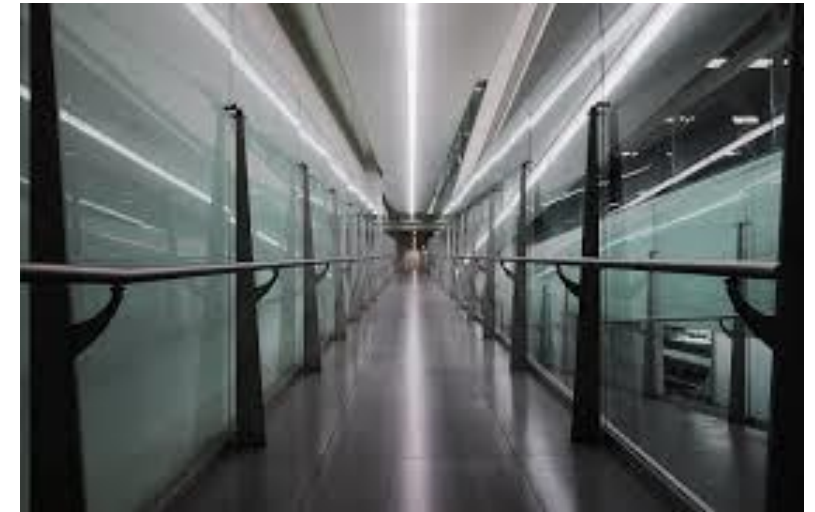
©Michael Paraskevas

2 dimensions



©Sebastian Dubiel

1 dimension

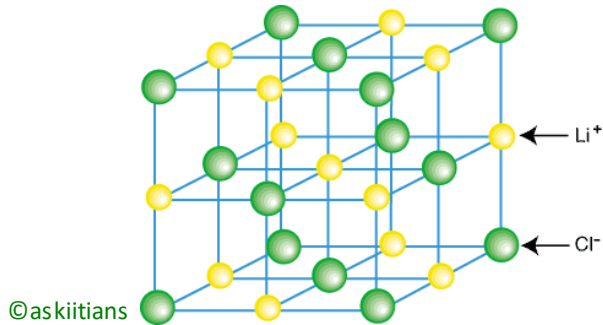


©Carlos Valenzuela

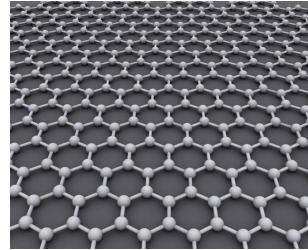
Interactions are never perturbative  
in 1 dimensión, even if  $U$  is small

# Quantum materials: lattice and dimensionality

3 dimensions

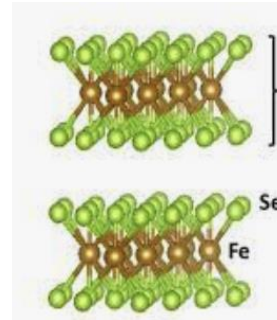
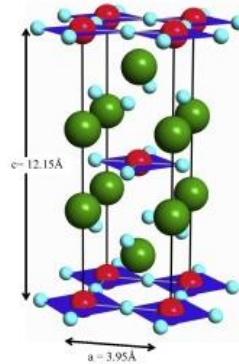


2 dimensions

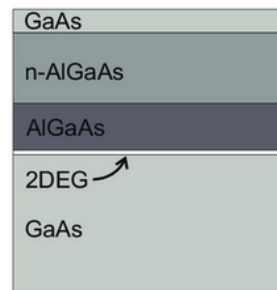


1 or  
few layers

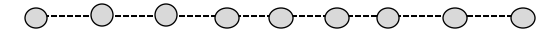
Layered quasi-2d materials



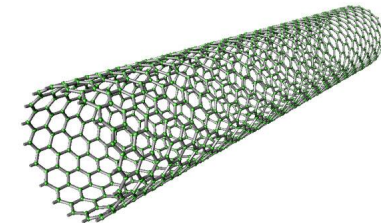
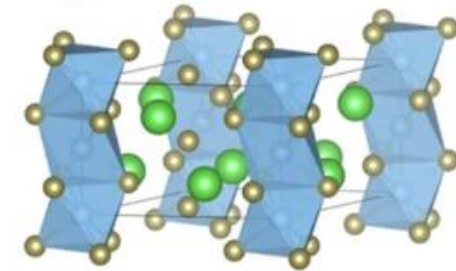
Interfaces



1 dimension



Quasi-1d materials



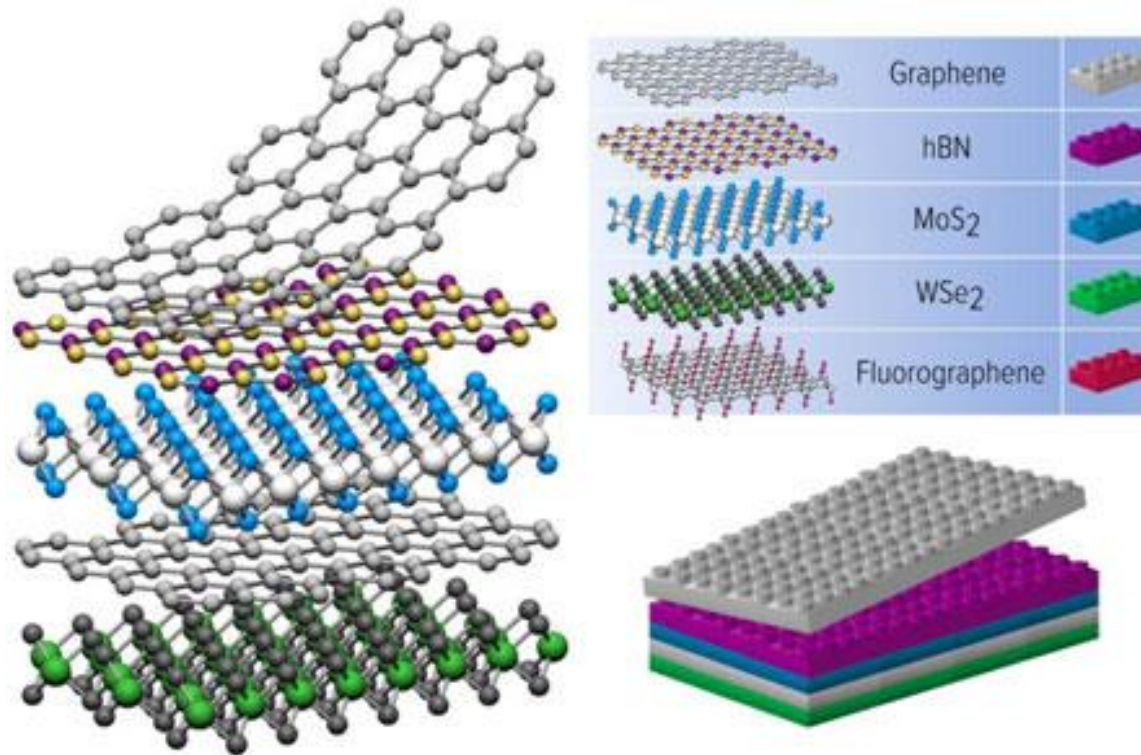
Interactions are never perturbative  
in 1 dimension

Fig: Guzmán-Verri et al,  
Nature 576, 429 (2019)

ABO<sub>3</sub> perovskite

# Engineering 2d materials and heterostructures

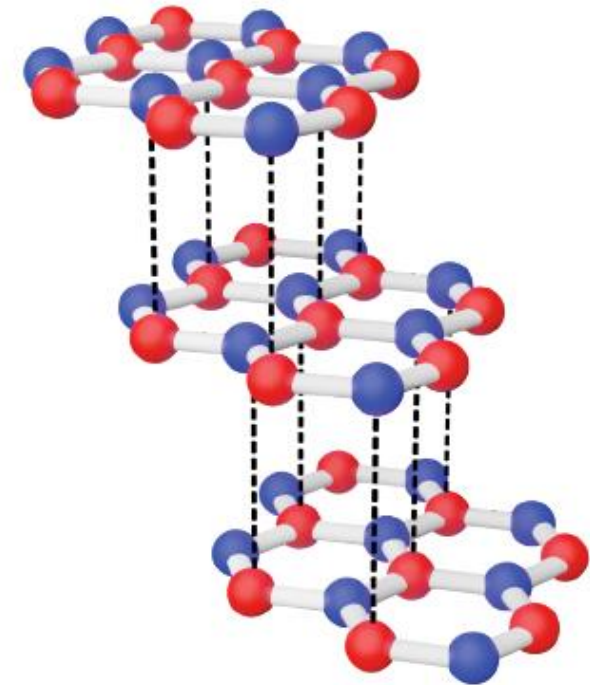
Stacking different 2d materials



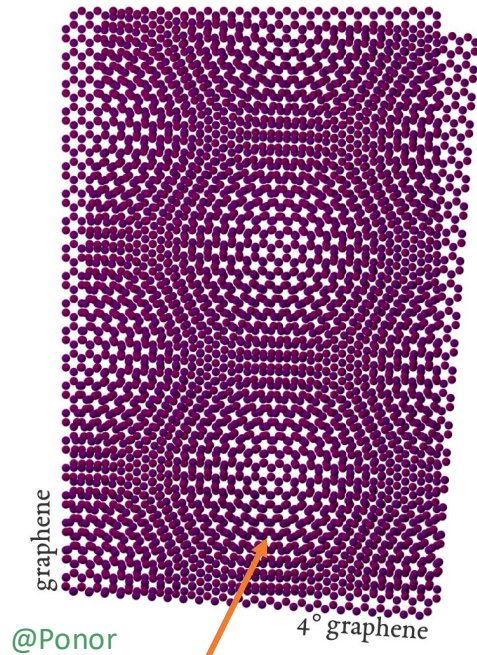
Geim & Grigorieva,  
Nature 499, 419 (2013)

Semimetal, insulating,  
metal, ferromagnetic ...

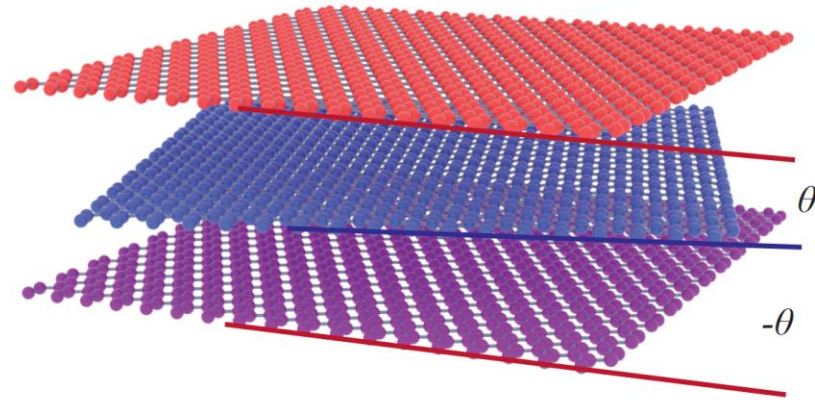
Multilayers with specific stacking



# Engineering 2d moiré heterostructures. Tunability

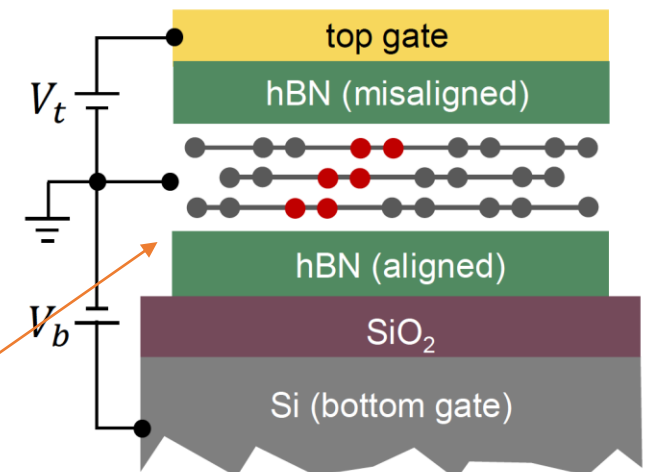
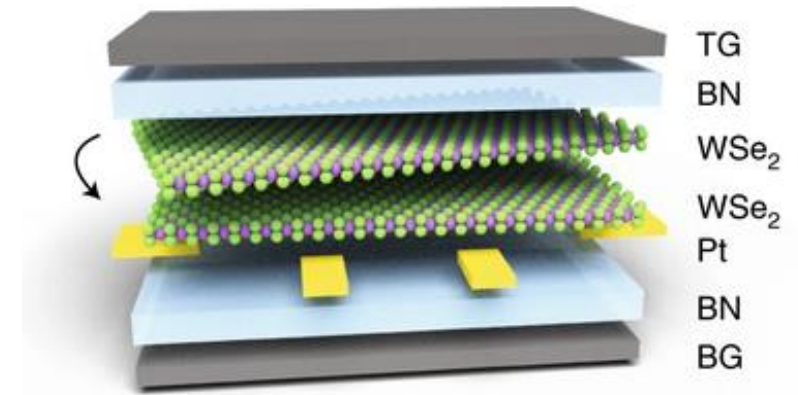


Moiré pattern with  
a much larger unit cell

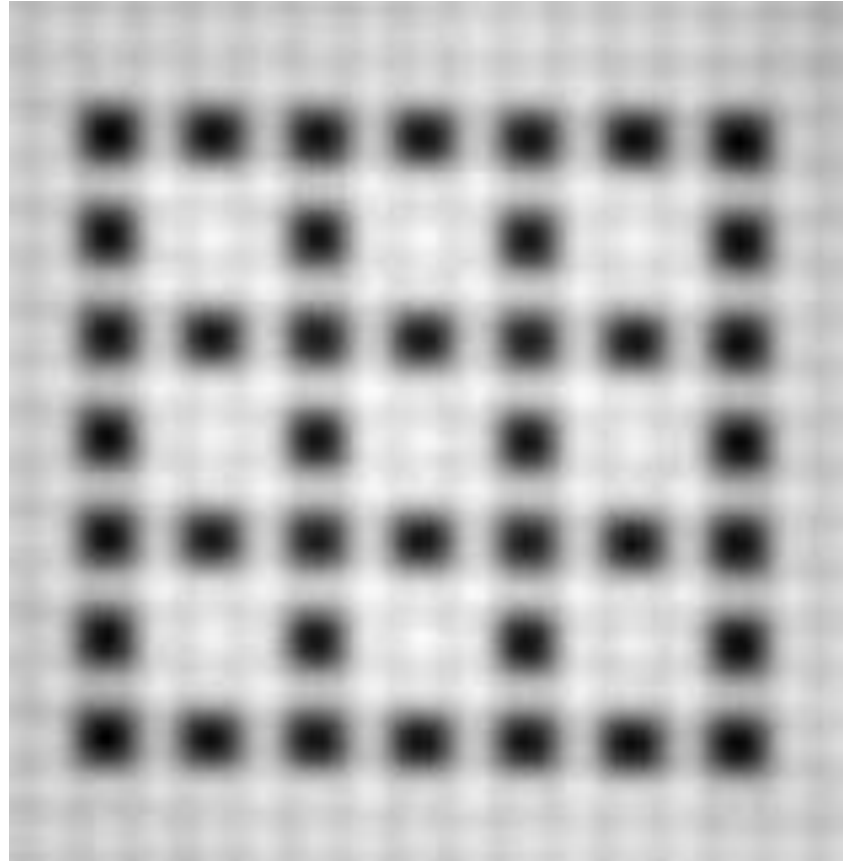


Variety of twisting arrangements  
with equal or different layers:  
graphene, dichalcogenides,  
magnetic 2D materials ...

Moiré also through slight mismatch  
or through ad-hoc engineered periodic potential



# Engineering 2d lattices: atoms on surfaces



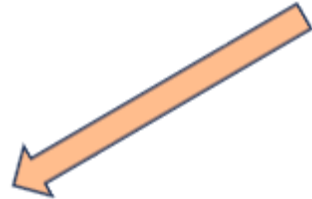
Yan & Liljeroth,  
Advances in Physics X, 4, 2019

# Emergence of Correlated Phases in Quantum Materials

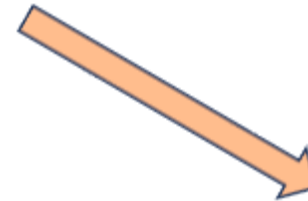
Interactions between many particles (electrons)



Correlated Quantum States  
in many different and novel materials  
(Tunability)



Symmetry breaking states



Formation of local moments



+ Interplay with topology

# Active electrons for correlated states

- Ion= nucleus + core electrons
- Focus on electrons close to Fermi level

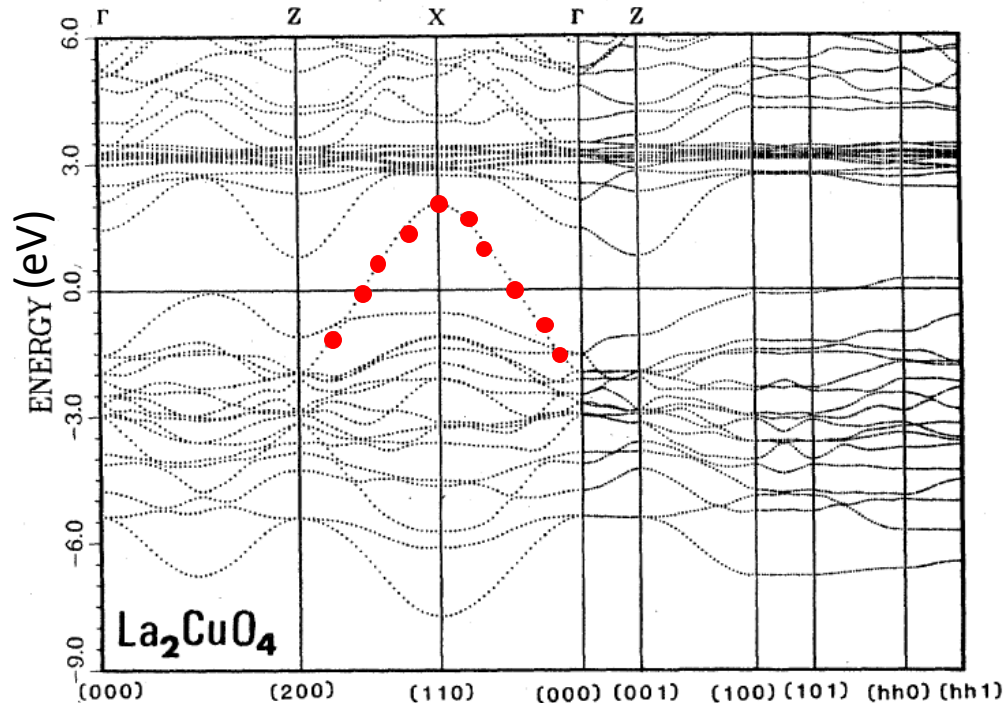
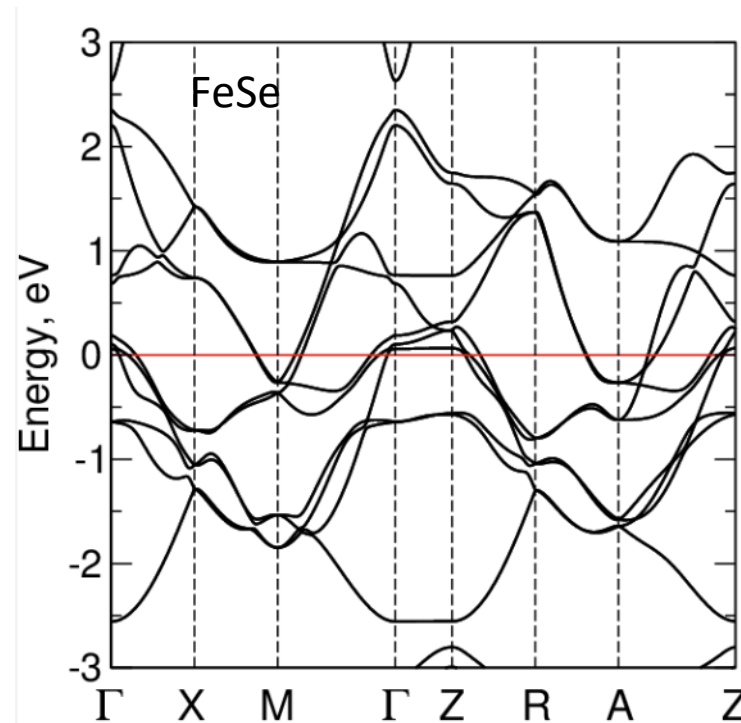
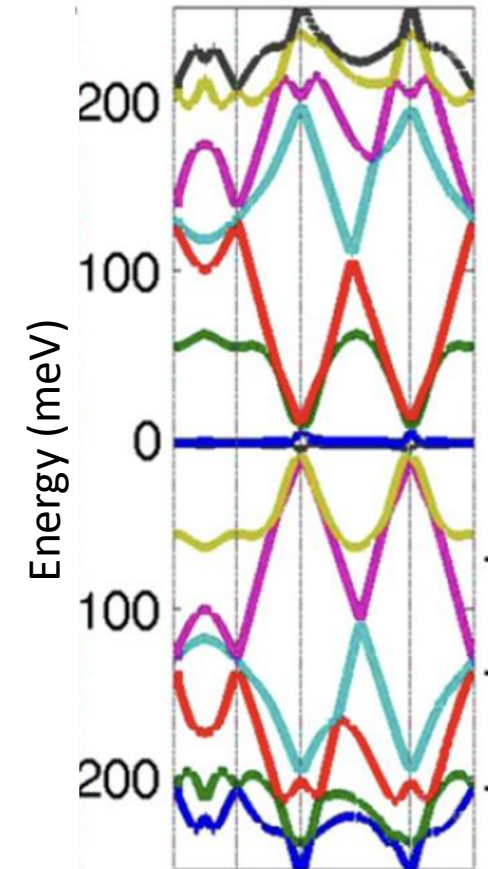


Fig: Pickett, RMP 61, 433 (1989)



Grechnev et al, Ukran. J. Phys 57, 171 (2012)



TBG  $\theta = 1.05^\circ$

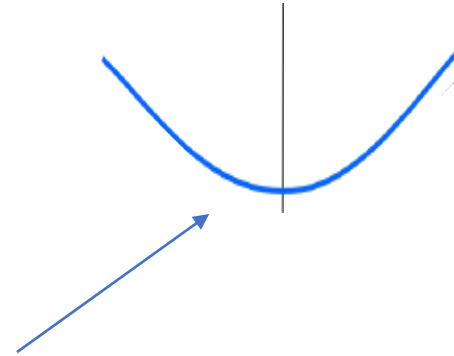
Bistritzer & MacDonald,  
PNAS 108, 12233 (2011),

# Kinetic energy: lattice versus continuum

## Free space: Parabolic band

- Isotropic
- No length scale
- Momentum conserved

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



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

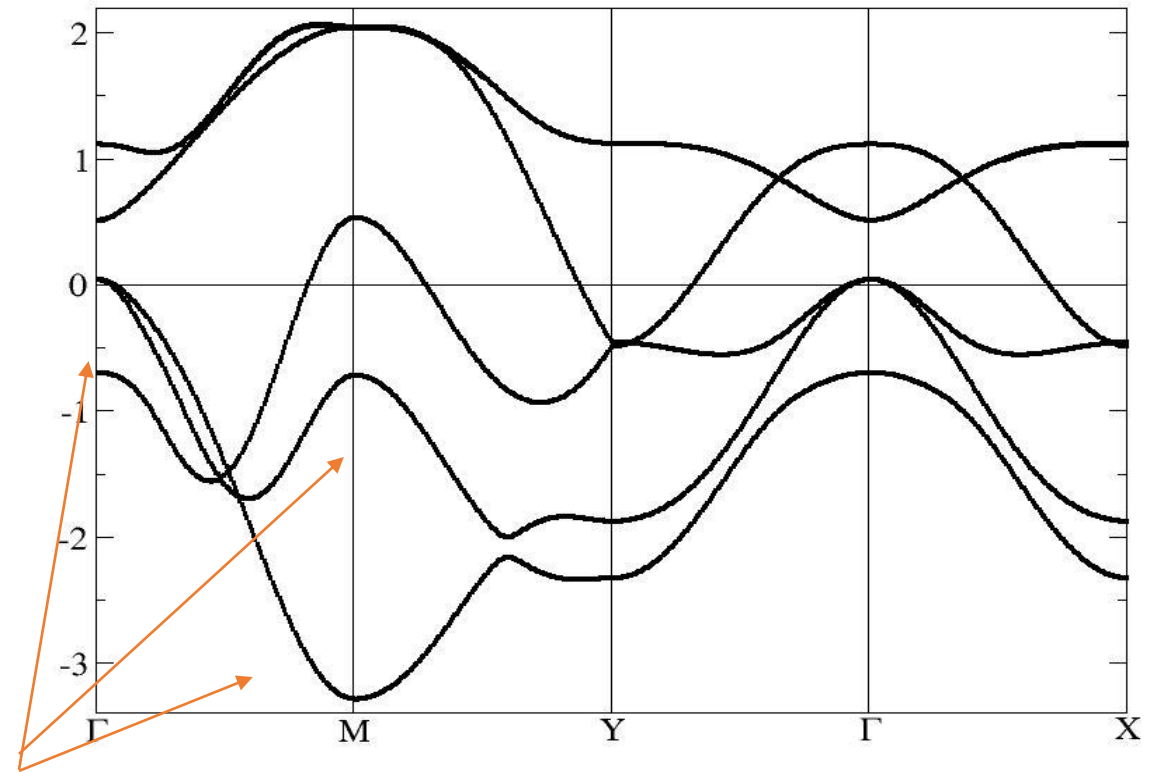
Inverse of second derivative  
of the energy gives the  
mass of the electron

# Kinetic energy: lattice versus continuum

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



Approximated to parabolic band  
very close to the bottom/top

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

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

Effective mass

# Kinetic energy: lattice versus continuum

In a solid:

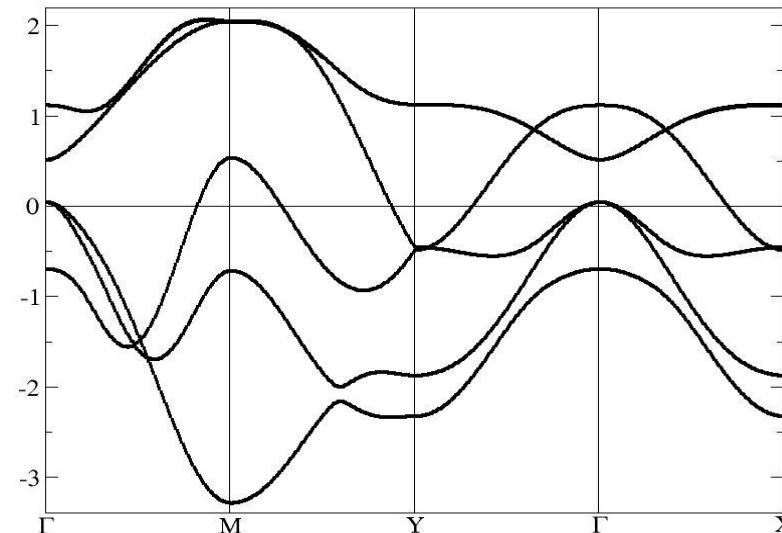
## Periodic potential of the ionic lattice

- 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

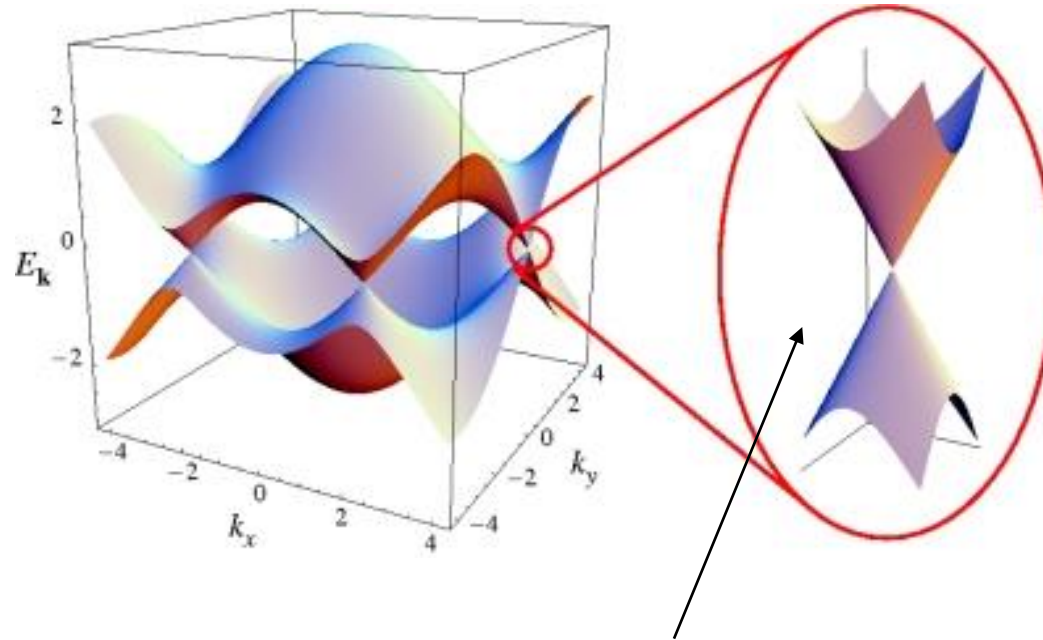
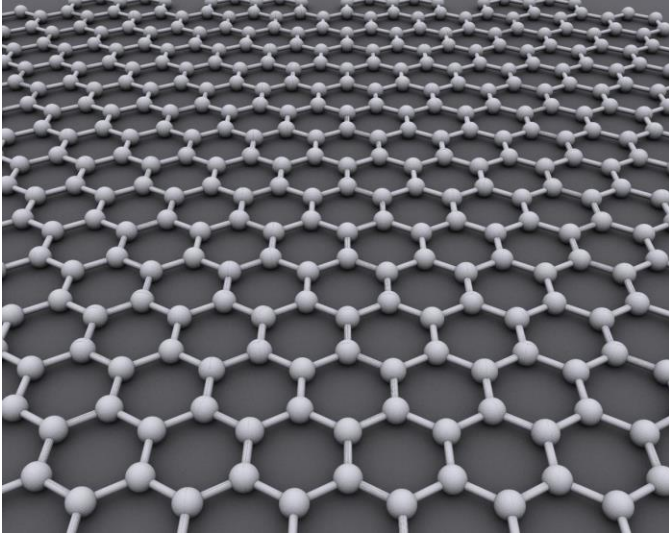
Free space:

- Isotropic
- No length scale
- Momentum conserved

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



# Kinetic energy: massless fermions



Linear Dirac dispersion

$$m^{-1} = |\partial^2 \epsilon / \partial k^2| = 0$$

Effective mass vanishes

massless fermions

# Quantum Effects: The degenerate 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  $\varepsilon$

chemical potential  $\mu$

## Zero temperature

Step function

States filled up to  
the Fermi Energy  $\varepsilon_F$

**Fermi surface**

(inside Fermi surface filled  
outside empty)

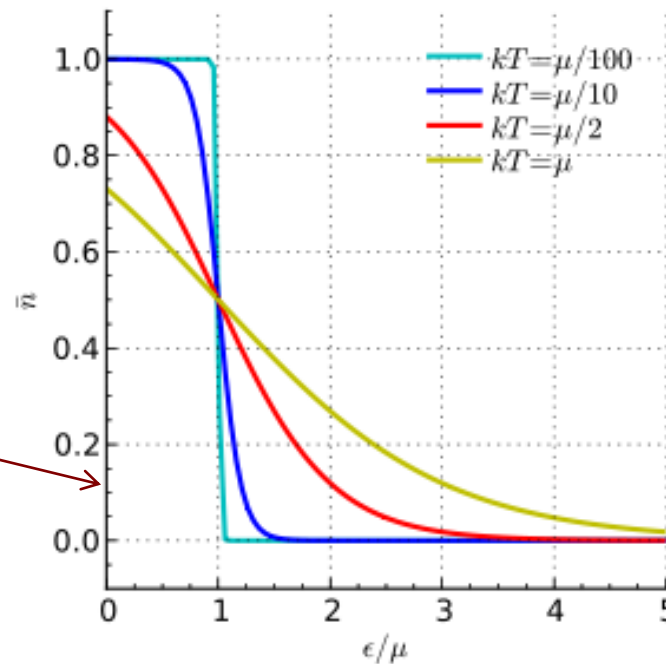


Fig: Wikipedia

**High temperatures**  
(classical gas)

$$K_B T \gg \mu$$

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

Maxwell-  
Boltzmann  
distribution  
function

# Quantum Effects: The degenerate Fermi gas

$$k_B T \ll \mu$$

(Fermi-Dirac: step)

$$k_B T \gg \mu$$

(Maxwell-Boltzmann)

## ○ Specific heat

Free energy

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

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

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

## ○ Spin susceptibility

Magnetization

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

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

independent of  $T$

Pauli susceptibility

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

Temperature dependences of different quantities tell us about correlations between the electrons

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

# Quantum Effects: The Fermi Temperature

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

In many metals

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

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

In doped semiconductors,  
TBG, heavy Fermions

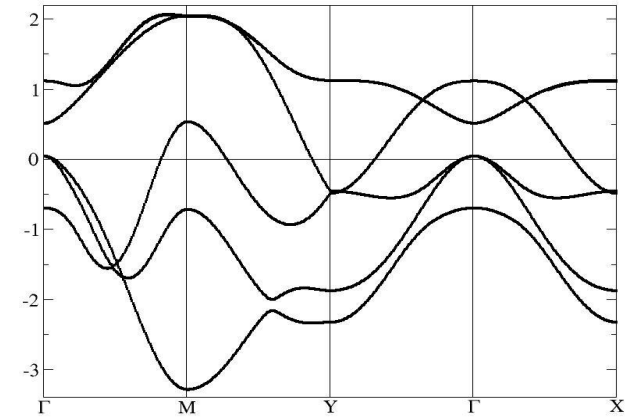
$$\epsilon_F \sim \text{few meV}$$

$$T_F \sim 50\text{-}100 \text{ K}$$

# Kinetic energy and bandwidth

Kinetic energy:  $\int_{-\infty}^{\epsilon_F} \epsilon N(\epsilon) d\epsilon$

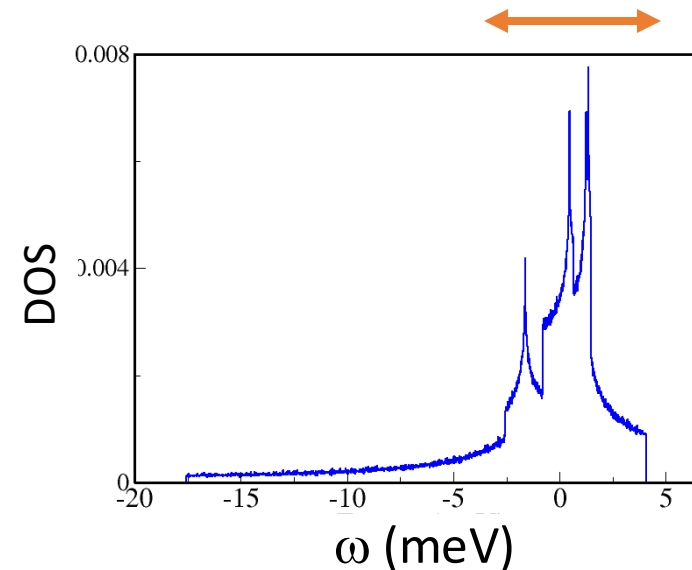
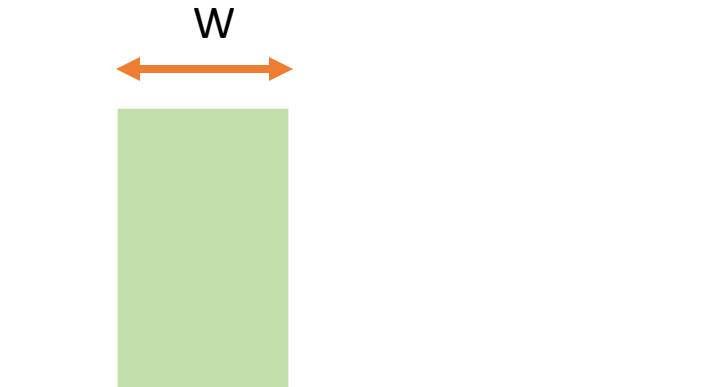
$N(\epsilon)$ : density of states



$N(\epsilon)$ : constant in  $[-W/2, W/2]$ , zero otherwise  $\longrightarrow$  Kinetic energy  $\propto W$

$W$ : bandwidth

Flat bands  
very sensitive  
to interactions



# Kinetic energy and bandwidth

Kinetic energy:  $\int_{-\infty}^{\varepsilon_F} \varepsilon N(\varepsilon) d\varepsilon$

$N(\varepsilon)$ : density of states

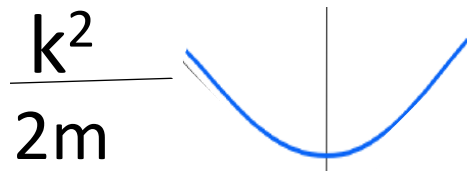
$N(\varepsilon)$ : constant in  $[-W/2, W/2]$ ,  
zero otherwise

$W$ : bandwidth

Kinetic energy  $\propto W$

Flat bands  
very sensitive  
to interactions

Larger mass  $\longrightarrow$  Narrower band  $\longrightarrow$  Smaller bandwidth  $W$   $\longrightarrow$  Smaller Kinetic energy



Careful! Not applicable to Dirac dispersion

# Kinetic energy and bandwidth

Kinetic energy  $\sim$  Bandwidth  $W$

$W \sim \text{eV}$  in most materials

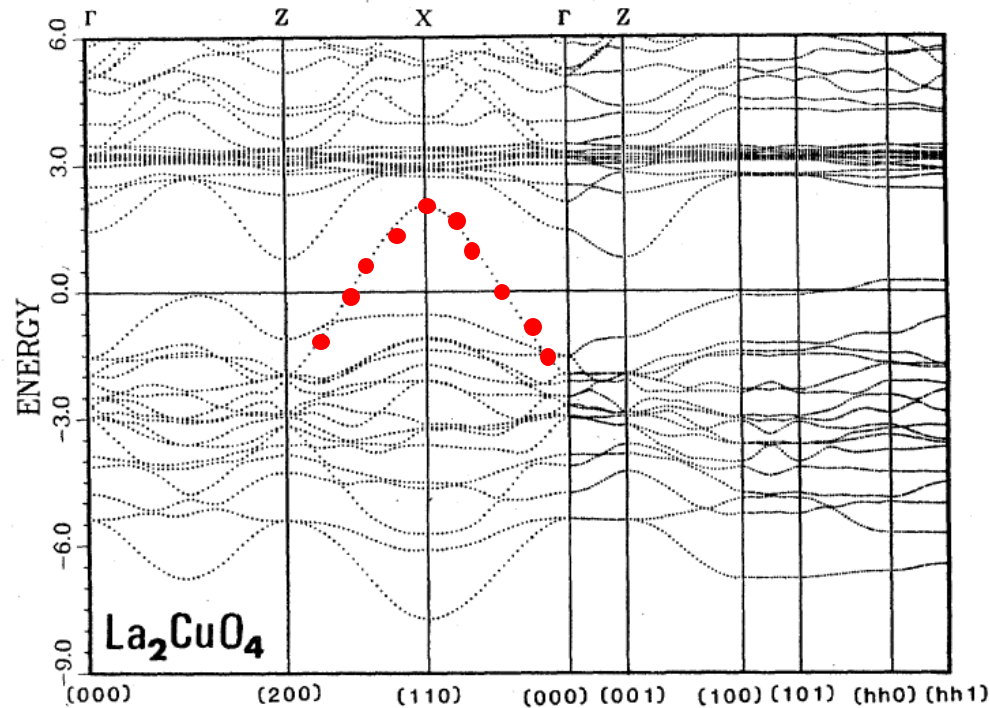
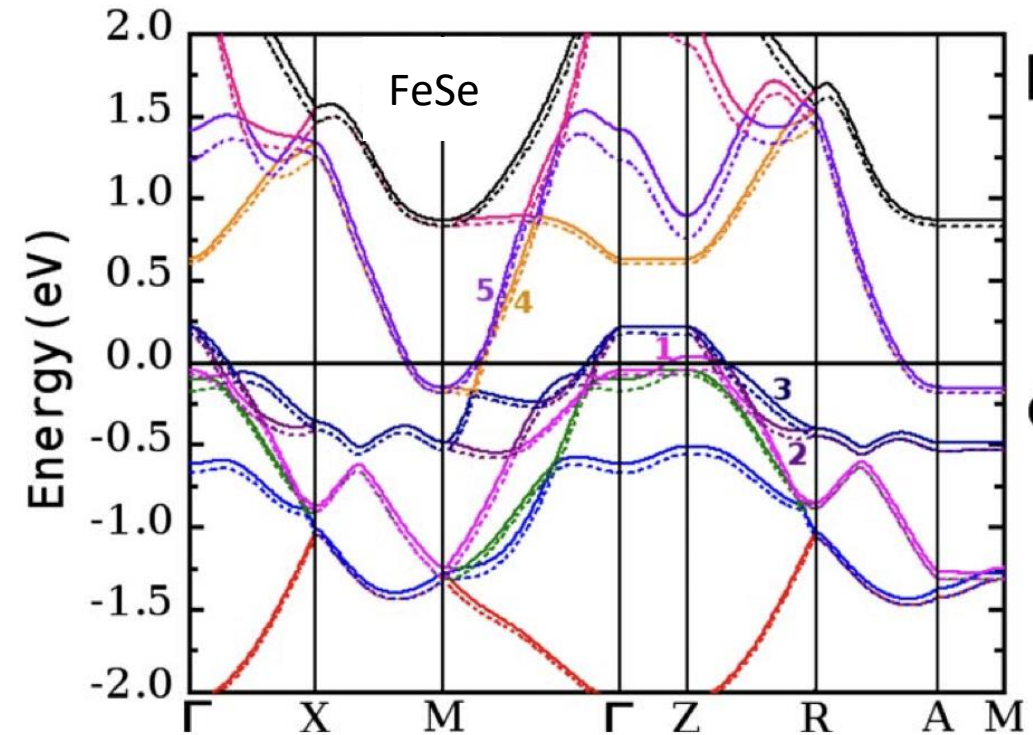


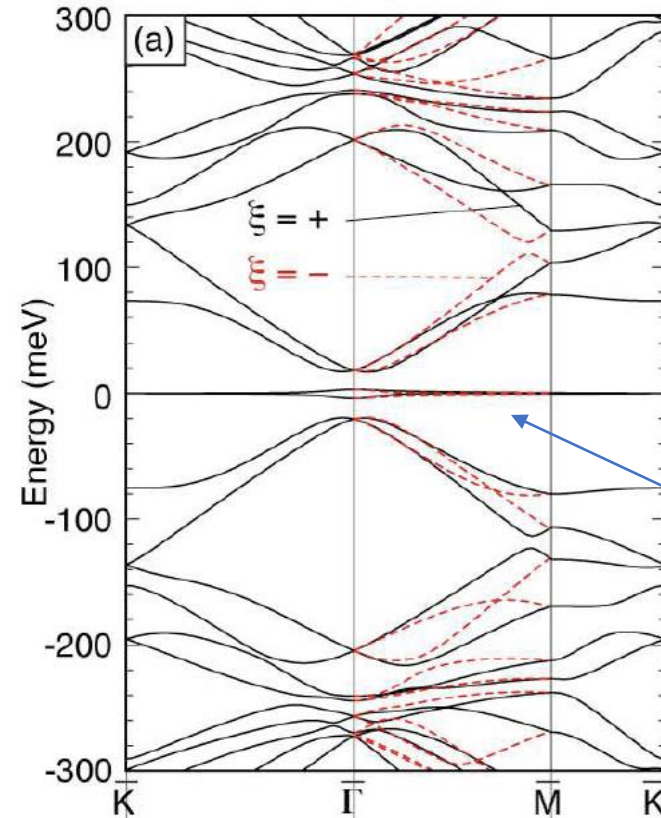
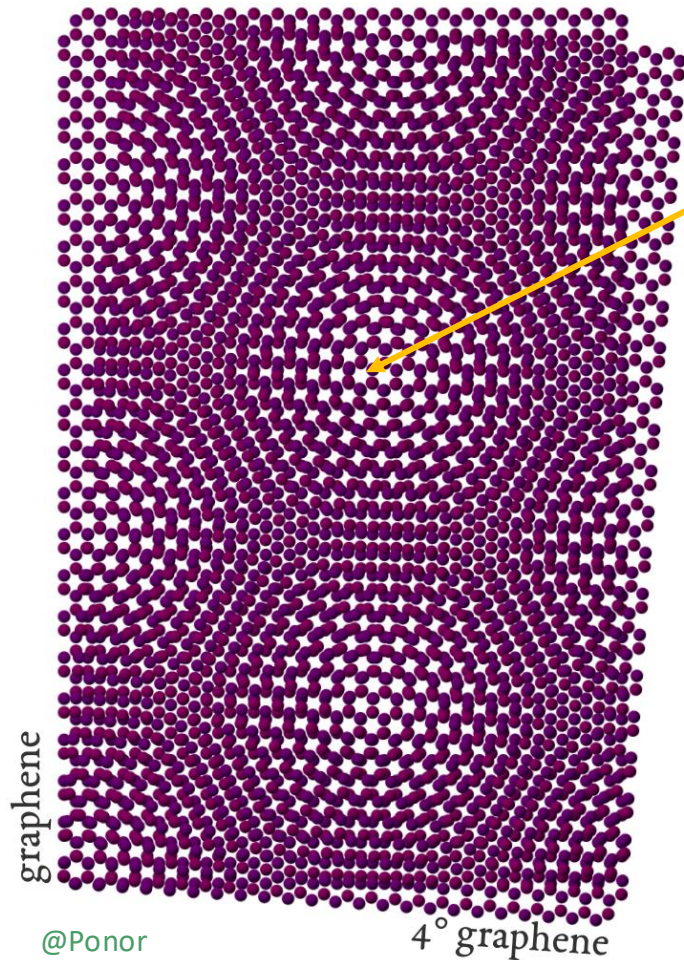
Fig: Pickett, RMP 61, 433 (1989)



Ma & Lu, PRB 78, 033111 (2008)

# Moiré heterostructures: flat bands

Moiré unit cell  $\sim 10$  nm lattice constant



Very narrow bands for certain twist angles (bandwidth 1-10 meV)

Very sensitive to interactions

# Strength of interactions

□ Ratio between Interaction and Kinetic energies  $U/W$

Kinetic energy  $\sim$  Bandwidth  $W$

$W \sim$  eV in most materials

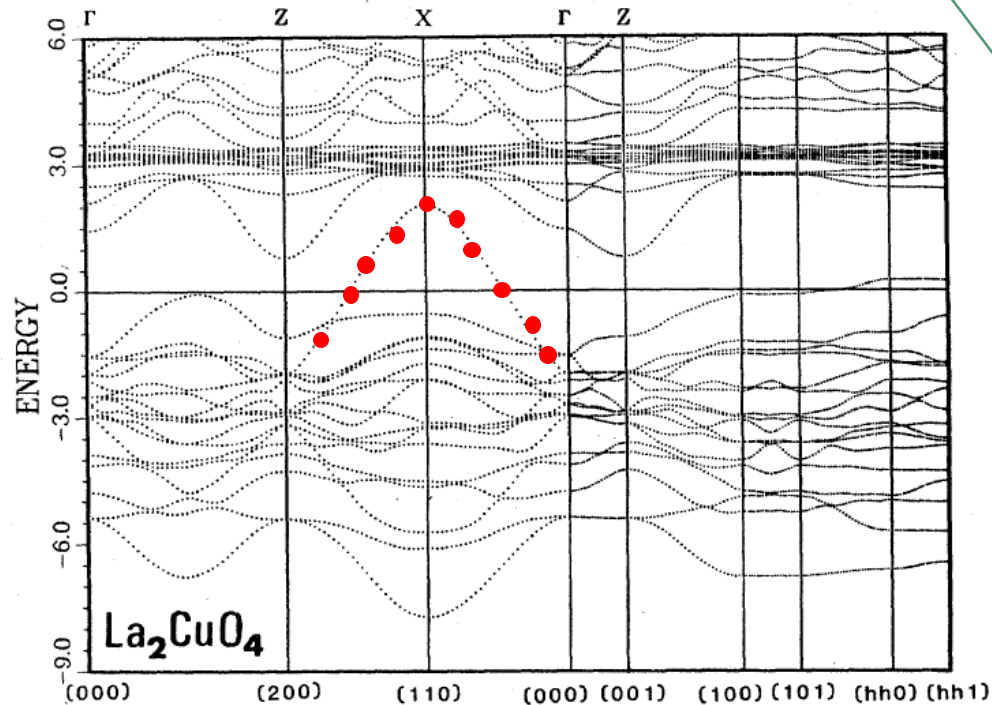


Fig: Pickett, RMP 61, 433 (1989)

Interaction energy:

$$U \sim \left( \frac{e^2}{4 \pi \epsilon_0} \right) \frac{1}{\epsilon_r r_0} = 14.37 \text{ eV } \text{\AA} \frac{1}{\epsilon_r r_0}$$

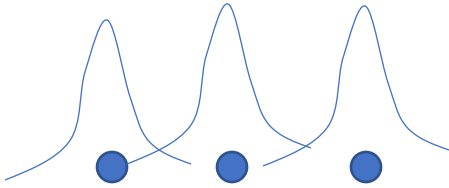
$r_0 \sim$  several  $\text{\AA}$   
in most materials

Similar energy scales

**$U/W$  not small**

# Strength of interactions

Bands: Tight binding model with atomic orbitals as a basis



Larger spread of wave function  
(less localized orbitals, larger  $r_0$ )



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



Onsite repulsion  
Two electrons in an atom less likely  
to be found very close  
(smaller effective interaction)

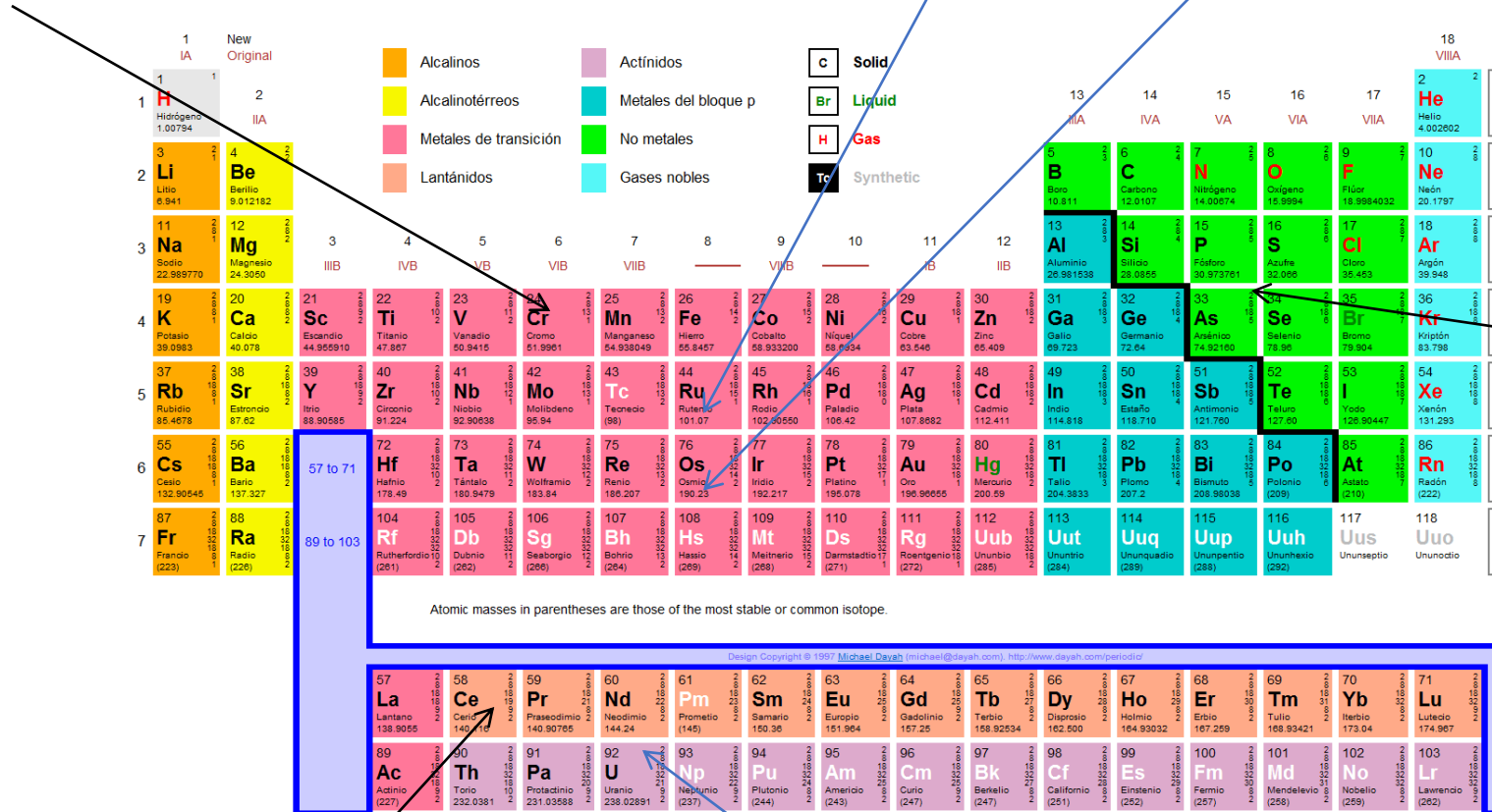
The type of atomic orbital matters

$$U \sim 14.37 \text{ eV} \frac{1}{\epsilon_r r_0}$$

# Strength of interactions.

3d: competition between kinetic energy & interaction

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



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

# Strength of interactions.

Periodic table showing element properties and categories.

**Legend:**

- Alcalinos (Orange)
- Alcalinotérreos (Yellow)
- Metales de transición (Pink)
- Lantánidos (Light Orange)
- Actínidos (Purple)
- Metales del bloque p (Cyan)
- No metales (Green)
- Gases nobles (Light Blue)
- Solid (C)
- Liquid (Br)
- Gas (H)
- Synthetic (Tc)

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

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Itinerant + local electrons  
Heavy fermion compound

# Effective models

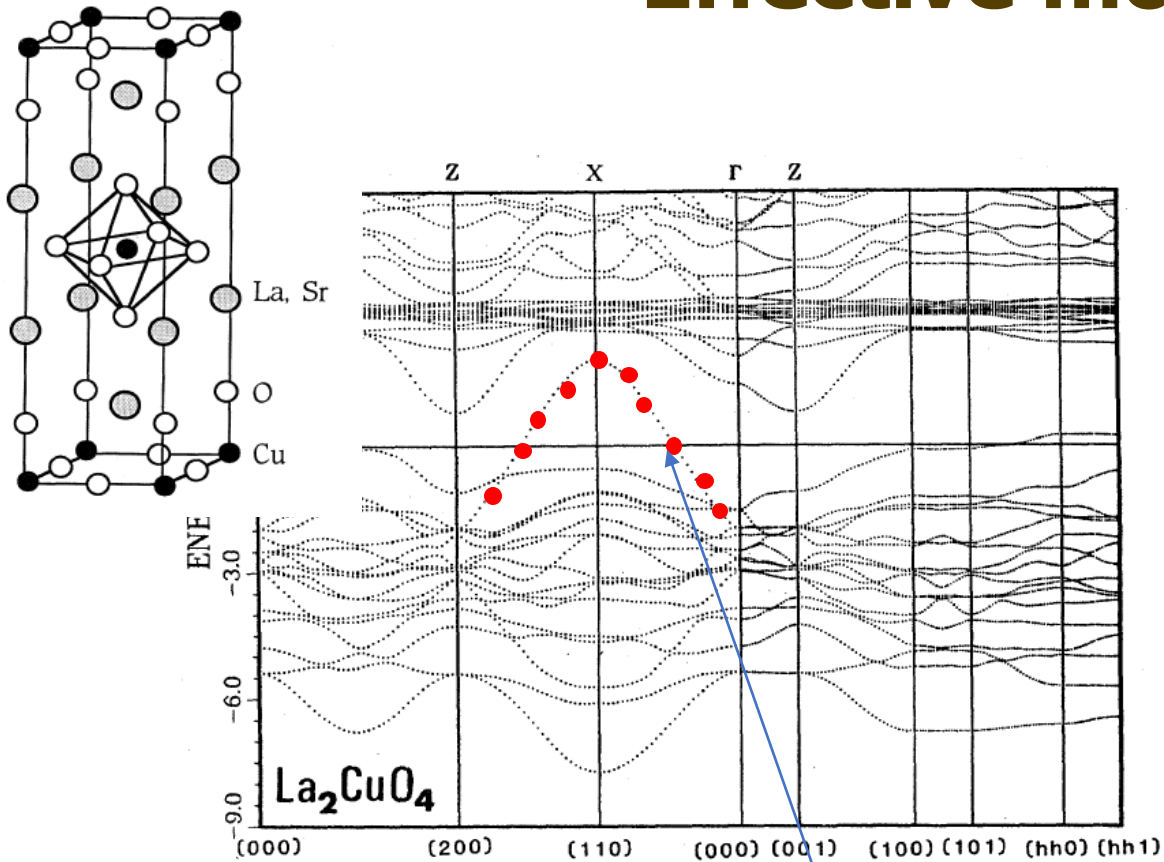


Fig: Pickett, RMP 61, 433 (1989)

Effective model for **Cu** electrons  
close to the Fermi level

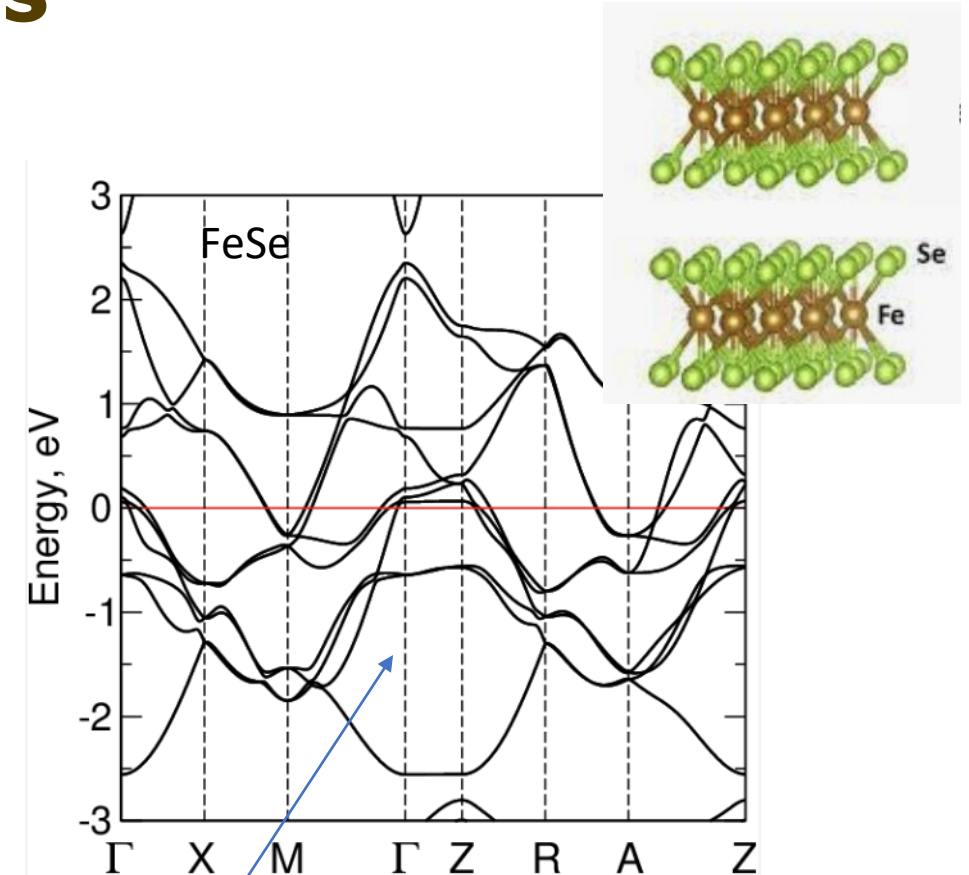
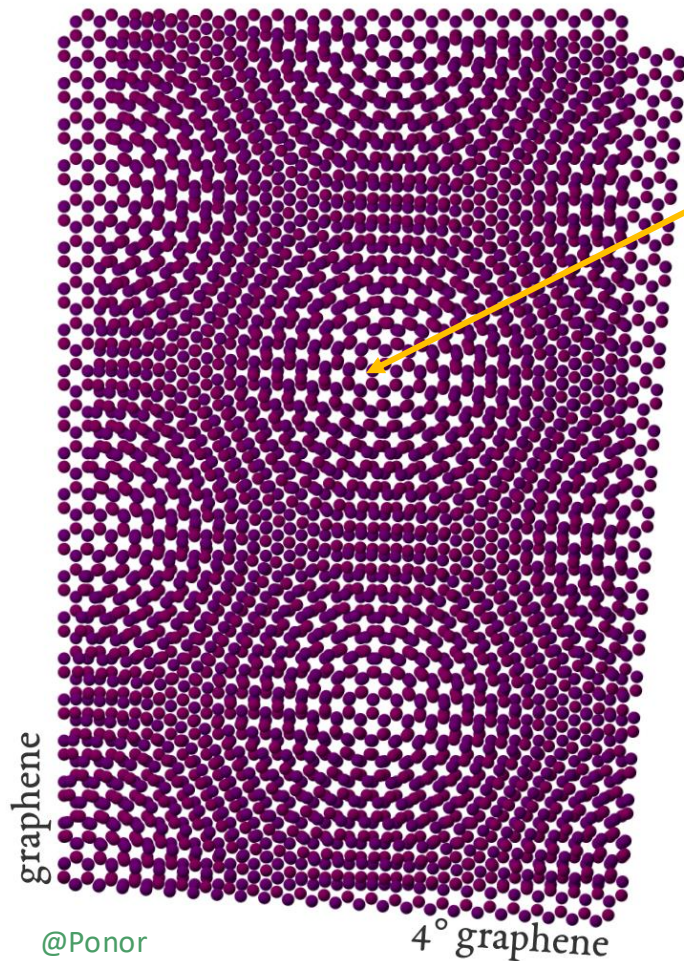


Fig: Grechnev et al, Ukran. J. Phys 57, 171 (2012)

Effective model for **Fe** electrons  
close to the Fermi level

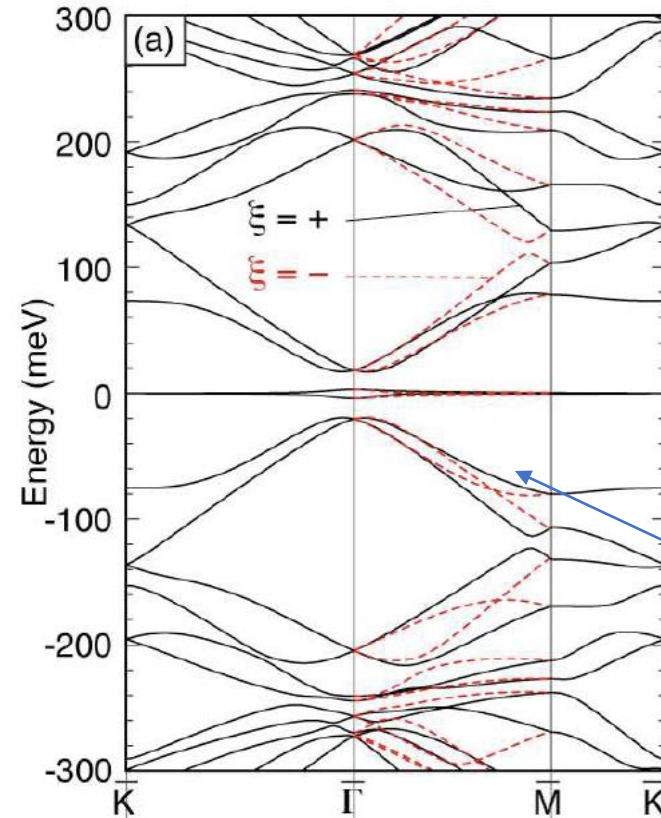
# Moiré heterostructures



Moiré unit cell  $\sim 10$  nm lattice constant

$$U \sim 30 \text{ meV}$$

$r_0$  several nm



Very narrow bands for certain twist angles (bandwidth 1-10 meV)

Energy scales of the system

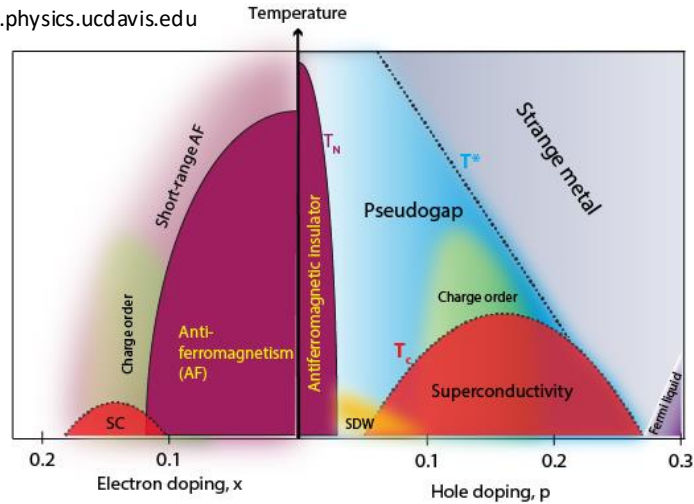


Temperature scale of correlated states

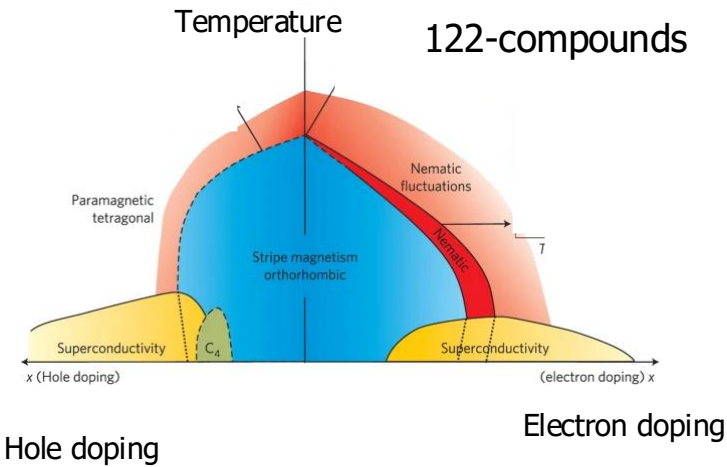
# Superconductivity in strongly correlated electron systems

## High-Tc superconducting cuprates

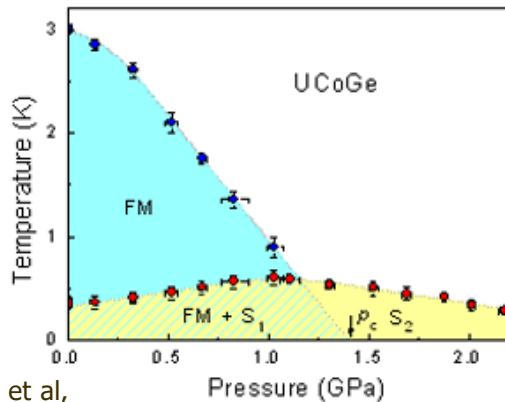
Fig: cme.physics.ucdavis.edu



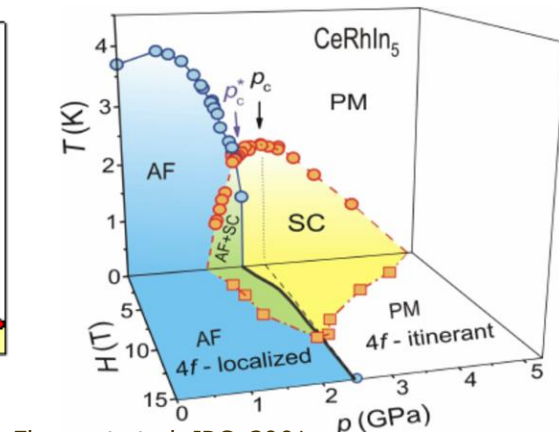
## High-Tc iron based superconductors



## Heavy fermion compounds

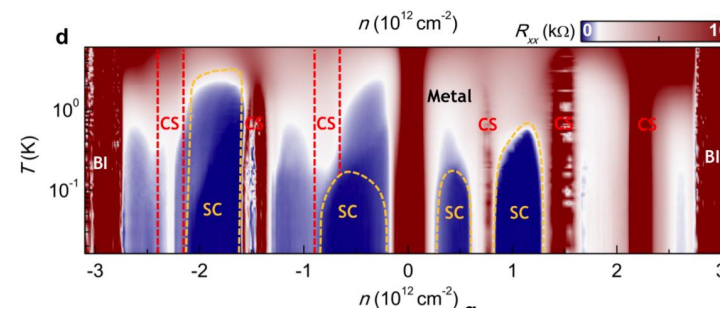


Slooten et al,  
PRL 103 , 097003(2009)



Flouquet et al, JPC, 2001

## Twisted bilayer graphene



Critical temperatures not small  
with respect to the relevant energy scales

# Metals and insulators

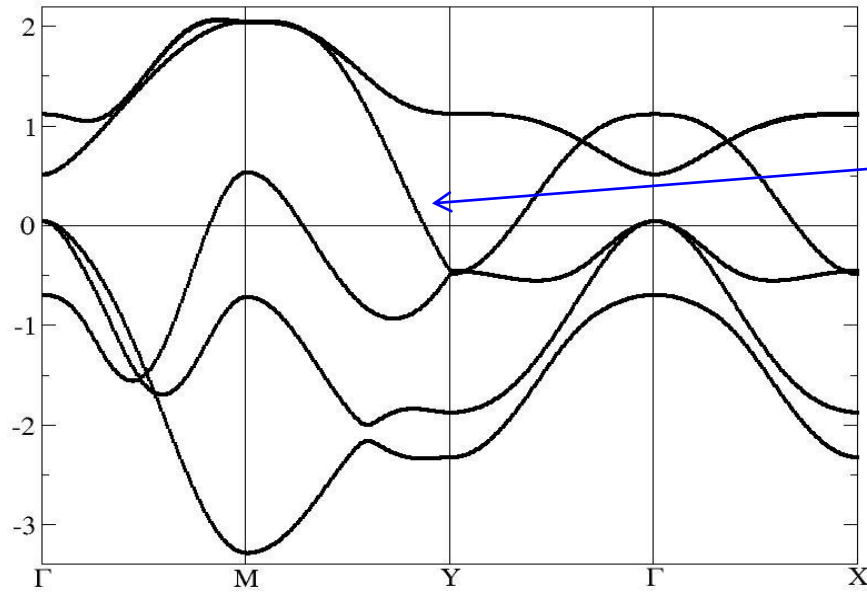


Fig: Calderón et al, PRB, 80, 094531 (2009)

**Metallicity**  
in clean systems  
Bands crossing the Fermi level  
(finite Density of States (DOS) at  $E_F$ )

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

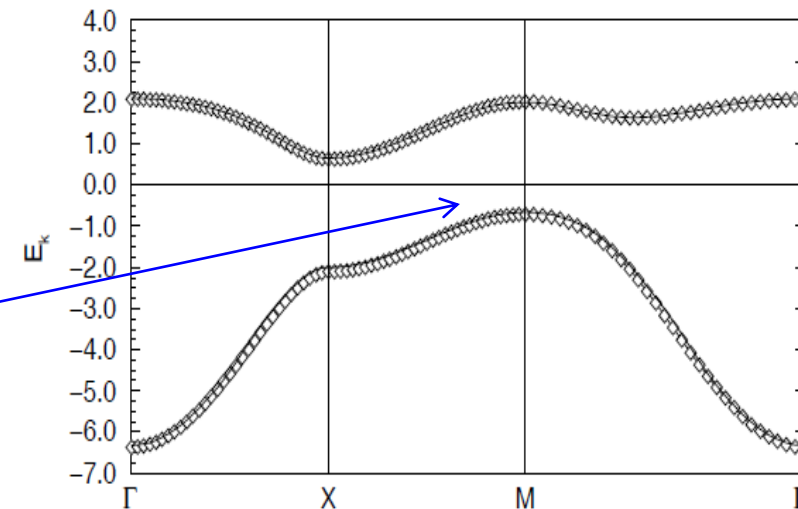


Fig: Hess & Serene, PRB 59, 15167 (1999)

# Metals and insulators

Assume a material with spin degeneracy:  
Each band can hold 2 electrons per unit cell

Odd number  
of electrons  
per unit cell



Metallic

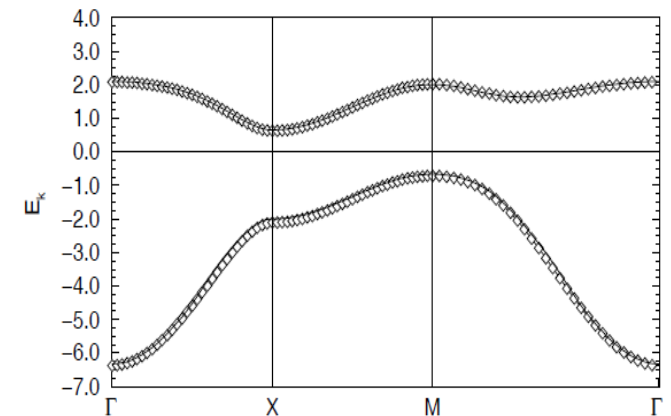
Even number  
of electrons  
per unit cell



Insulating



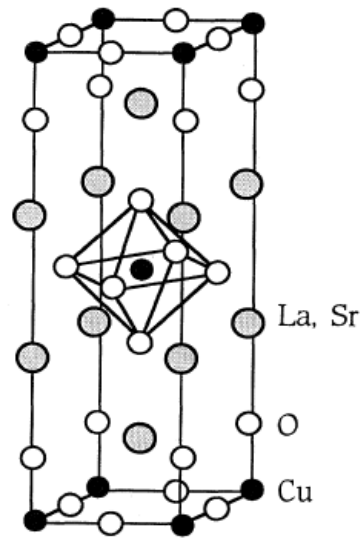
Metallic (in case  
of band overlap)



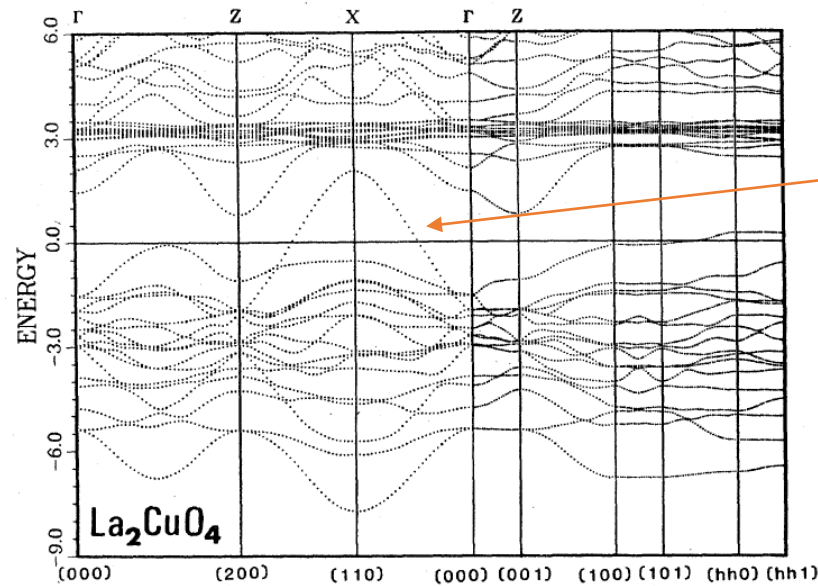
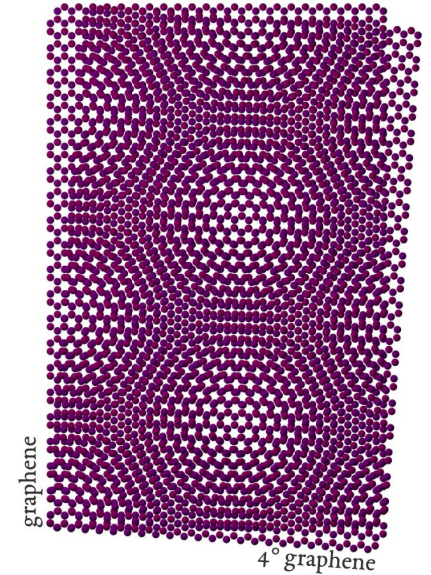
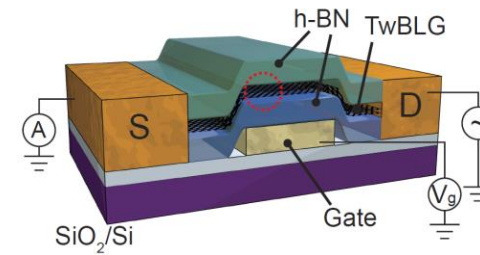
# Correlated states and electronic filling

High- $T_c$   
superconducting cuprates

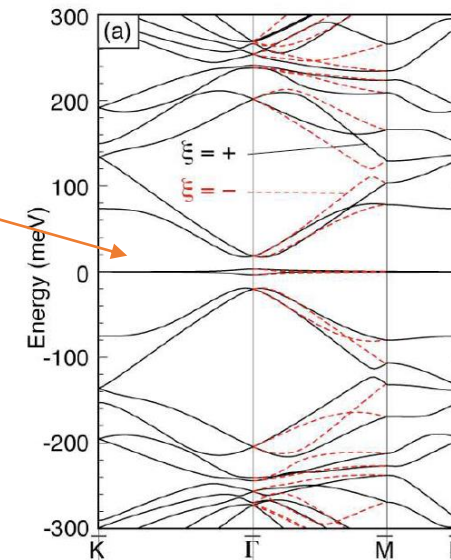
Doping through  
chemical  
substitution



Twisted  
bilayer graphene

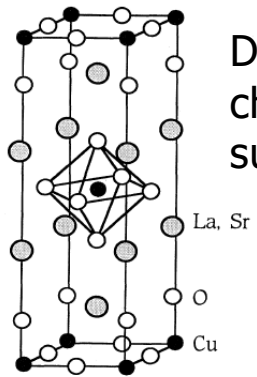


Expected to be metals

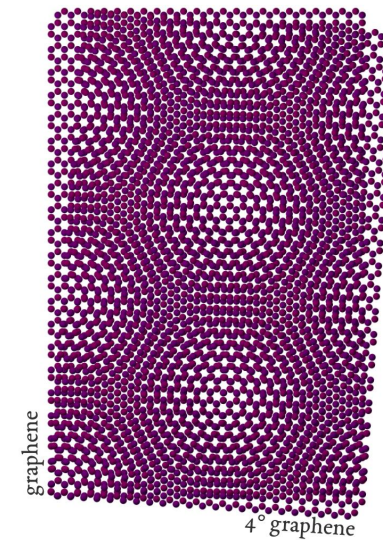
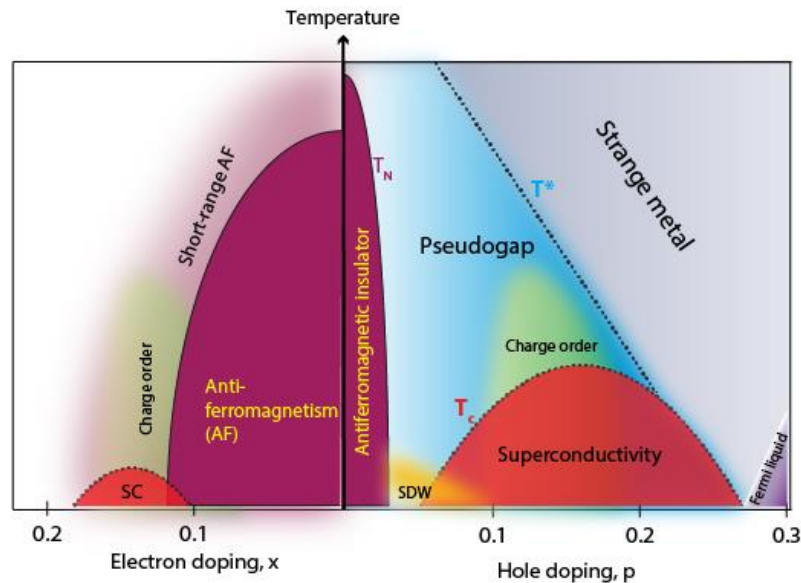
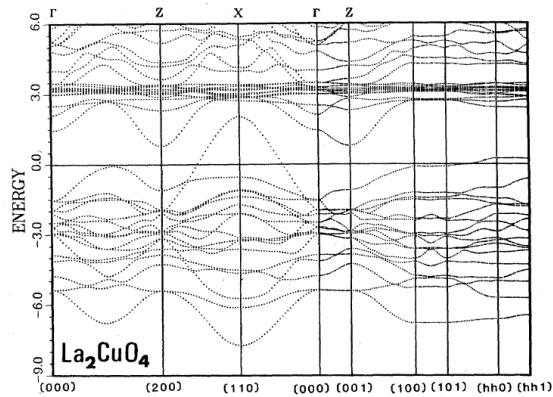


# Correlated states and electronic filling

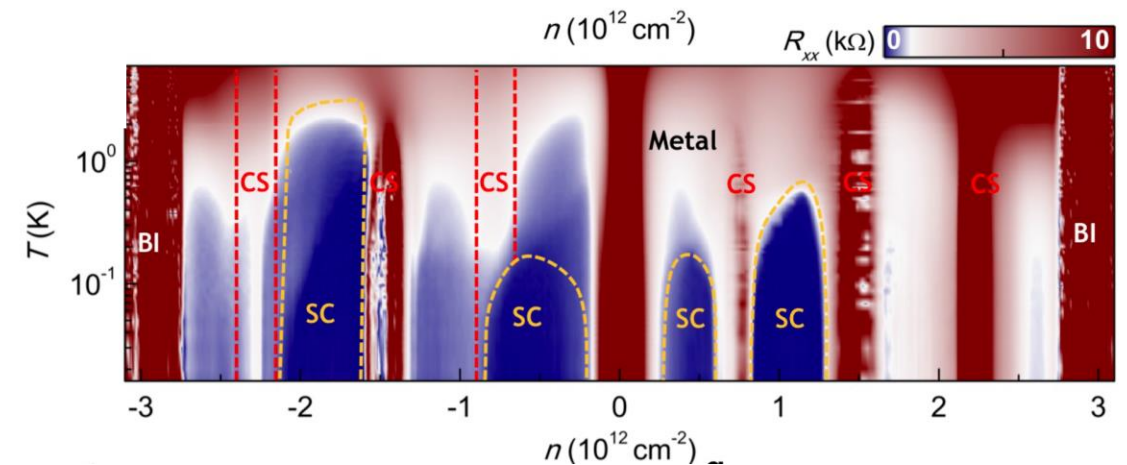
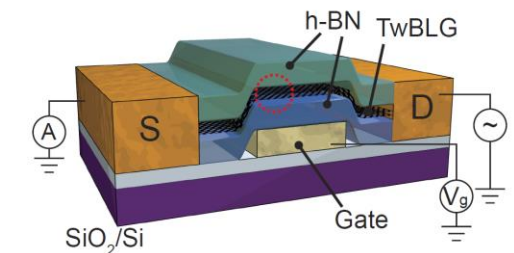
## High-Tc superconducting cuprates



Doping through chemical substitution

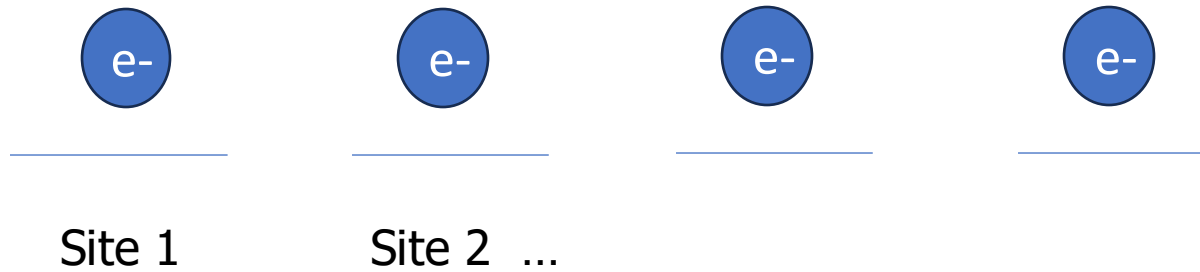


## Twisted bilayer graphene



# Correlated states and electronic filling

Onsite repulsión  $U$   
Hopping energy  $t$

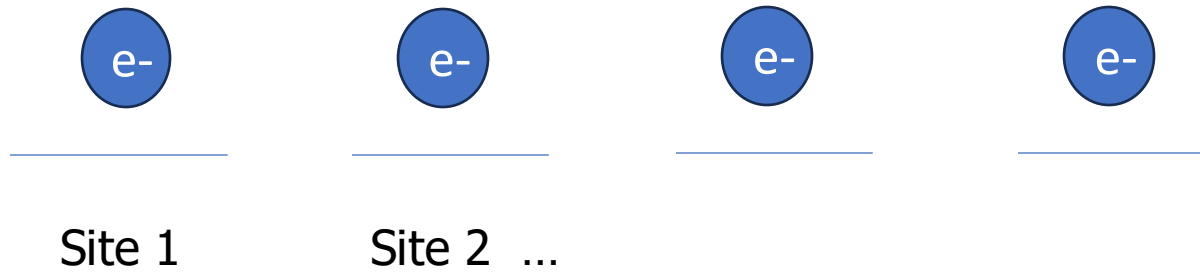


1 electron per site/atom

$U \gg t$  Metal insulator transition  
due to localization of electrons

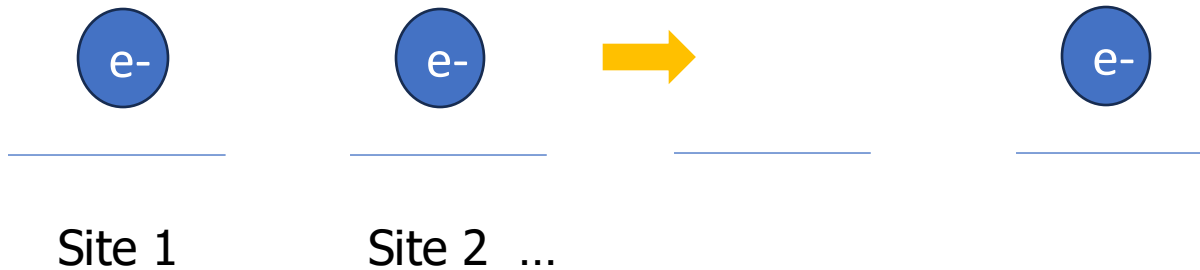
# Correlated states and electronic filling

Onsite repulsión  $U$   
Hopping energy  $t$



1 electron per site/atom

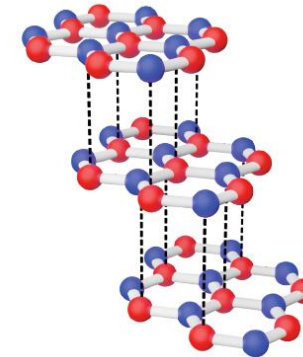
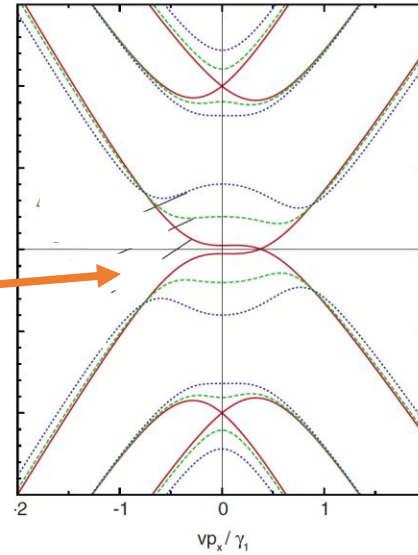
$U \gg t$  Metal insulator transition  
due to localization of electrons



Partial electronic filling per site/atom  
Always metallic (if no symmetry breaking)  
But maybe correlated metal!

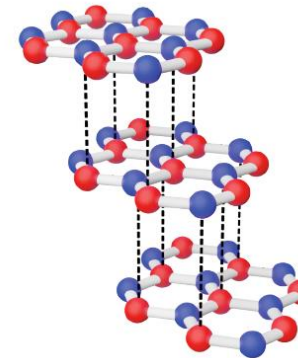
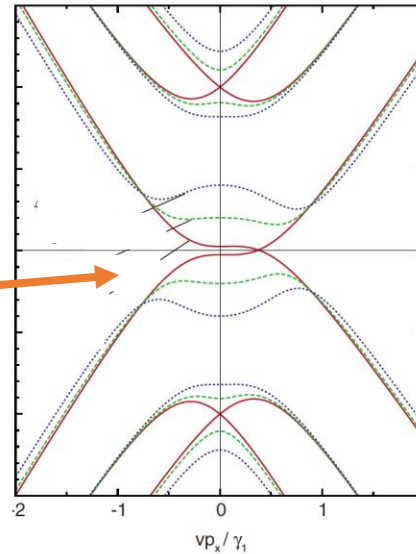
# Band structure "details"

- ❑ Dimensionality
- ❑ Bandwidth  $W$  (flat bands)
- ❑ Flat band regions  
(large density of states at  $E_F$ )

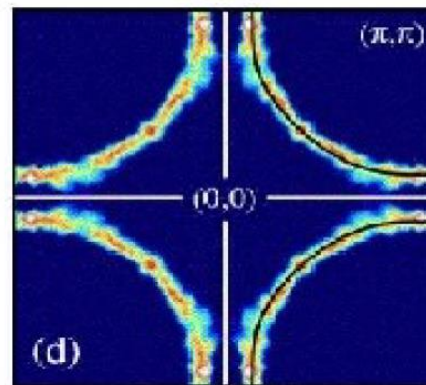
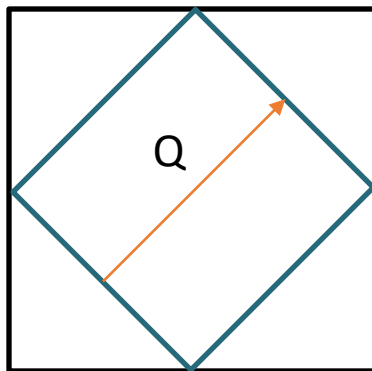


# Band structure "details"

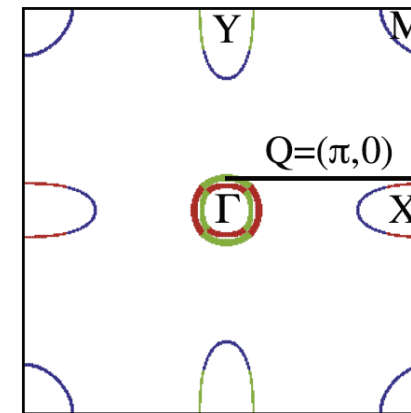
- Dimensionality
- Bandwidth  $W$  (flat bands)
- Flat band regions  
(large density of states at  $E_F$ )
- Nesting with momentum  $Q$   
(always in 1D)



Fermi surfaces  
in 2D



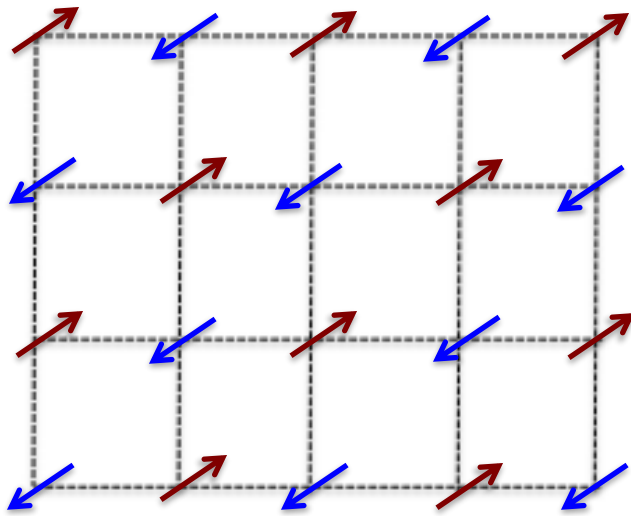
Fermi Surface of Cuprates



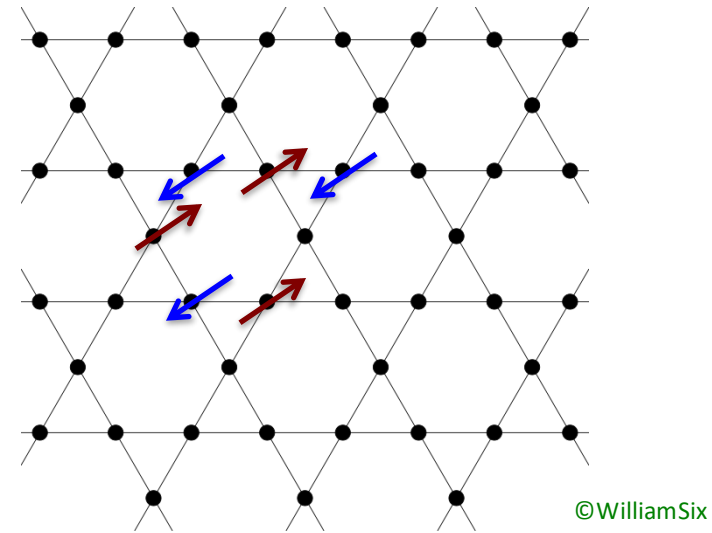
Fermi Surface of Iron superconductors

# Dimensionality and crystalline lattice

Bipartite lattice

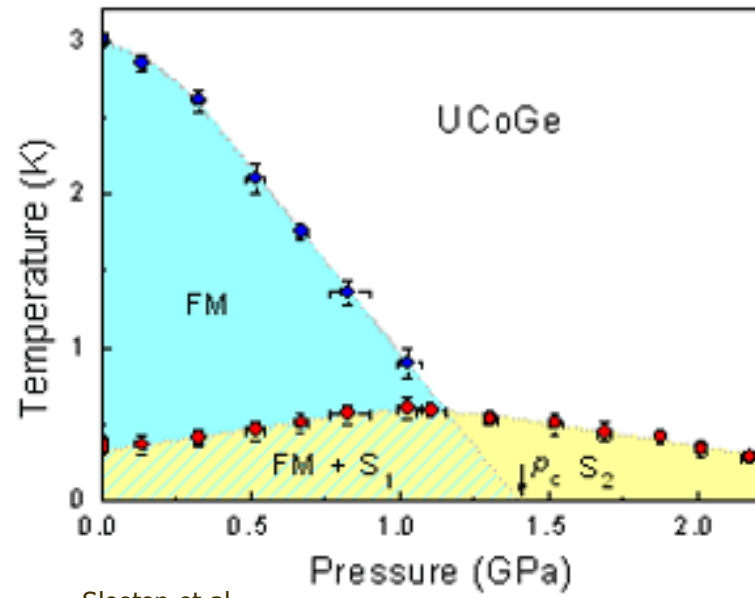
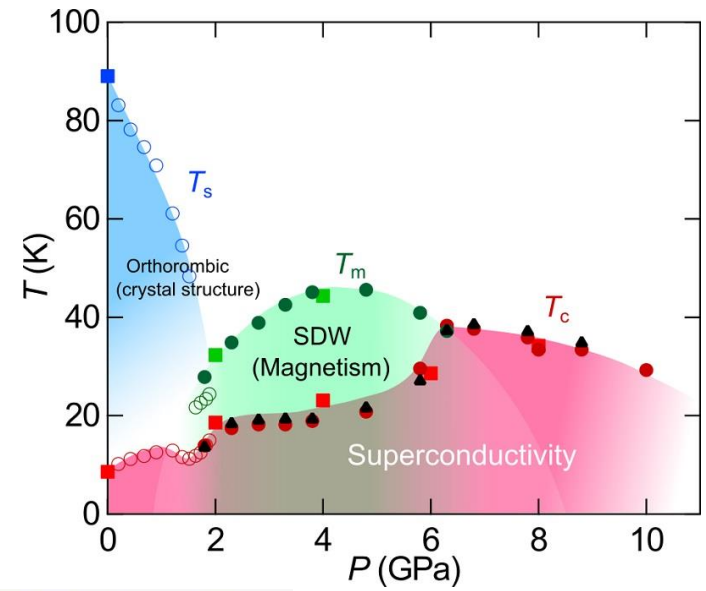


Frustrated lattice

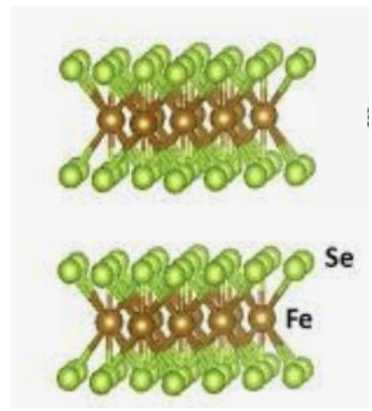
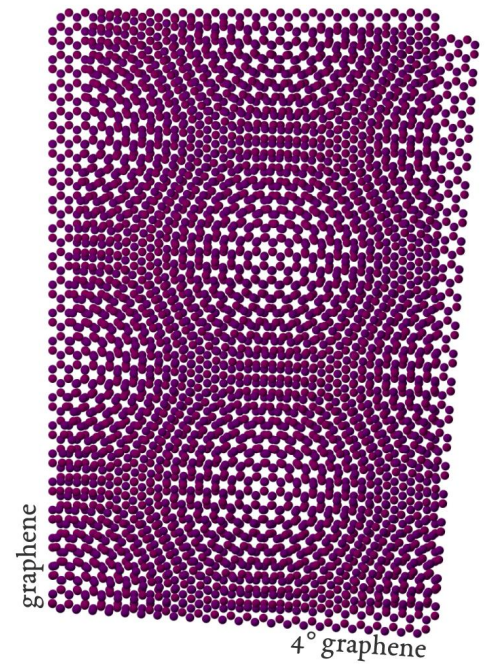


©WilliamSix

# External knobs to control the correlated states: pressure, strain ...



Slooten et al,  
PRL 103 , 097003(2009)

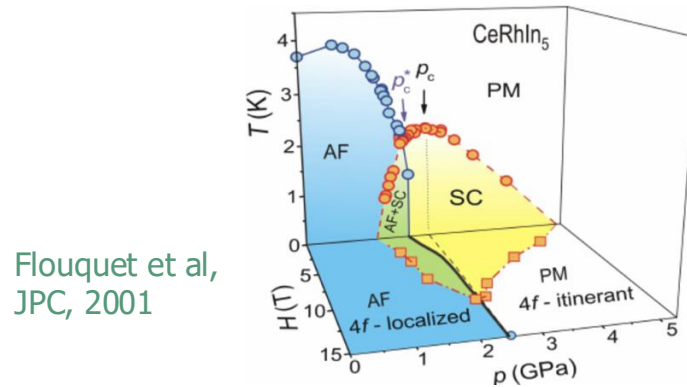


Modification of kinetic energy (lattice constant, Fermi Surface details ...)

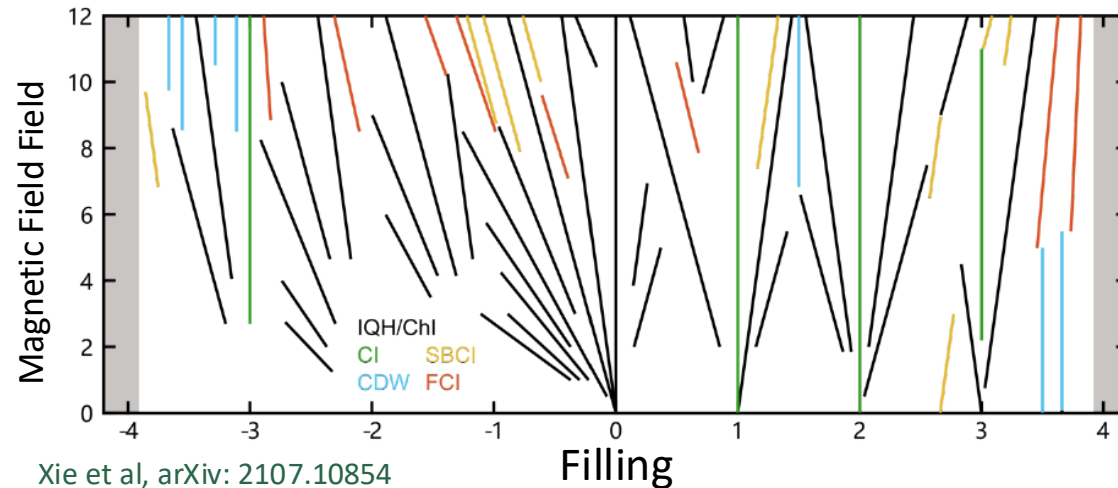
In a given material certain correlated states appear only under pressure

# External knobs to control the correlated states: magnetic and electric field...

Magnetic field: spin and orbital effect

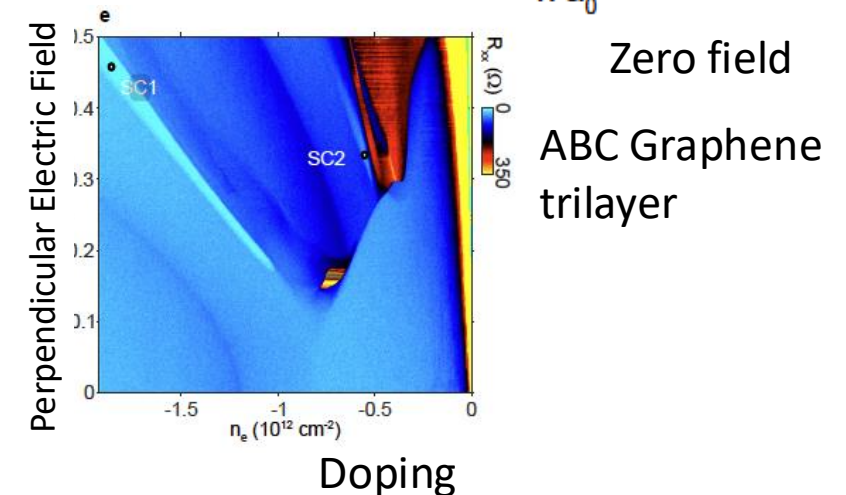
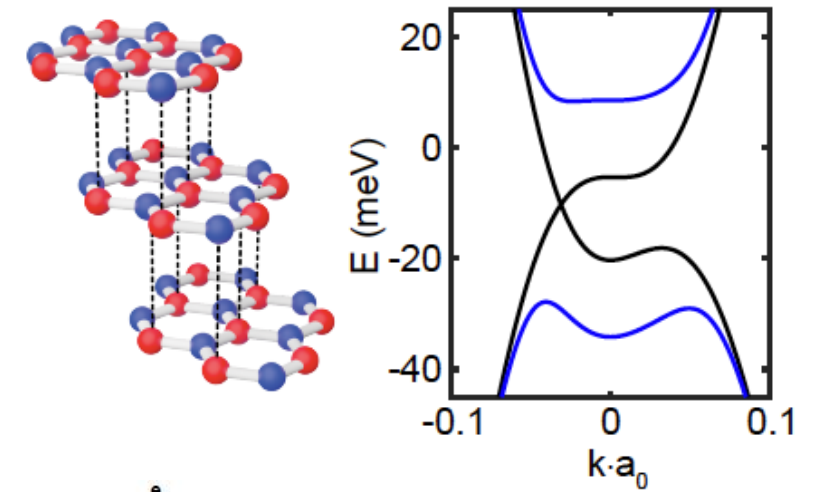


Twisted Bilayer Graphene (compressibility measurements)



Different types of insulating correlated states

Perpendicular electric field

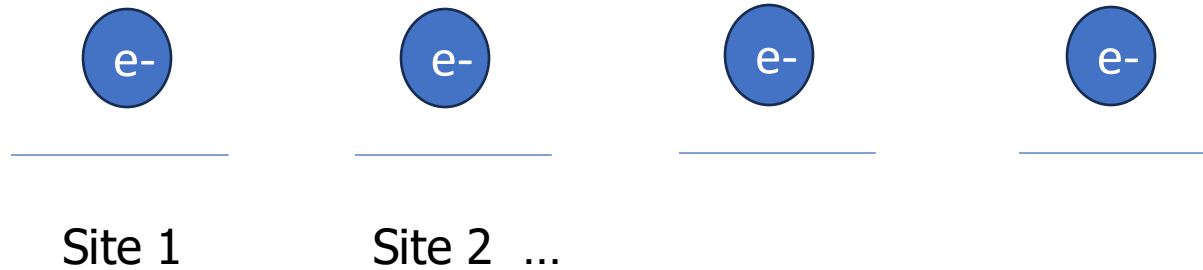


# The role of screening: from Coulomb to Hubbard

Coulomb interaction

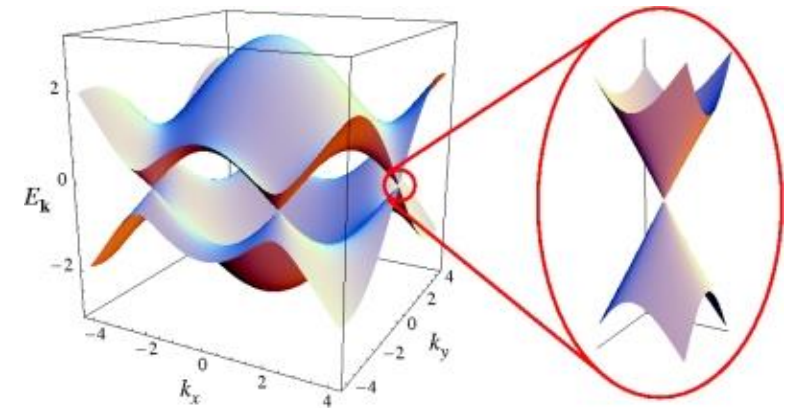
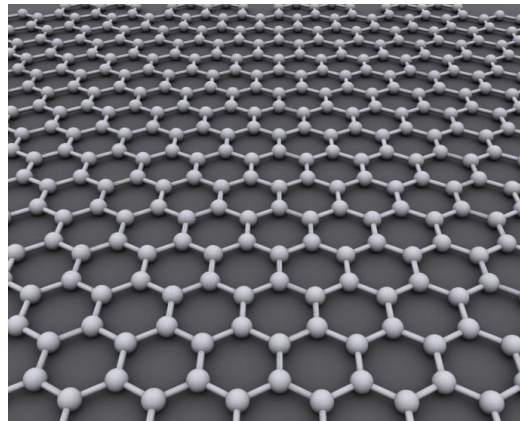
$$\left( \frac{e^2}{4 \pi \epsilon_0} \right) \frac{1}{\epsilon_r r_0} = 14.37 \text{ eV } \text{\AA} \frac{1}{\epsilon_r r_0}$$

Tuning  $\epsilon_r$  and maximum interaction length  $r_0$



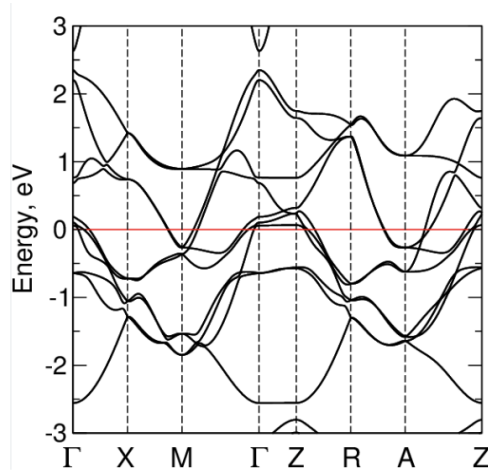
If not screened the electronic interaction decays a  $1/r$

Graphene:  $1/r$  interaction

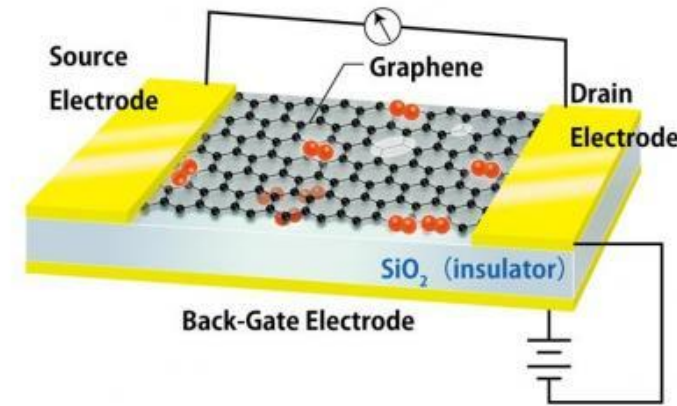


# The role of screening: from Coulomb to Hubbard

## Screening in metals



## Screening with a gate



## Coulomb interaction

$$\left( \frac{e^2}{4 \pi \epsilon_0} \right) \frac{1}{\epsilon_r r}$$



## Screened interaction

$$\left( \frac{e^2}{4 \pi \epsilon_0} \right) \frac{1}{\epsilon_r} \frac{\text{Exp}(-r/\lambda_0)}{r}$$

The interaction decreases faster with distance



Tune interaction length

$\epsilon_r$  also determined by screening from deep bands, substrate, gates...:

# The role of screening: from Coulomb to Hubbard

$$\left( \frac{e^2}{4 \pi \epsilon_0} \right) \frac{1}{\epsilon_r} \frac{\text{Exp}(-r/\lambda_0)}{r}$$

$\lambda_0 \sim$  lattice constant

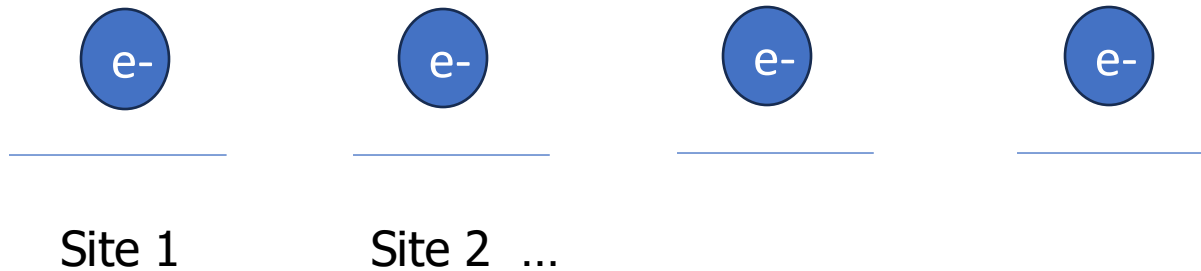
Only onsite repulsión U :

**Hubbard model**

$$\lambda_0 \rightarrow \infty$$

**Coulomb 1/r**

Interaction decays slowly  
and extends to all neighbors

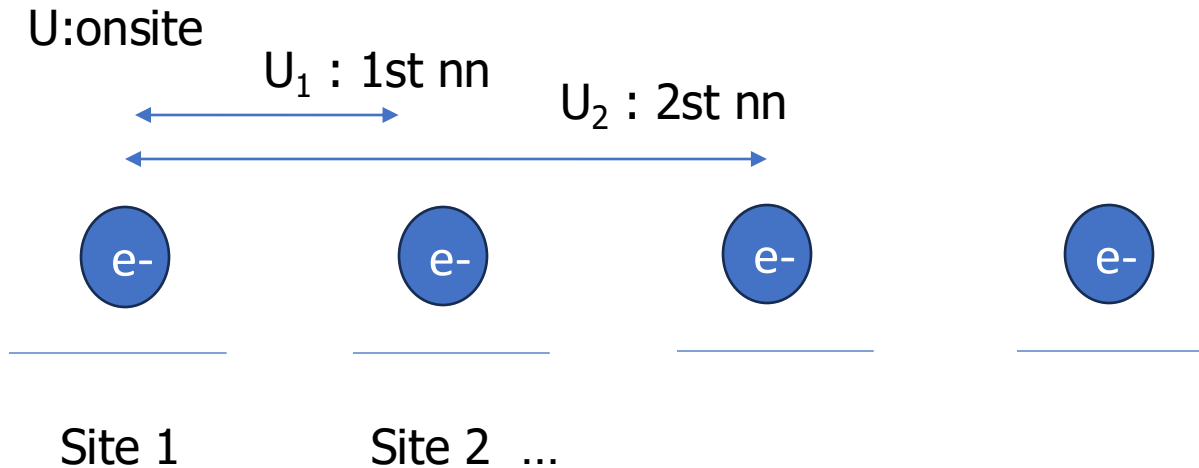


# The role of screening: from Coulomb to Hubbard

$$\left( \frac{e^2}{4 \pi \epsilon_0} \right) \frac{1}{\epsilon_r} \frac{\text{Exp}(-r/\lambda_0)}{r}$$

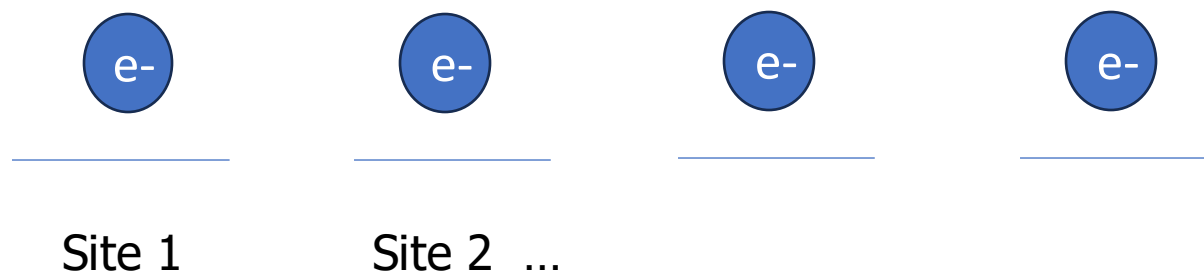
## Extended Hubbard model

Interaction up to first or second neighbors



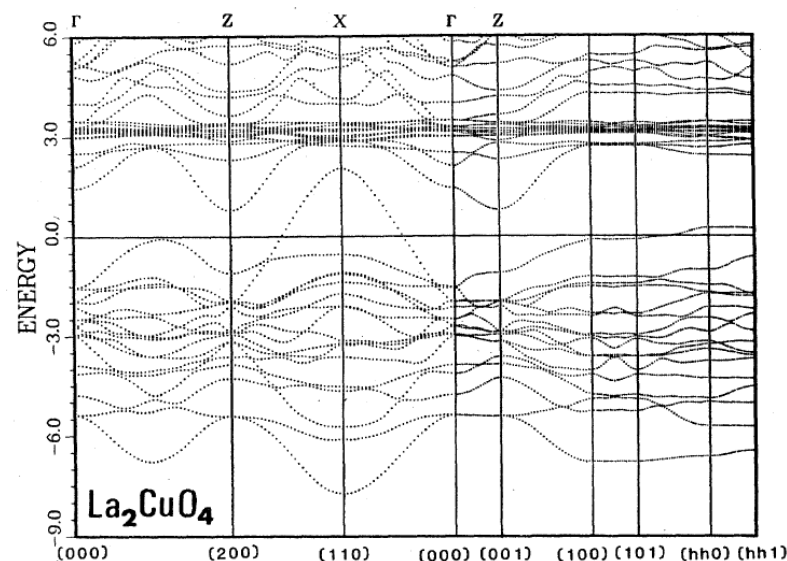
# The role of screening: from Mott to Wigner

Onsite repulsión  $U$   
Hopping energy  $t$



1 electron per site/atom

$U \gg t$  Metal insulator transition  
due to localization of electrons



Mott insulator  
(Mott-Hubbard)

Large density of electrons,  
onsite repulsion  
& role of lattice

# The role of screening: from Mott to Wigner

Assume: { 3D, free space (continuum)  
Coulomb  $\propto \frac{e^2}{r}$

Electronic density

$$n = N_e / V$$

$N_e$ : Number of electrons  
 $V$ : Volume

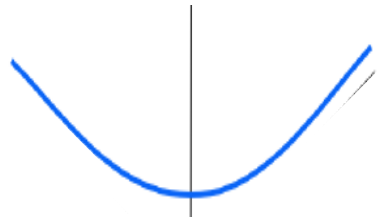
Kinetic energy

$$\int_{-\infty}^{\epsilon_F} \epsilon N(\epsilon) d\epsilon \propto n^{2/3}$$

$N(\epsilon)$ : density of states

Interaction energy

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

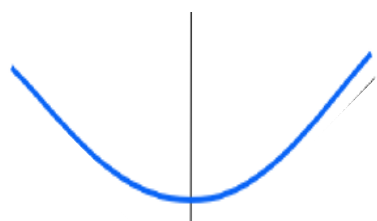


Interaction energy  
Kinetic energy

$$\propto n^{-1/3}$$

← Larger for small density  
Important in semiconductors

# The role of screening: from Mott to Wigner



Interaction energy  
Kinetic energy

$$\propto n^{-1/3}$$

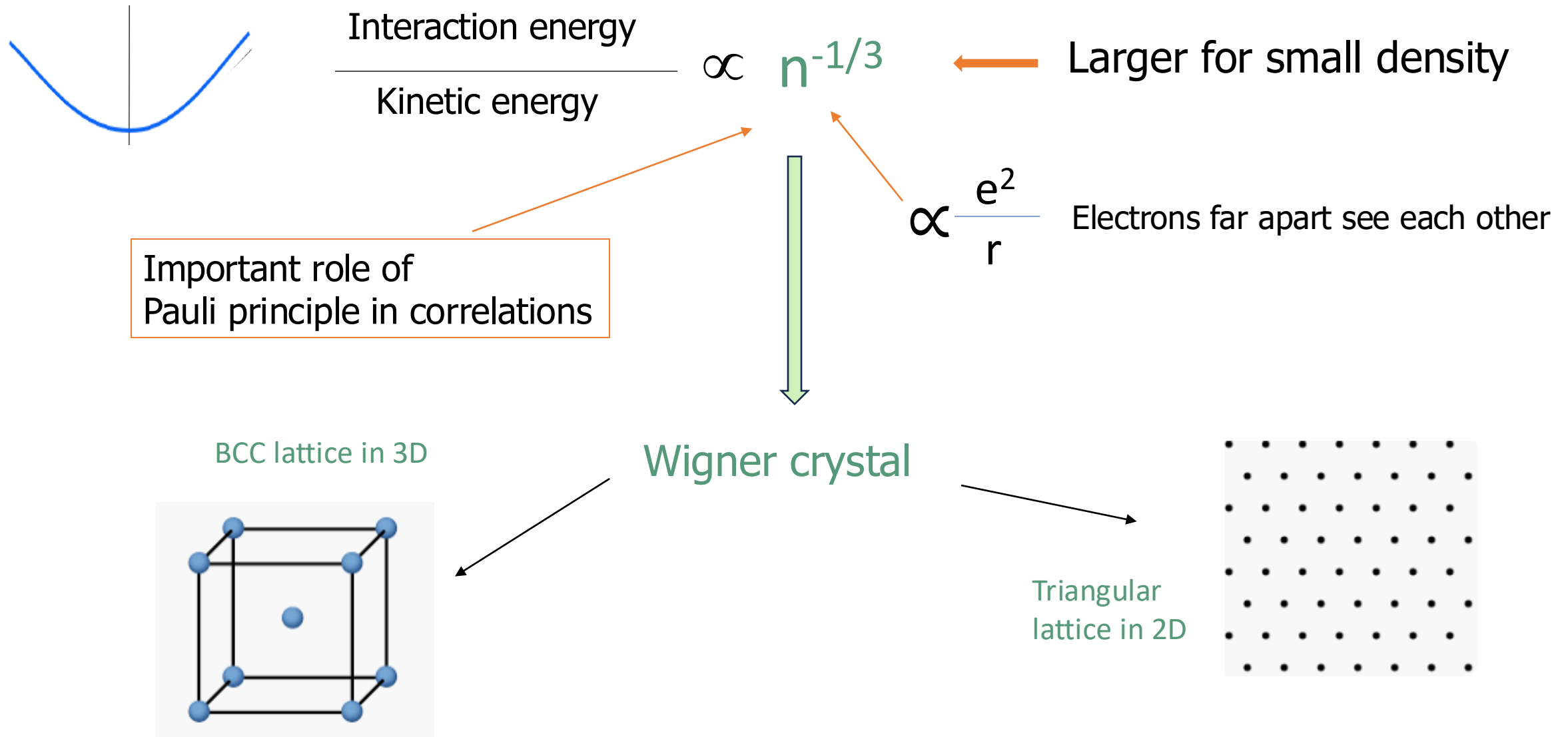
← Larger for small density

$$\propto \frac{e^2}{r}$$

Electrons far apart see each other

Important role of  
Pauli principle in correlations

# The role of screening: from Mott to Wigner



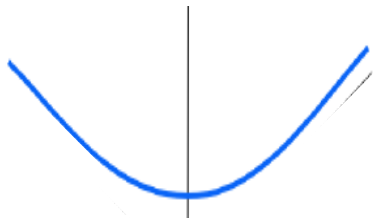
# The role of screening: from Mott to Wigner

## Wigner crystal

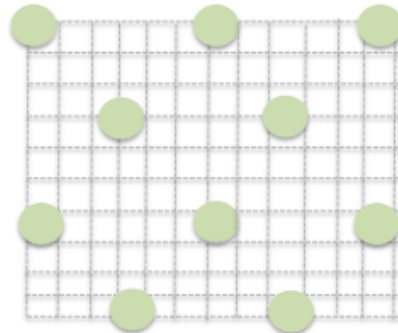
Free space (continuum)

$$\text{Coulomb interaction} \propto \frac{e^2}{r}$$

Insulating for small densities (incommensurate)



Close to the bottom of the band  
The lattice less important



Breaks lattice symmetry

## Mott insulator

Lattice (unit cell)

Onsite interaction  $U$



Larger effect of interactions  
at integer filling of the lattice sites  
(commensurate filling)

Does not break  
the lattice symmetry

Onsite repulsion only:  
Electrons far apart  
do not interact  
(Pauli principle still matters)

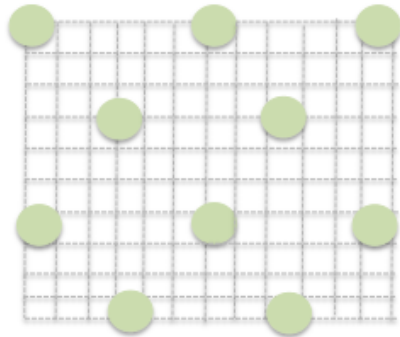
# The role of screening: from Mott to Wigner

## Wigner crystal

Free space (continuum)

$$\text{Coulomb interaction} \propto \frac{e^2}{r}$$

Insulating for small densities (incommensurate)



## Mott insulator

Lattice (unit cell)

Onsite interaction  $U$



Larger effect of interactions  
at integer filling of the lattice sites

Charge localization (spin not invoked in insulating behavior)

# Generalized Wigner or Wigner-Mott

Extended Hubbard: finite range of interaction

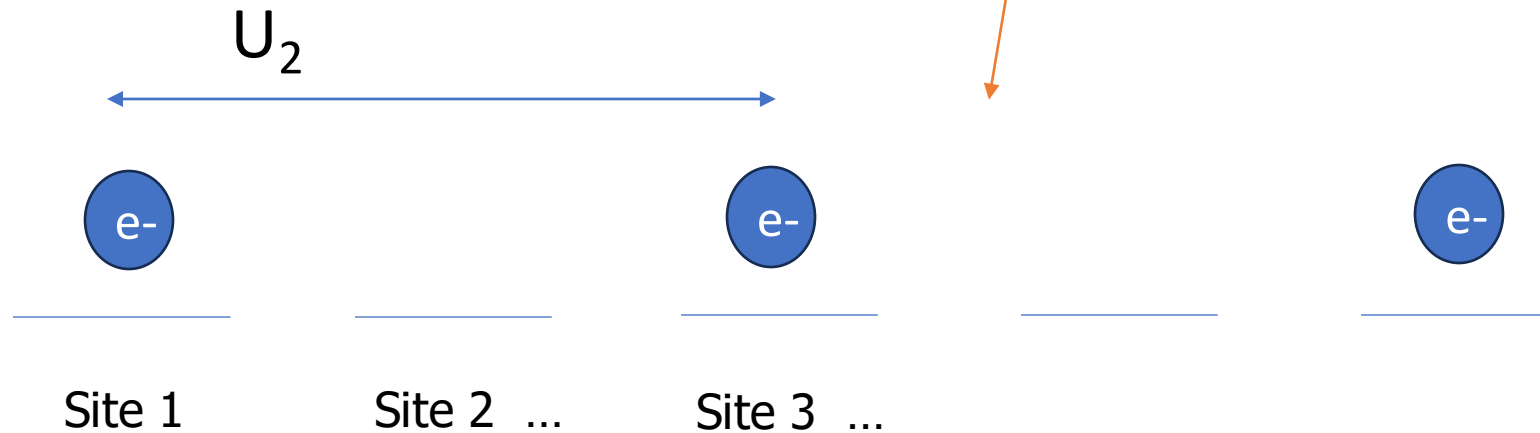
Commensurate filling



Repulsion up to  
1st nearest neighbors

Break the lattice symmetry

An orange arrow points from Site 2 to Site 3, indicating a transition or a change in the lattice symmetry.



Repulsion up to  
2nd nearest neighbors

# Generalized Wigner or Wigner-Mott

Extended Hubbard: finite range of interaction

Commensurate filling

Repulsion up to  
1st nearest neighbors

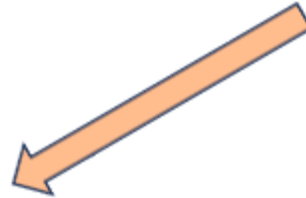


# Emergence of Correlated Phases in Novel Materials

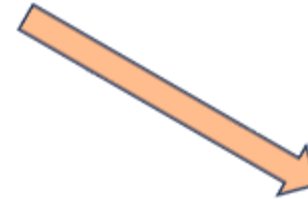
Interactions between many particles (electrons)



Correlated Quantum States  
(Tunability)



Symmetry breaking states



Formation of local moments



Among other effects

# Tuning parameters for correlated states

Interaction energy vs Kinetic energy (& Topology)

- ☐ Filling of electronic bands
- ☐ Electronic bands details
- ☐ Dimensionality
- ☐ Crystalline lattice
- ☐ Screening
- ☐ External knobs (pressure, ...)
- ☐ Interaction with lattice
- ☐ Other (spin-orbit, ...)

40 years of intensive research effort and continuously new surprises appear

# Emergence of quantum phases in novel materials

## Basic ideas & generic concepts

Different kinds of phenomena  
& why they happen

## Theoretical description

Many different approaches and  
analytical & numerical methods

Experimental signatures  
of the quantum states. Novel  
ways to probe these states

Materials and platforms  
where these quantum phases appear