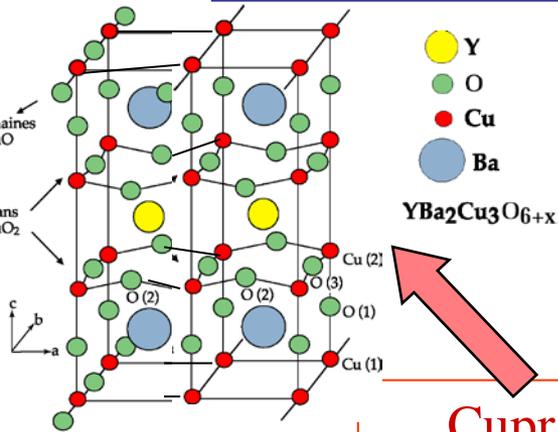
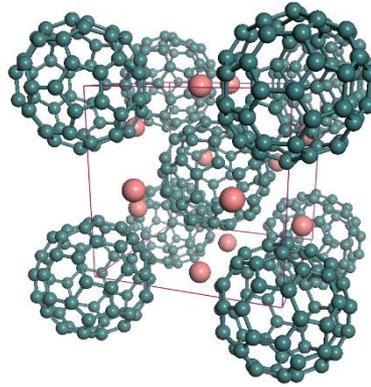


Correlated quantum matter: Mott transition, unconventional superconductivity,... charge order

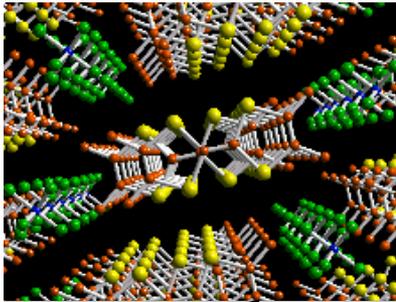
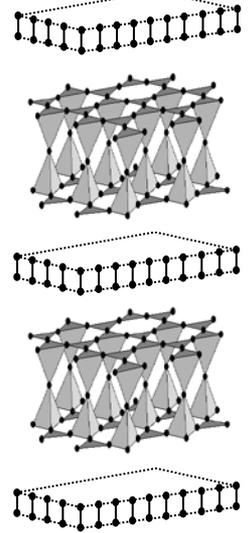


Cuprates

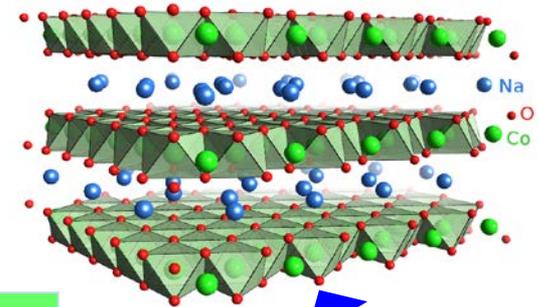


Fullerites

Highly frustrated Magnets (Kagome lattices)



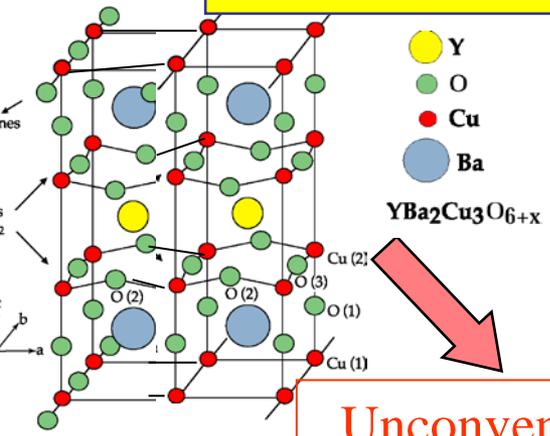
Organic Superconductors



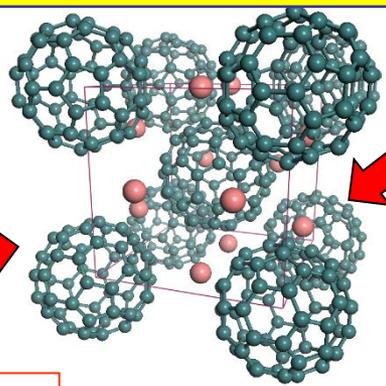
Cobaltates

Those are new materials discovered and synthesized within the last 40 years

Correlated quantum matter: Mott transition, unconventional superconductivity,... charge order

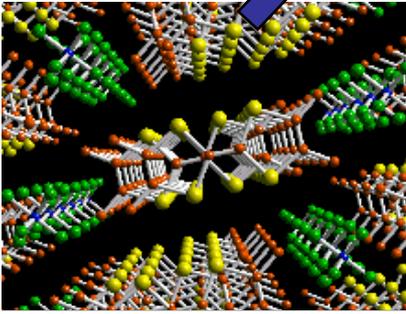
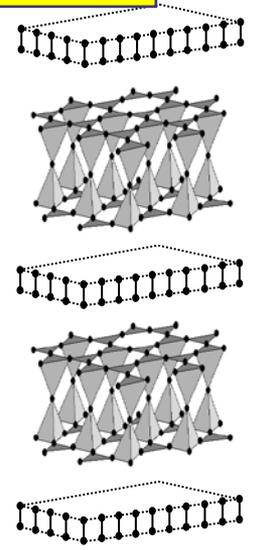


Unconventionnal Superconductivity



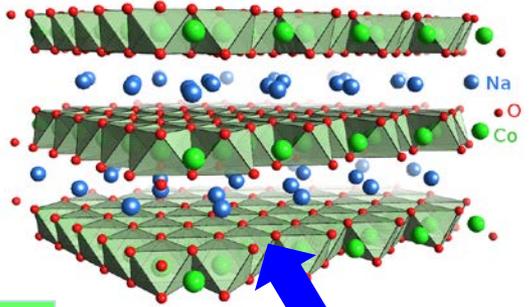
Mott transition
 Cs_3C_{60}

2D Quantum Spin Liquids



1D Luttinger liquids

High Thermoelectric power



Charge Order

Those emergent observations require interactions between electrons

Correlated quantum matter: Mott transition, unconventional superconductivity,... charge order

Correlated electron systems, an introduction

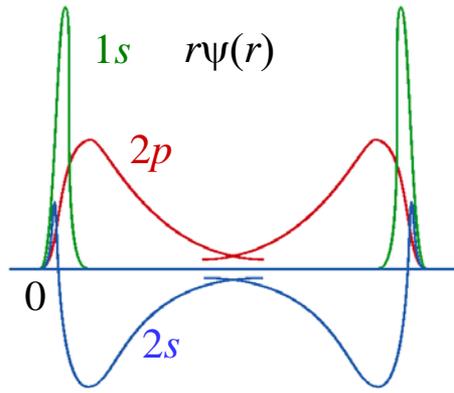
- **Band theory: insulators , metals , Fermi liquids**
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- *Mott transition in fullerenes*
 - **Band structure Mott transition in Cs_3C_{60}**
 - **Jahn Teller Distortions**
 - **Phase diagram**
- *Unconventional superconductivity*
 - **Cuprates : doped Mott insulators**
 - **Pseudogap - Incidence of impurities**
 - **SC gap in Cs_3C_{60}**
 - **Pseudogap and SC fluctuations in cuprates**
- *Charge orders*
 - **Charge order and phase diagram in cuprates**
 - **Disproportionation in sodium cobaltates Na_xCoO_2**

Conclusions

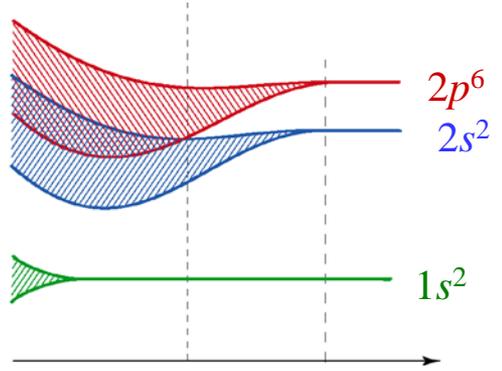


Independent electron band structures: Ne and Na

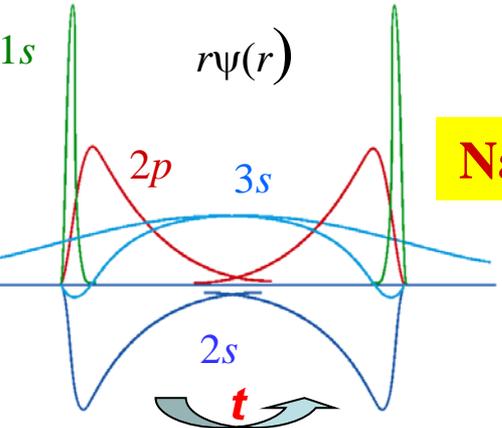
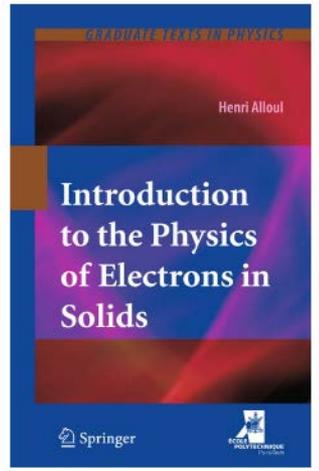
$3s^1$



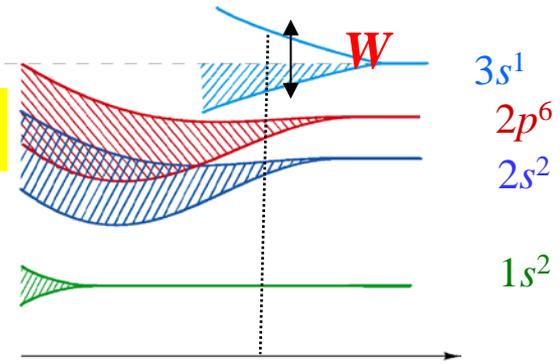
Ne



**Last band is full
INSULATOR**



Na



**Last band partly filled
METAL**

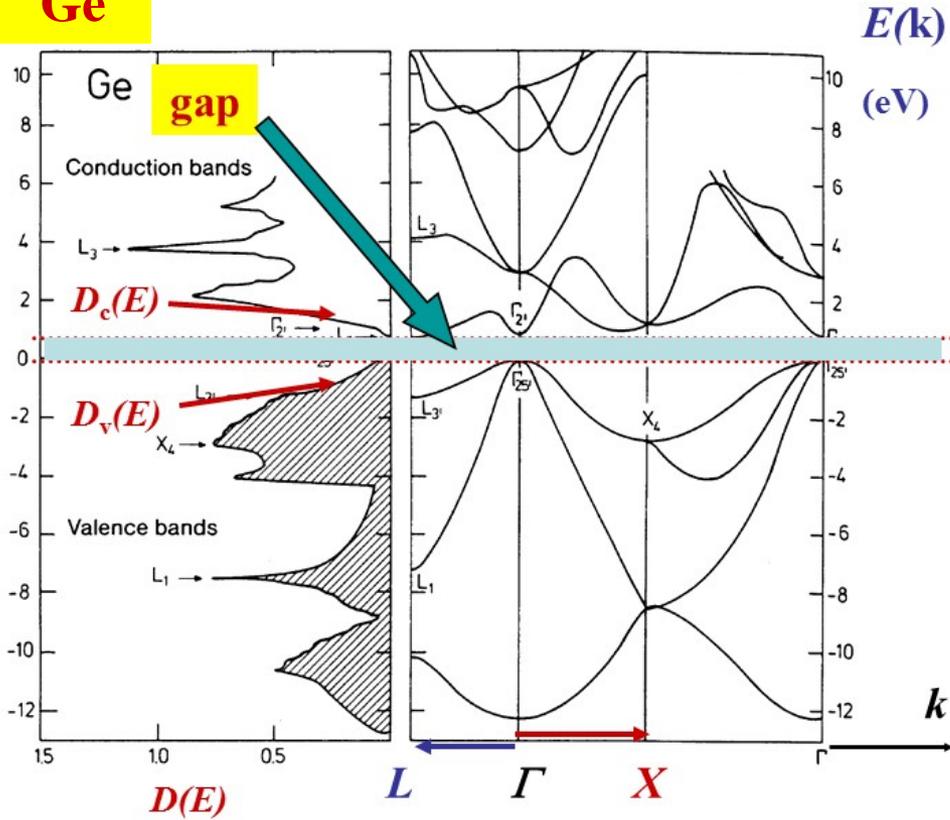
Transfer integral
from site to site

**t determines the bandwidth $W = z t$
Both increase with decreasing d**

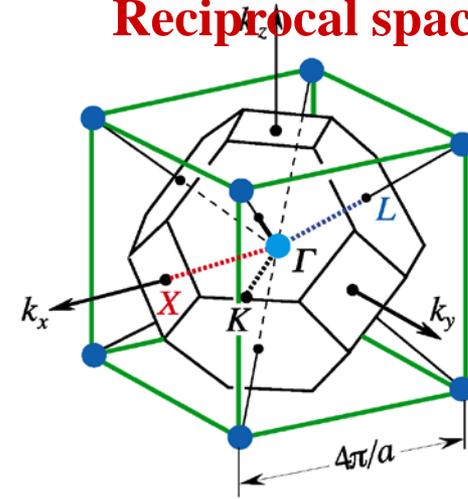
z near neighbours

Band Structure and Brillouin zone

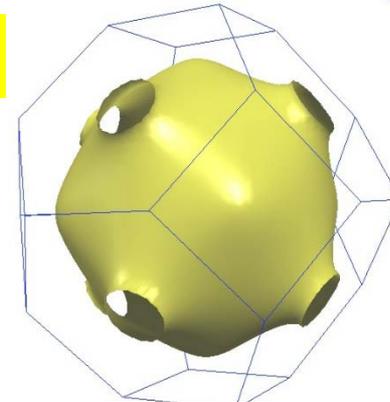
Ge



Reciprocal space



Cu



Even number of electrons
Valence bands are full at $T=0$
SEMICONDUCTOR
insulator with low energy gap

Odd number of electrons
METAL
Last band half filled
Delimited by the Fermi surface

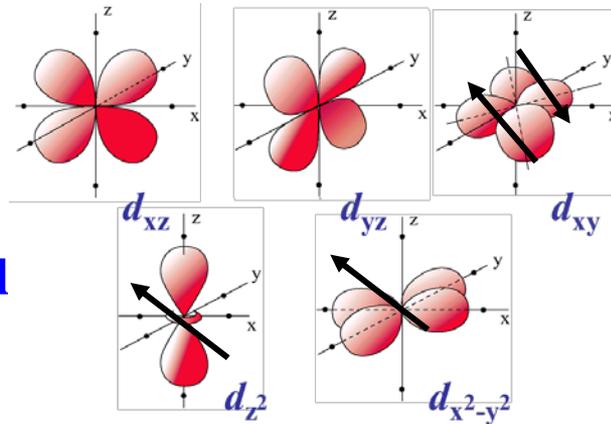
Broad bands : quasi free electron metals (small U)

WHAT ABOUT MAGNETISM?

ATOMIC PHYSICS

One needs to take into account local correlation effects in partly filled atomic shells

***d* orbitals**



Weaker interorbital
coulomb energy J

Large intraorbital
coulomb energy U

Filling of the electronic states
follows Hund's rules

For instance Mn^{2+}



$S=5/2$

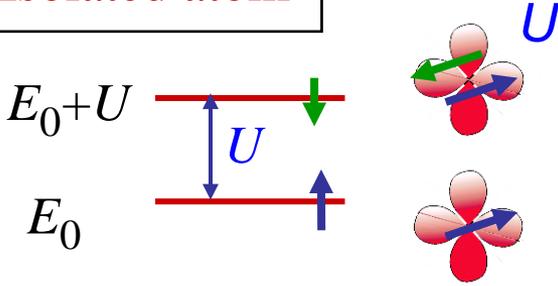
U Localise the electrons on the given orbitals

**U induces local moments on atomic sites
This yields a Mott insulator in the solid state
Which can be magnetic**

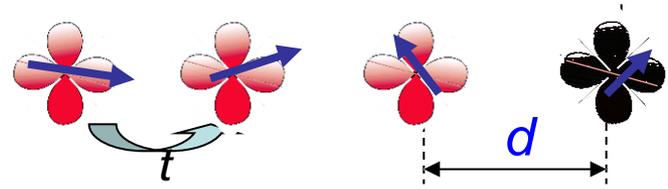
Hubbard model and Mott insulator to metal transition

A single orbital per site

Isolated atom



Solid state

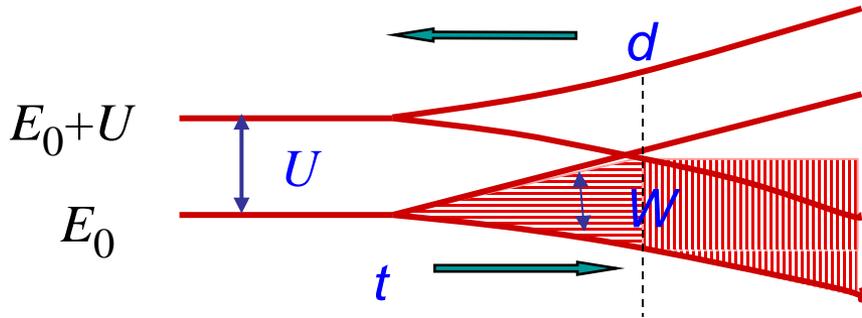


Electrons quasi localised on each site

t competes with U

t and bandwidth $W = zt$ increase with decreasing d

Coulomb repulsion U

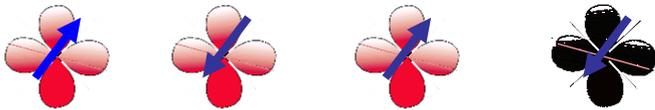


Bandwith $W = z t$
 z near neighbours

U Charge localization
Magnetism

MOTT INSULATOR $U > W$

METAL $W > U$



insulating AF ground state

Mott transition to a metallic state
Should be induced by pressure

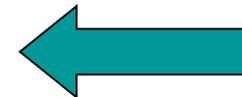


N. Mott
Nobel prize 1977

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Correlated electron systems, an introduction

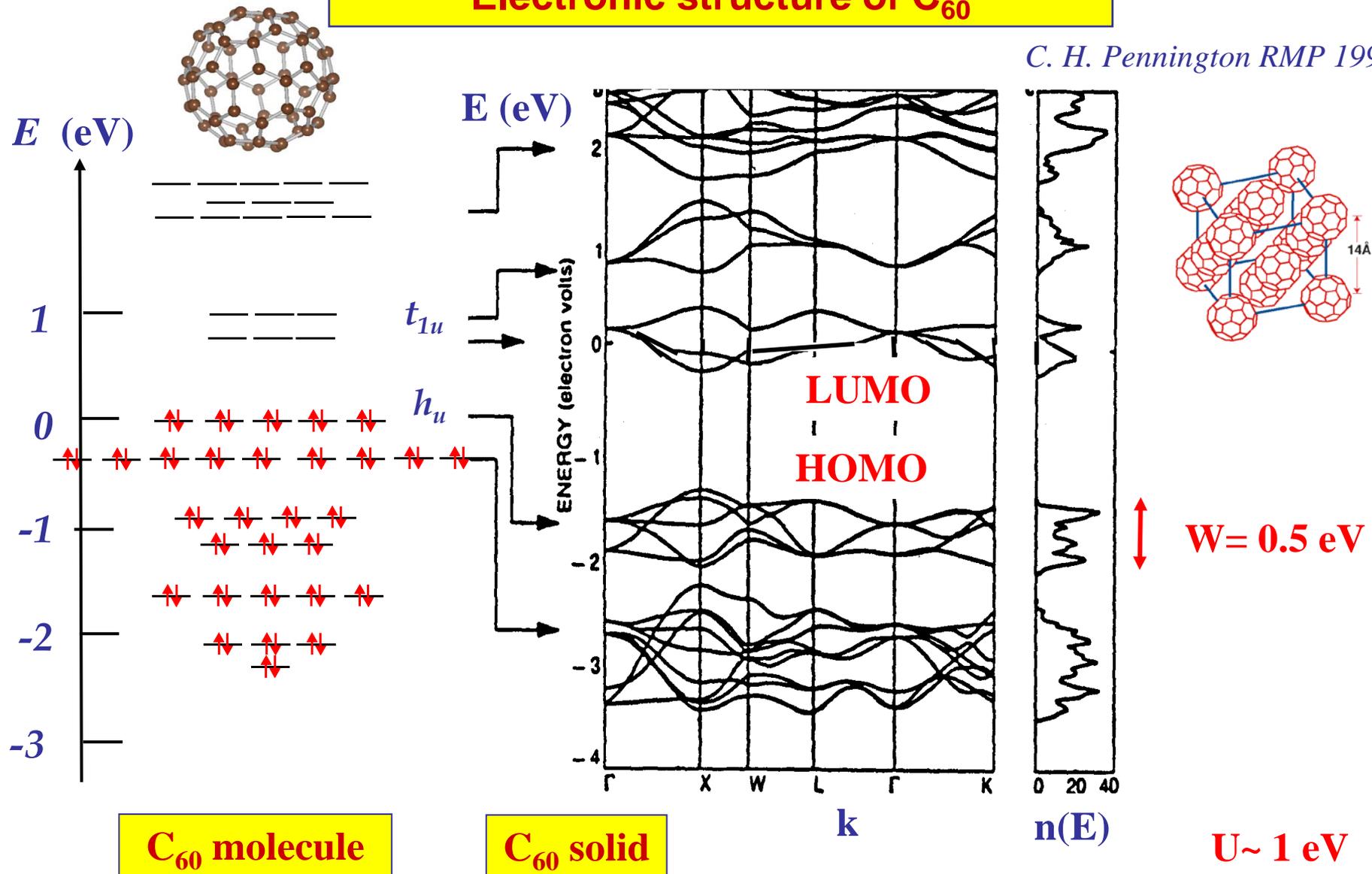
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Conclusions

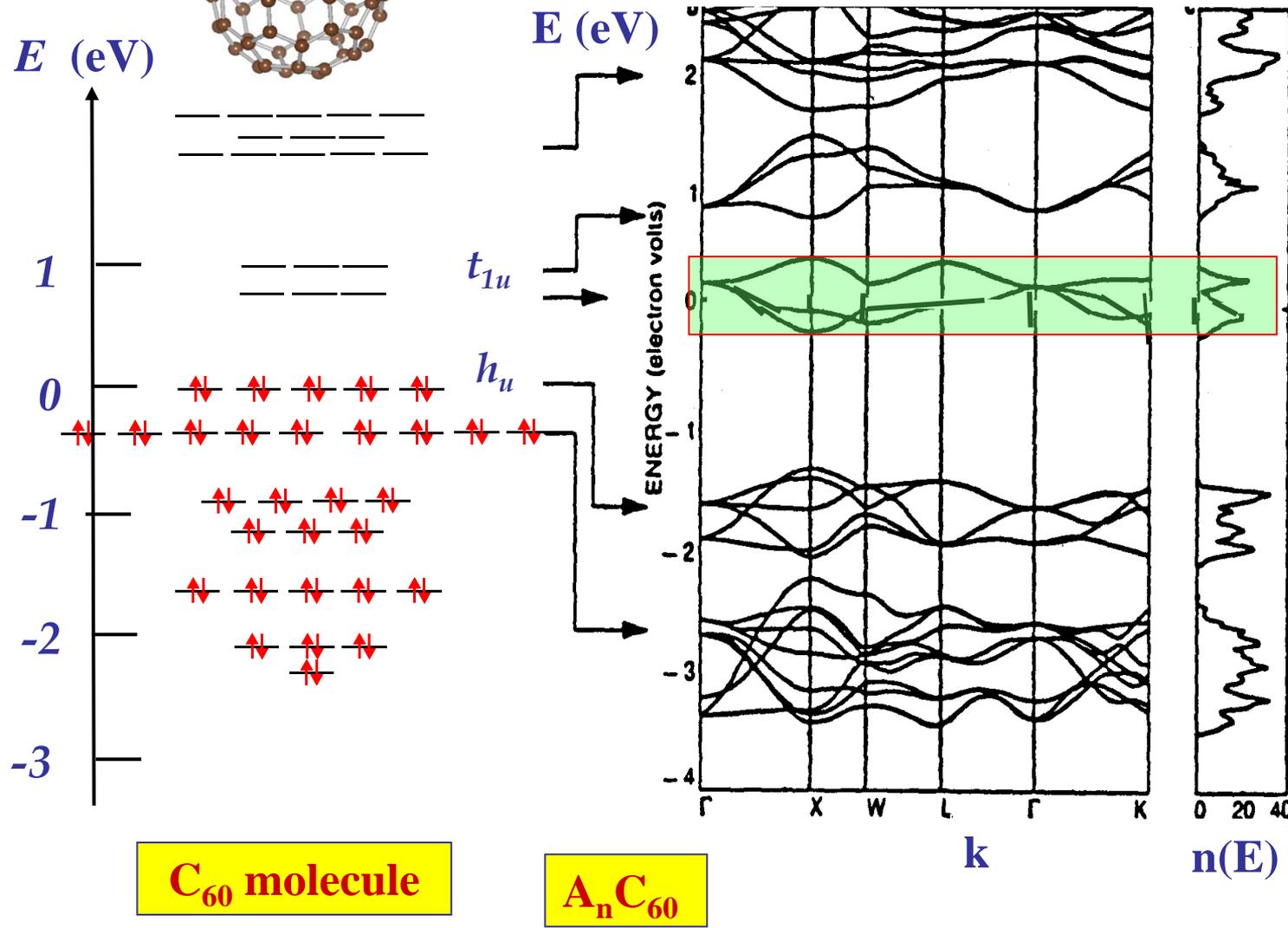
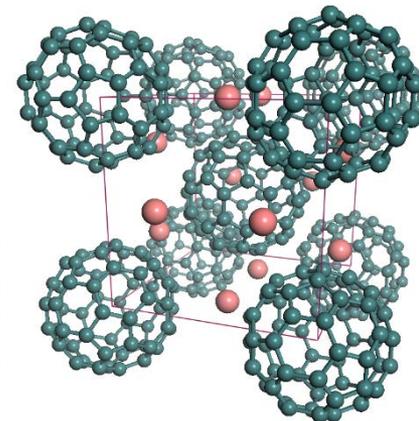
Electronic structure of C_{60}

C. H. Pennington RMP 1995.



Electronic structure of doped fullerides

C. H. Pennington RMP 1995.



n charges transferred from alkali to C_{60}

$W = 0.5 \text{ eV}$

$U \sim 1 \text{ eV}$

C₆₀ molecule

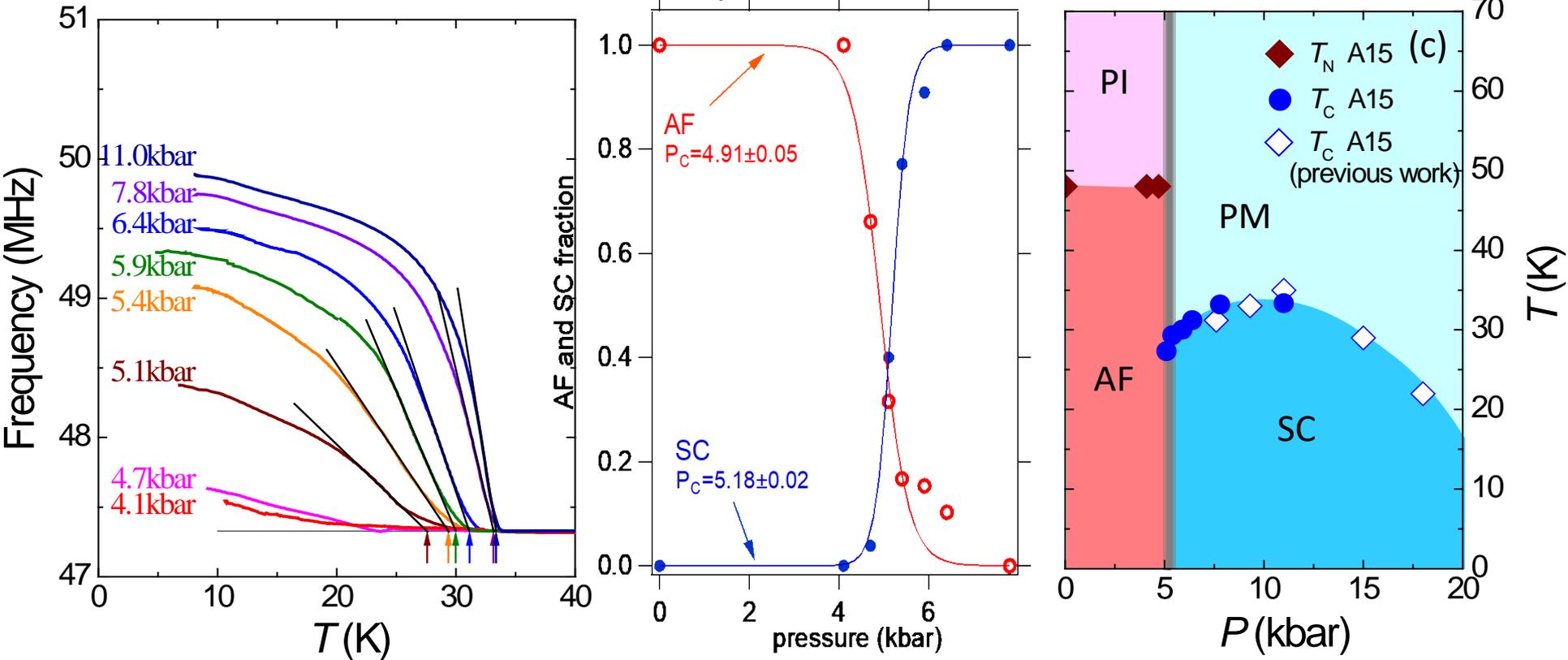
A_nC₆₀

A_nC₆₀ should be metallic for any doping 0 < n < 6

Mott transition to the metallic state in a clean A15 sample

Sharp establishment of the SC state

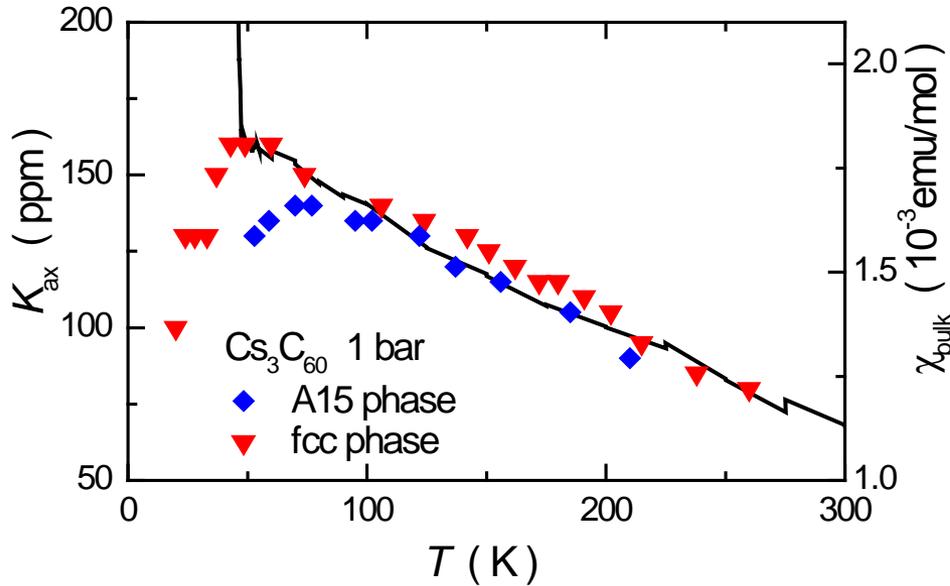
P. Wzietek, et al, Phys. Rev. Lett. 112, 066401 (2014), arXiv1310.55



Insulating Paramagnetic state

^{13}C NMR

$$K_{\text{ax}} = A \chi_s$$



High T Curie-Weiss behavior

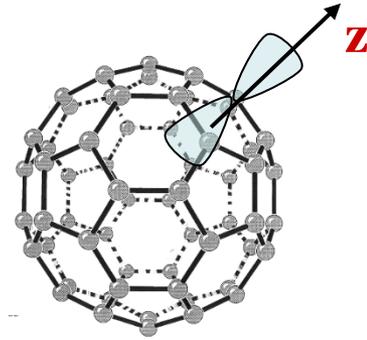
$$\chi = p_{\text{eff}}^2 / 3k_B(T + \theta)$$

$$\theta \sim 100 \text{ K}$$

Effective moment : $p_{\text{eff}} \sim 1.70 \mu_B$

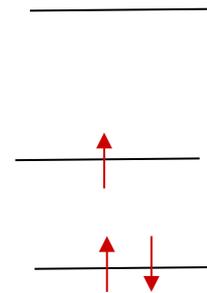
S ~ 1/2 on the C₆₀ balls?

Molecular orbitals:
constructed from p_z orbitals



Here A is dipolar $A_{\text{exp}} \sim 700 \text{ Oe}/\mu_B$
Calculated value : $A = 640 \text{ Oe}/\mu_B$

**Local moment is indeed
on the C₆₀ balls!**



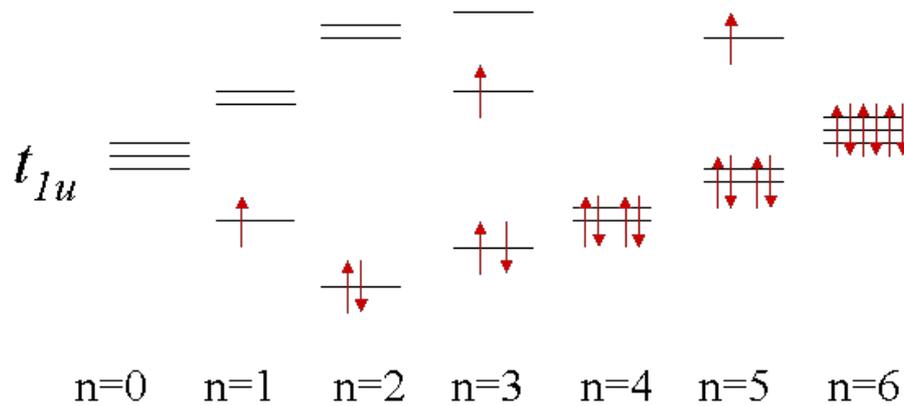
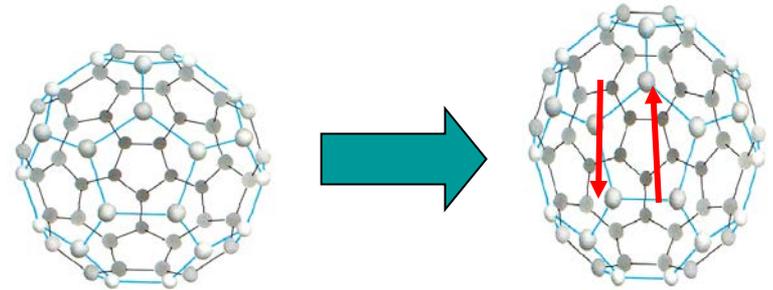
Low spin state (JTD)

Strong electronic correlations on the molecular orbitals

In A_nC_{60} the coulomb repulsion for two electrons on a ball is $U \sim 1\text{eV}$

For a charged molecule

The degeneracy of the t_{1u} level is lifted by a **Jahn Teller distortion**



Here Hund's rules are inverted

Manini, Tosatti PRB94

For $n=3$

Low spin $S=1/2$

rather than high spin $S=3/2$



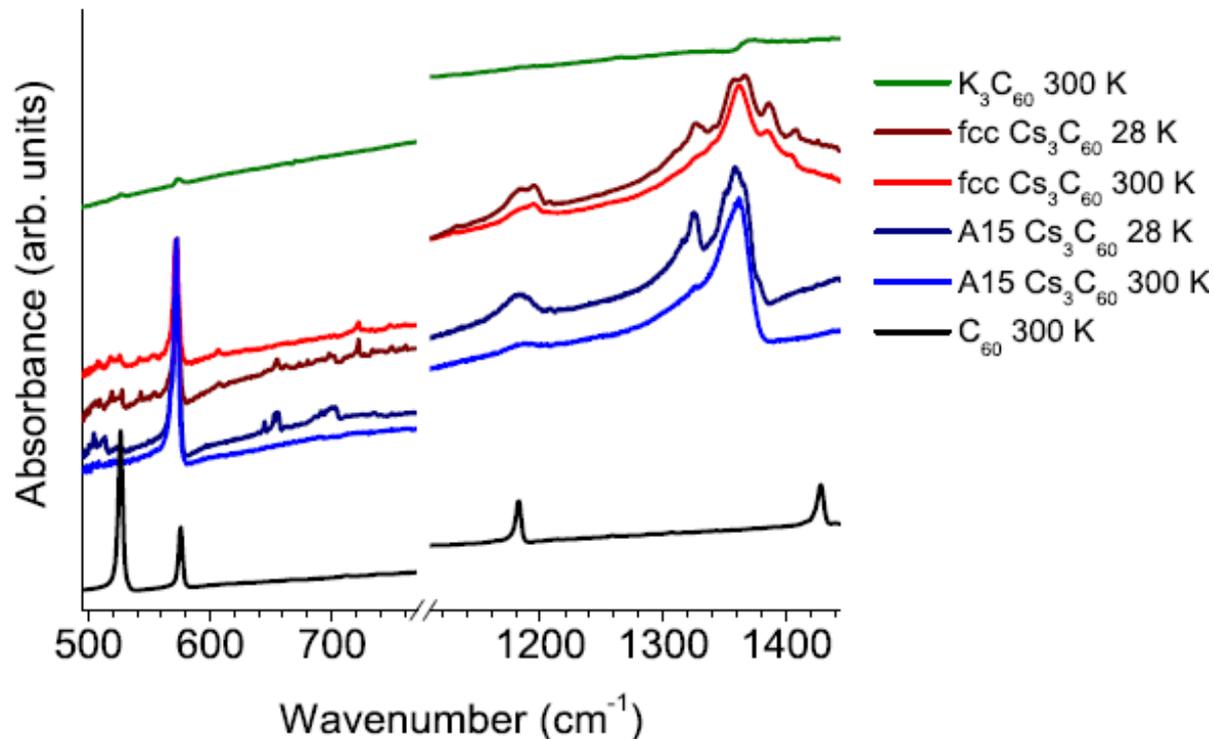
*M. Héritier, W. Victoroff,
O. Gunnarson,
M. Fabrizio, E. Tosatti*

The Jahn-Teller splitting of the t_{1u} level depends on the C_{60} charge

Interplay of electronic interactions and JTD

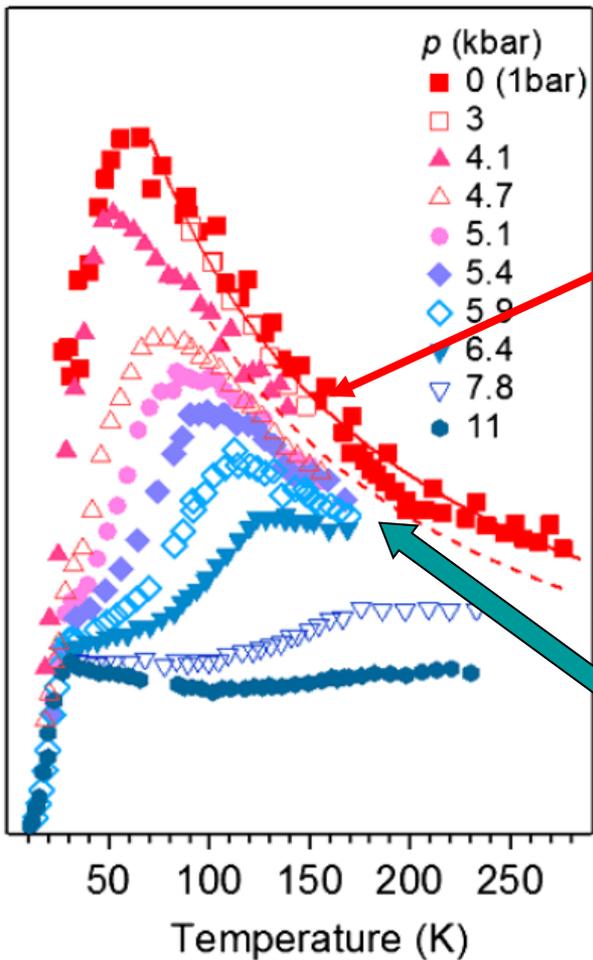
IR experiments give direct confirmation of the JTD state

Klupp G, Matus P, Kamarás K, et al, Nature Communications 3 912 (2012)



The C_{60} balls are indeed JT distorted on a large T range in both A15 and fcc phases hence the low spin state

Second step transition varies with applied pressure



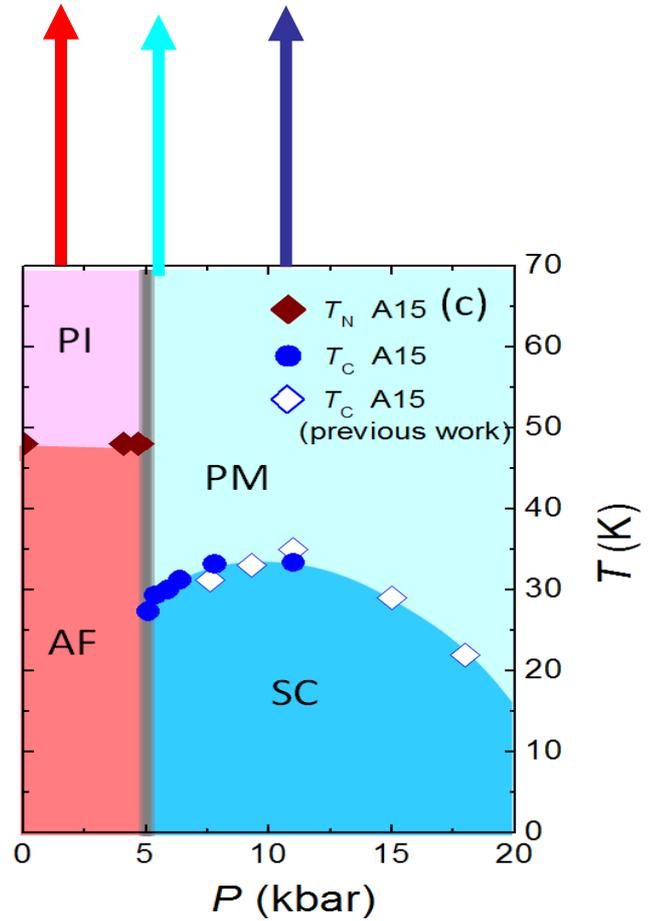
0.15 Dense paramagnet phase well above T_N

$$\frac{1}{T_1} = A_{hyf}^2 \frac{\sqrt{\pi S(S+1)/3}}{\gamma_e \mu_B k_B z J}$$

0.10
0.05
0.00

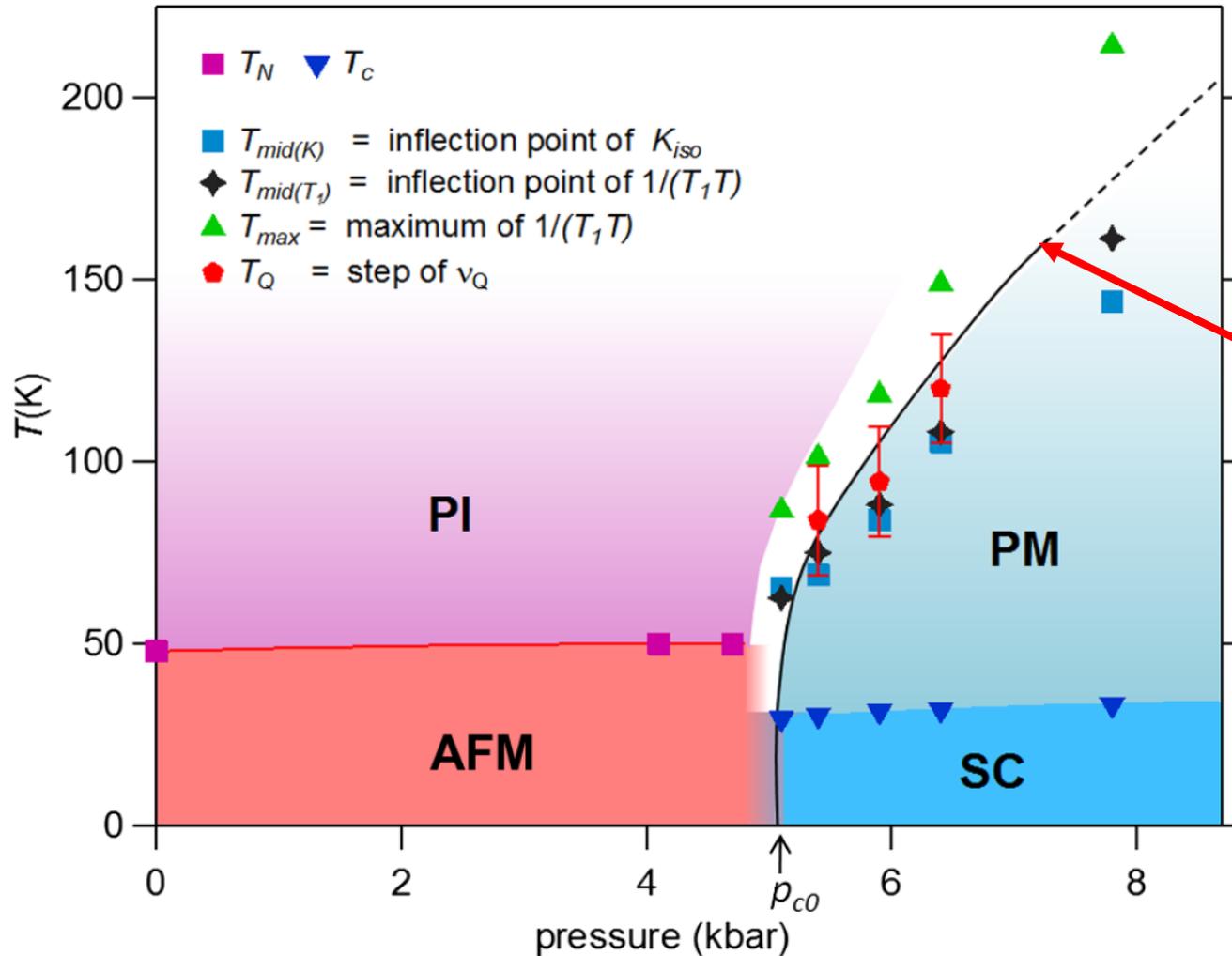
$1/T_1 T$ ($s^{-1} K^{-1}$)

The insulating phase behaviour is recovered with increasing T



The second step transition corresponds to the restoration of the insulating paramagnetic state (MIT)

Overall phase diagram with critical point



At high p
Step of v_Q disappears

Transition broadens

Critical point p_c
as for liquid vapor

*H. Alloul et al
PRL (2017)*

MIT varies upon lattice expansion that is t/U ?

Correlated quantum matter: Mott transition, unconventional superconductivity,... charge order

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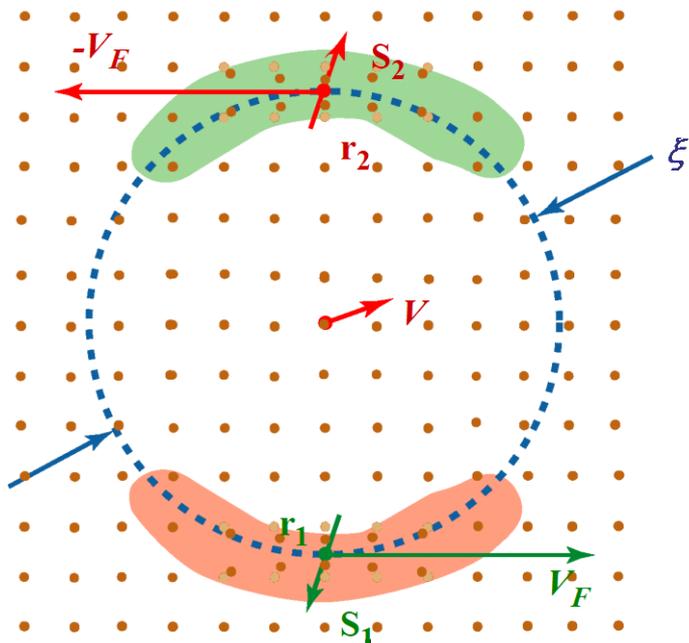
Conclusions

Phonon BCS Superconductivity opposes Mott physics

Attractive coupling between electrons mediated by the lattice phonons



Bardeen, Cooper and Schrieffer
Nobel prize 1972



BCS superconductivity in metallic alloys
Cooper pairs of electrons

Repulsive electron electron interaction U does not favor superconductivity

Up to the 1980's
Mott physics and magnetism were considered as detrimental to SC

Upper limit for T_c (23K) ?



New superconductors : the discovery of high T_c cuprates in 1986

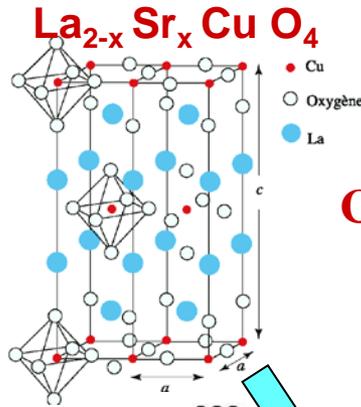


A. Mueller and G. Bednorz

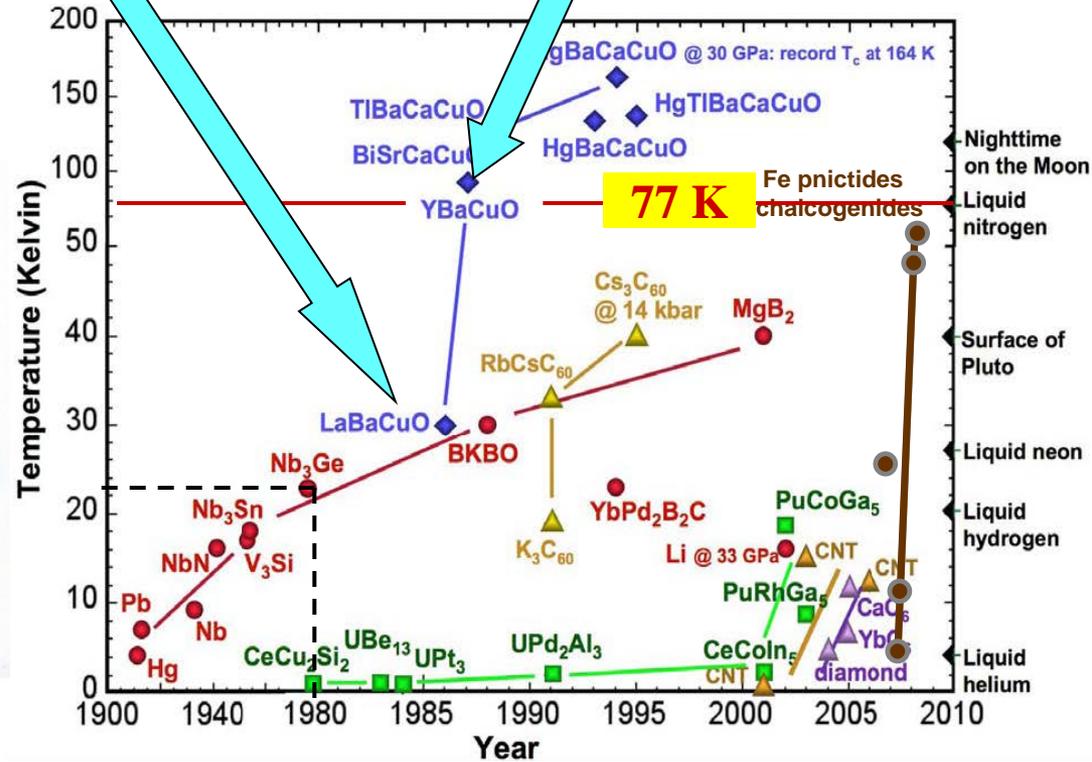
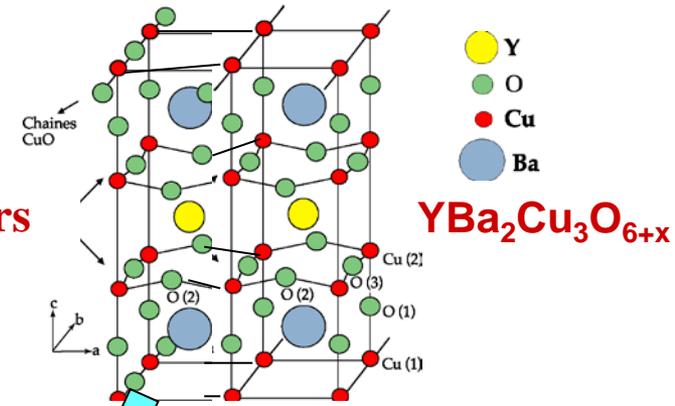
Nobel prize 1987

High T_c : applications!!

Popular demonstrations of SC



CuO₂ layers



H.Alloul, « Introduction to the physics of electrons in solids », Springer (2011)



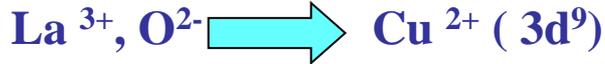
Laboratoire d'Excellence
Physique : Atomes Lumière Matière

H.Alloul, ICAM Annual Meeting Hsinchu (Taiwan), January 15th (2019)



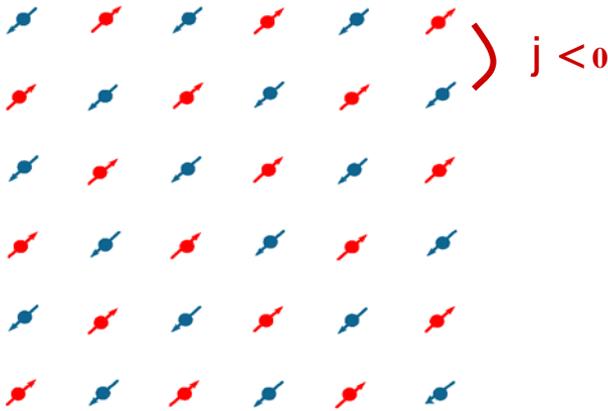
From the Mott insulator to the high T_c superconductor

Physical properties of cuprates are controlled by **doping**

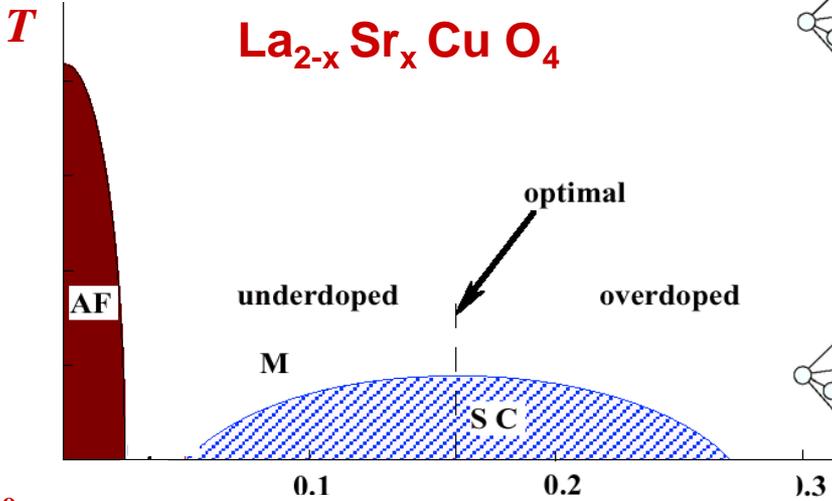
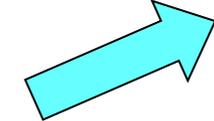


One hole per Cu on 3d level

S=1/2 Mott insulator
AF ground state



Large coulomb repulsion U

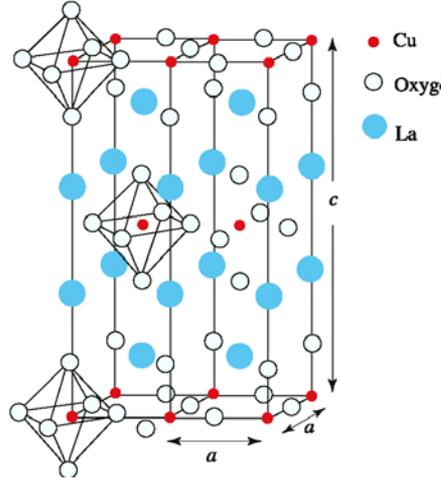


Sr²⁺ replaces La³⁺
 x extra holes per Cu



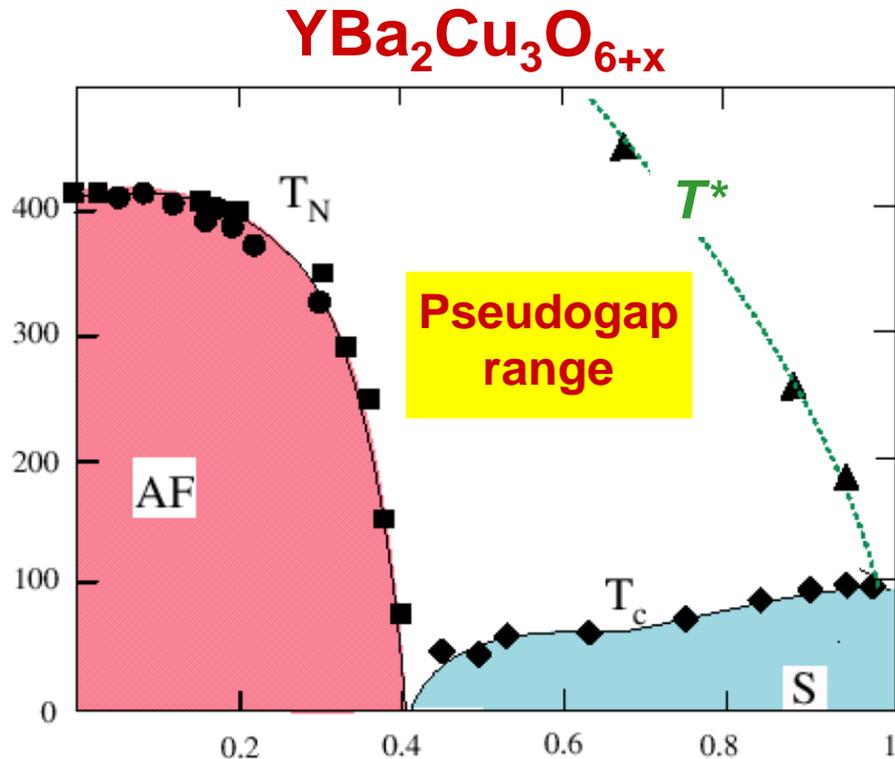
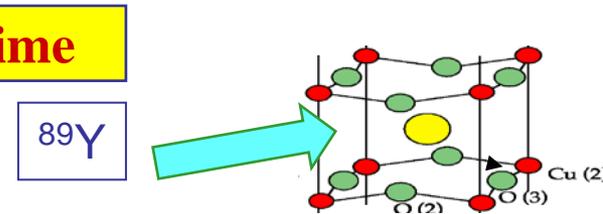
**Doped Mott insulators
are Superconducting metals
with high T_c**

**Persistence of correlations
in the doped materials?**



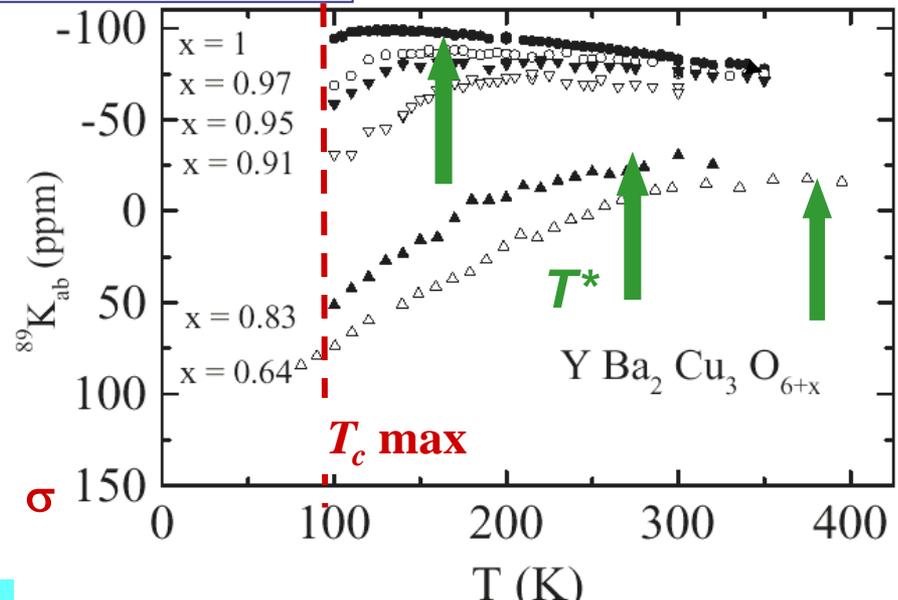
NMR evidence for a pseudogap regime

H.Alloul, T. Ohno and P. Mendels, PRL 1989



Chemical shift \rightarrow $^{89}\text{Y NMR shift}$

Hyperfine coupling \rightarrow $^{89}\text{K} = \sigma + A\chi_s(T)$



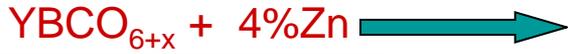
In usual metals χ_s is T independent (as for $x=1$) and vanishes at $T=0$ in the SC

Large loss of $\chi_s(T)$ well above T_c

For $x < 1$ (underdoped range)

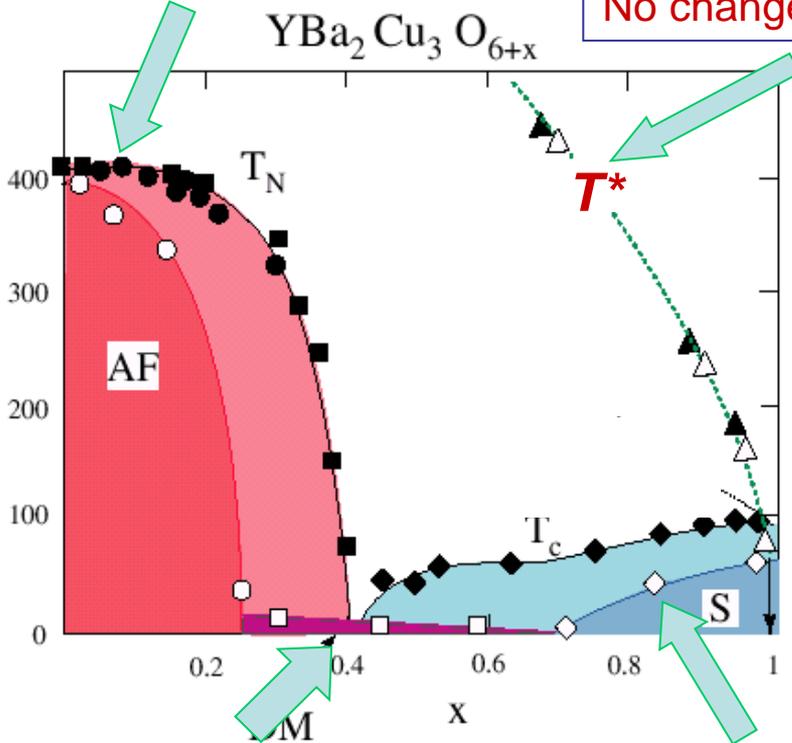
Origin of the pseudogap?

Influence of defects on T_c and on the pseudogap



Dilution effect on T_N

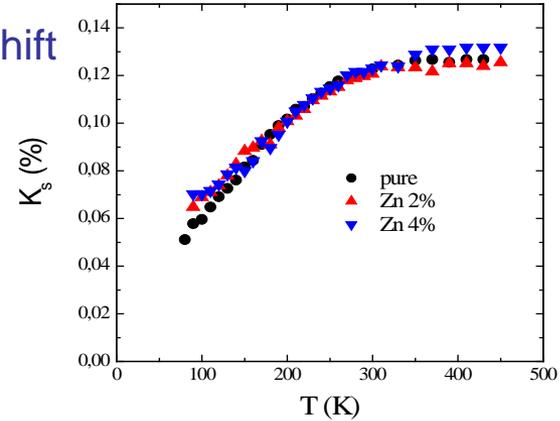
No change of T^*



Increase of the disordered magnetism range

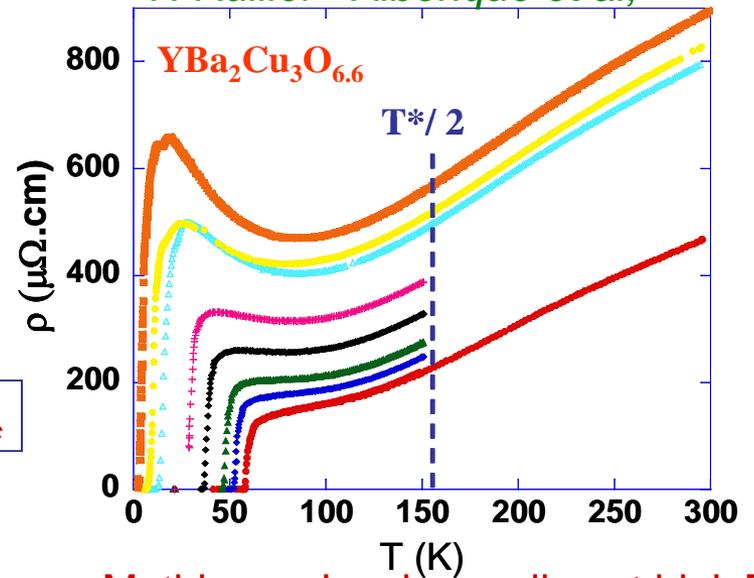
Large depression of T_c

H. Alloul et al, PRL 67, 3140 (1991)



$\rho(T)$ + irradiation by electrons

F. Rullier-Albenque et al,

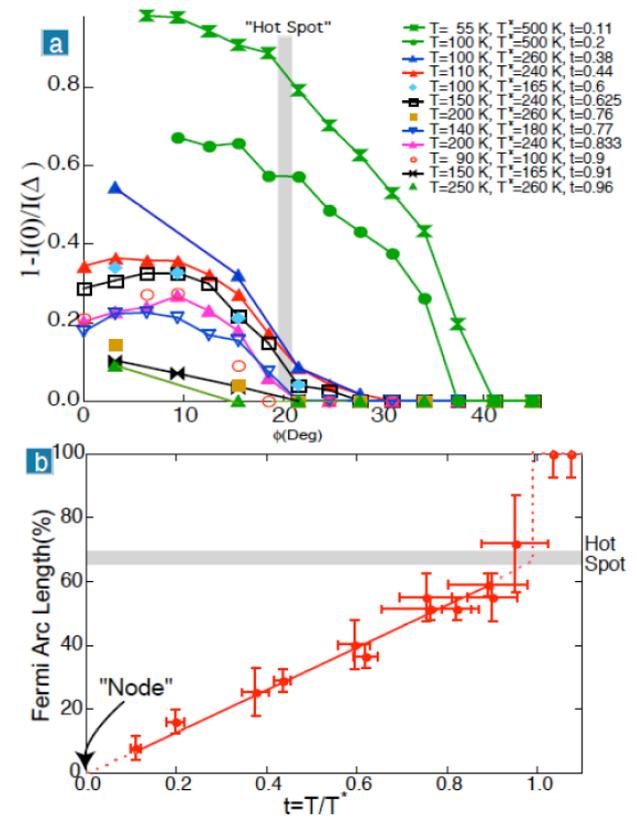
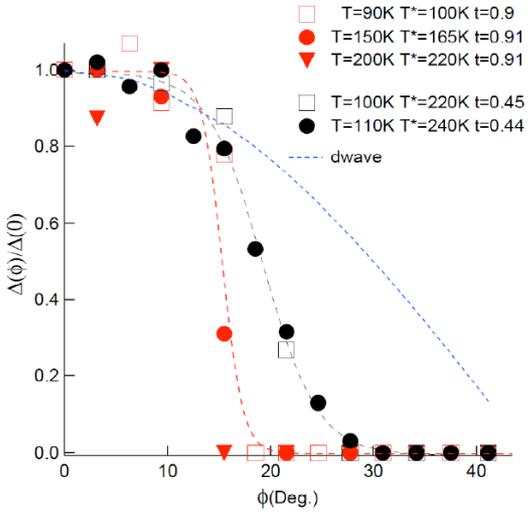
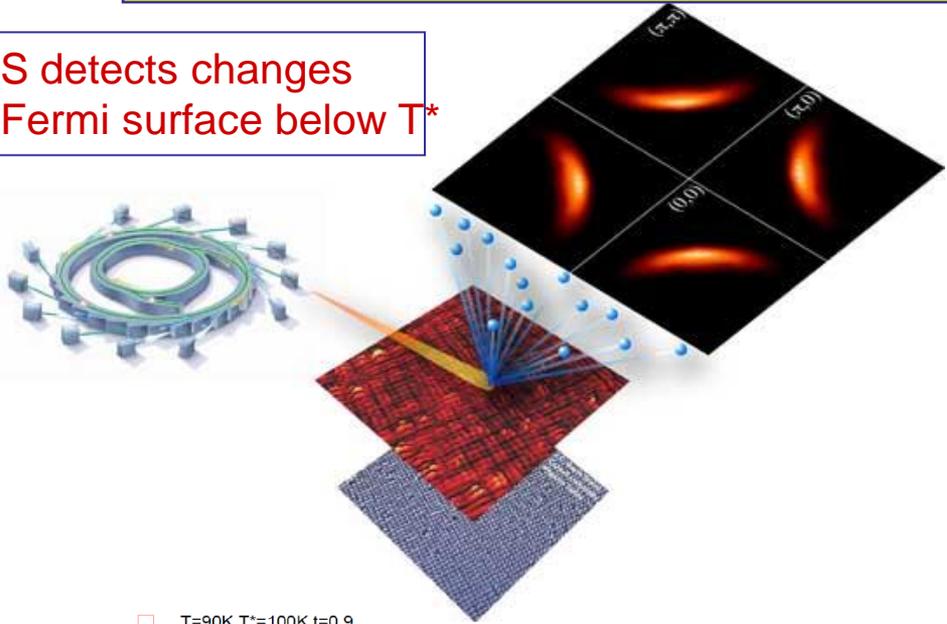


Mathiessen's rule applies at high T

The pseudogap is robust and insensitive to disorder

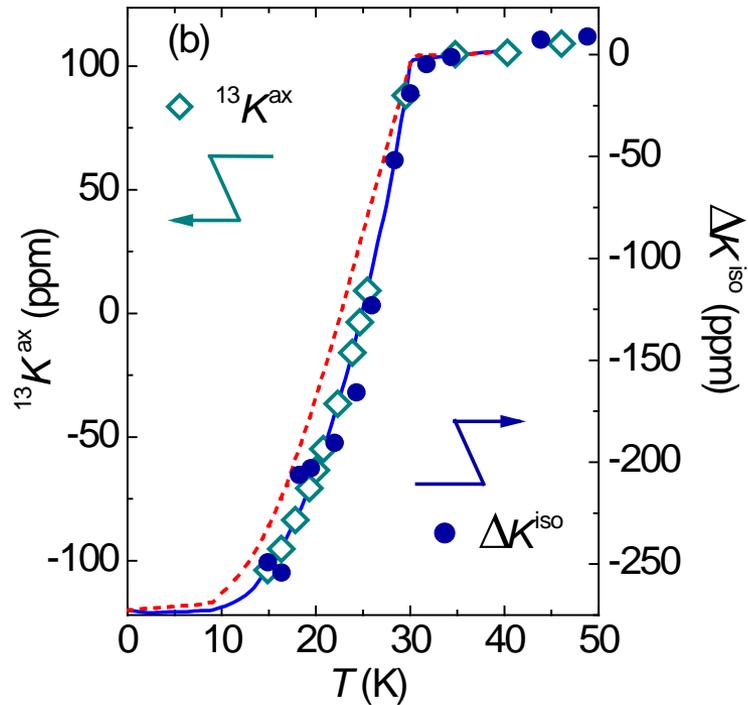
Fermi surface differentiation : Fermi arcs below T^*

ARPES detects changes in the Fermi surface below T^*

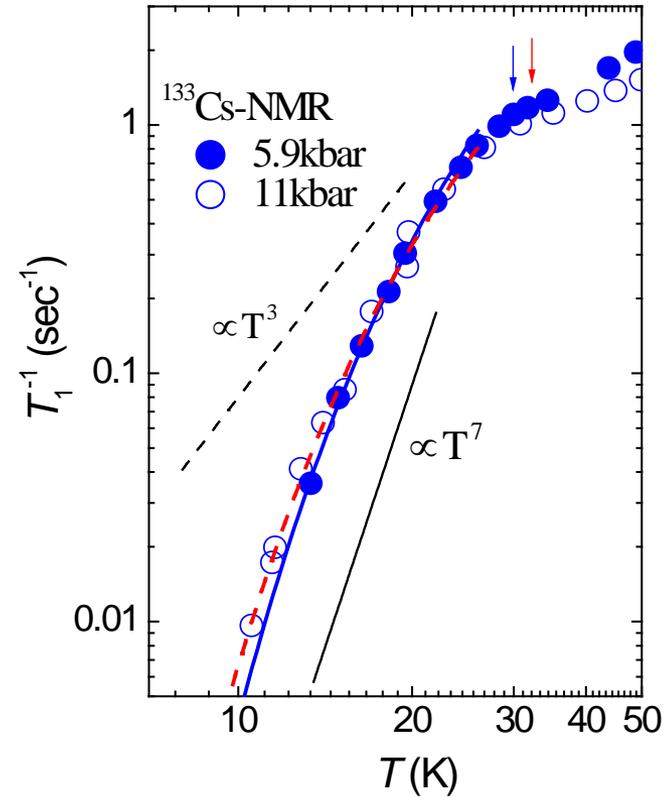


The gap opens in the antinodal directions and progressively extends in the BZ
Decrease of Fermi arc length with decreasing T

Superconducting gap in Cs_3C_{60}



Suppression of the spin susceptibility
in the paired **singlet state**

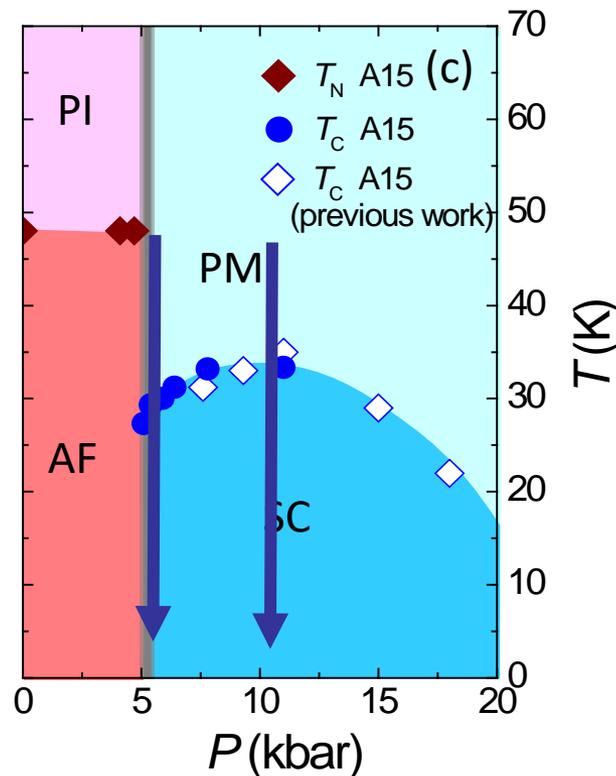
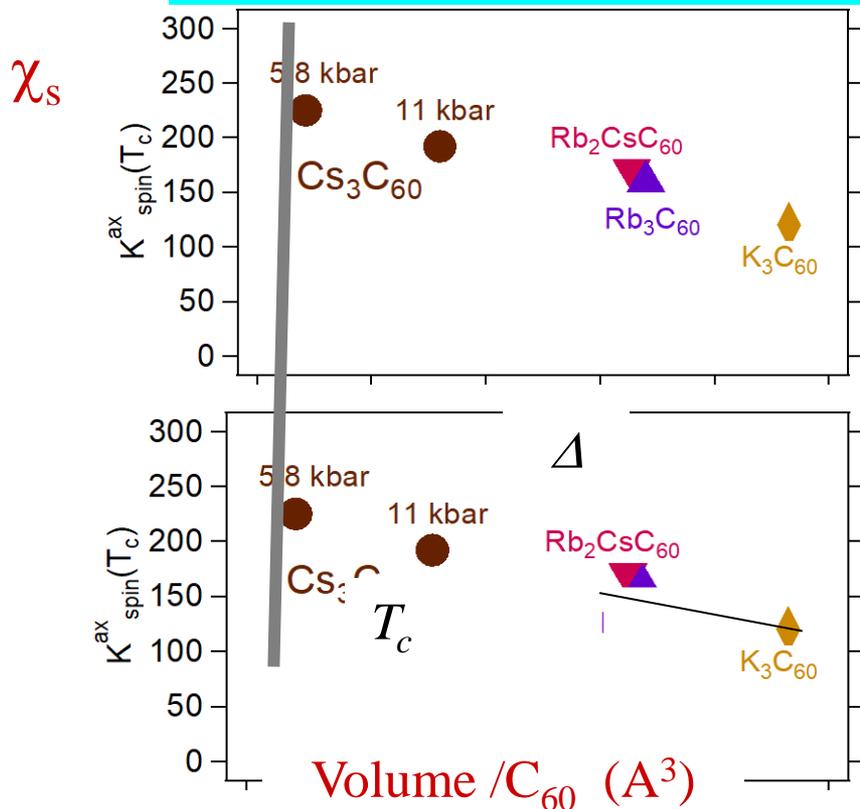


Low T variation of $1/T_1$
Probes the SC excitations
 $1/T_1 \propto \exp(-\Delta/k_B T)$

Isotropic gap (s wave)

Variation of the physical quantities with pressure near the Mott transition

No pseudogap on χ nor on $1/T_1$ near the Mott transition



$$\Delta = 1.75 k_B T_c \text{ for weak coupling BCS}$$

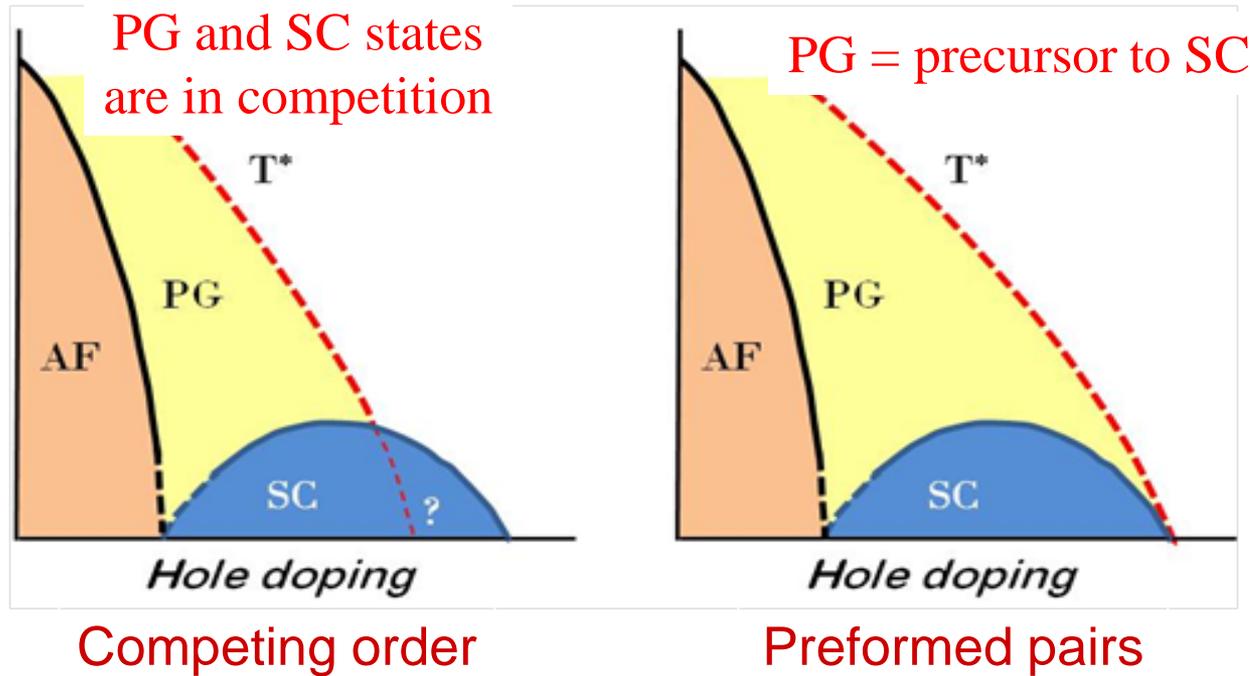
Here the SC gap increases up to the Mott transition and reaches $\Delta = 3 k_B T_c$

But: long lasting controversies on the pseudogap

Google quotations 2014

- « BCS superconductor » 14 200
- « Cuprate superconductor » 31 000
- « Pseudogap in cuprates » 9 700

Competing order or preformed pairs?



Two energy scales in the underdoped range?

How can one probe the SC fluctuations?

Superconducting fluctuations up to T^* ?

Influence of disorder?

H. Alloul, F. Rullier-Albenque et al EPL (2010)

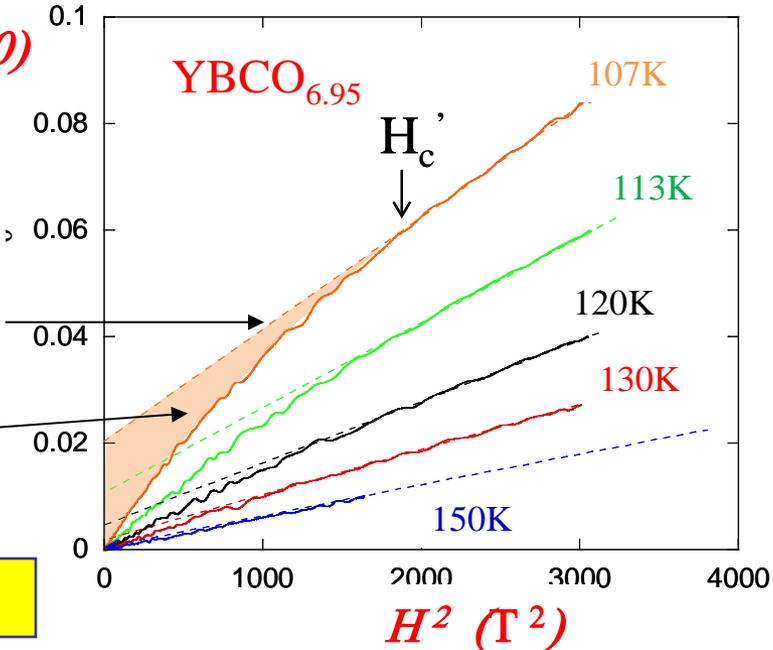
Superconducting fluctuations contribution to the conductivity

F. Rullier-Albenque, H. A. et al, PRL PRB (2011) $\delta\rho/\rho(0)$

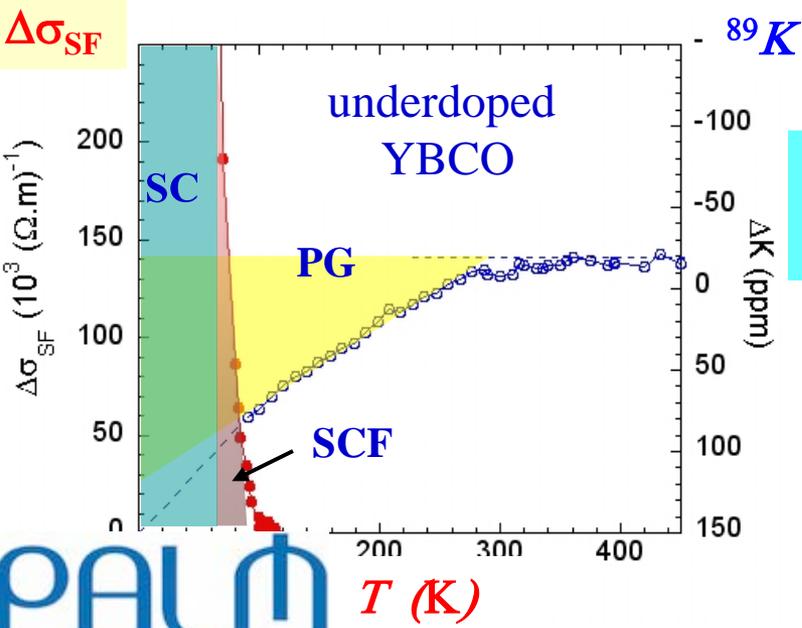
The normal state H^2 magnetoresistance is restored by high fields (up to 55 Tesla)

$$\delta\rho / \rho(0) = (\delta\rho / \rho)_0 + a_{\text{trans}} H^2$$

Permits to extract the SCF conductivity $\Delta\sigma_{\text{SF}}$

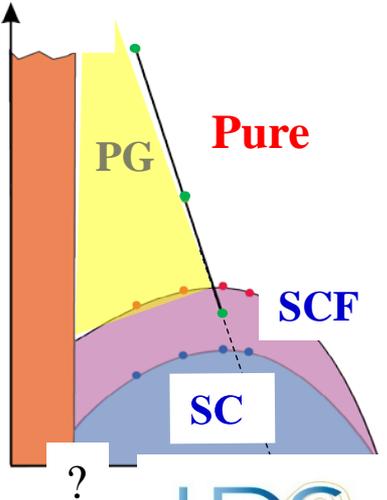


Quantitative comparison of PG and SCF ranges



The pseudogap cannot be a precursor state for SC

Two distinct phenomena



Correlated quantum matter: Mott transition, unconventional superconductivity,... charge order

Correlated electron systems, an introduction

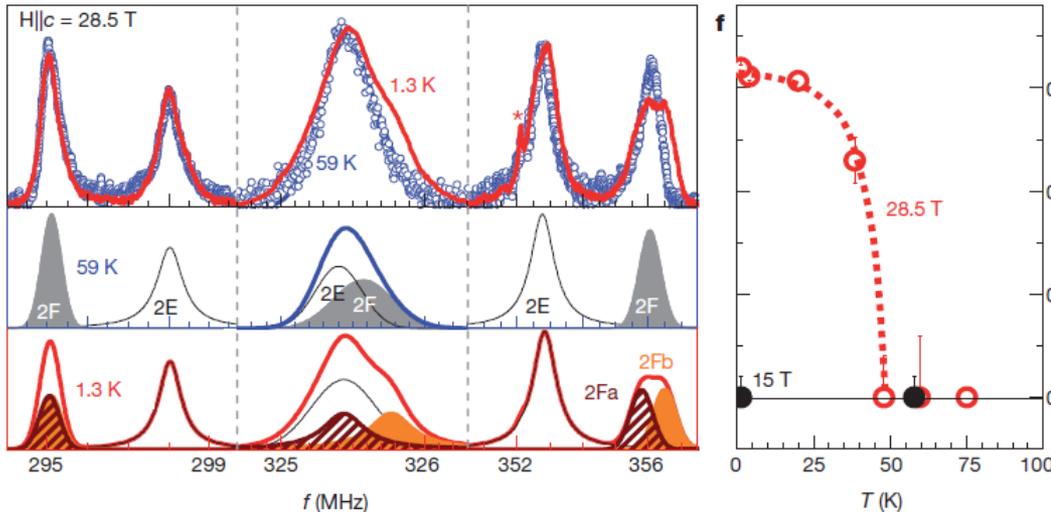
- **Band theory: insulators , metals , Fermi liquids**
- **Mott insulators and Mott Metal insulator transition**
- *Mott transition in fullerenes*
 - **Band structure Mott transition in Cs_3C_{60}**
 - **Jahn Teller Distortions**
 - **Phase diagram**
- *Unconventional superconductivity*
 - **Cuprates : doped Mott insulators**
 - **Pseudogap - Incidence of impurities**
 - **SC gap in Cs_3C_{60}**
 - **Pseudogap and SC fluctuations in cuprates**
- *Charge orders*
 - **Charge order and phase diagram in cuprates**
 - **Disproportionation in sodium cobaltates Na_xCoO_2**



Conclusions

CDW order in YBCO: Incidence of chain oxygen order?

NMR: Charge modulation at low T, high field Wu et al. Nature **477** 191 (2011), MH. Jullien)

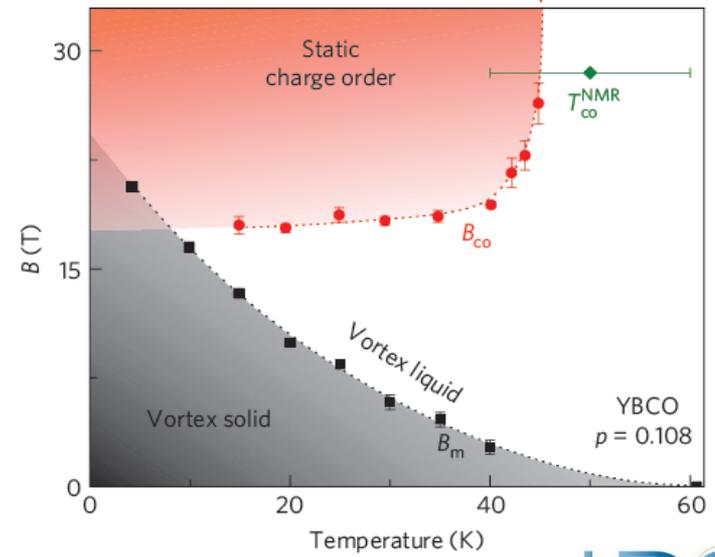
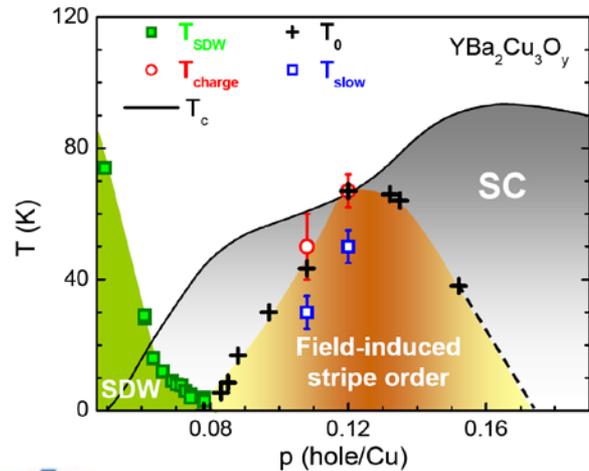


Quantum oscillations
(Taillefer + Proust)
(Sebastian + Harrison)

Fermi Surface reconstruction
below 60K

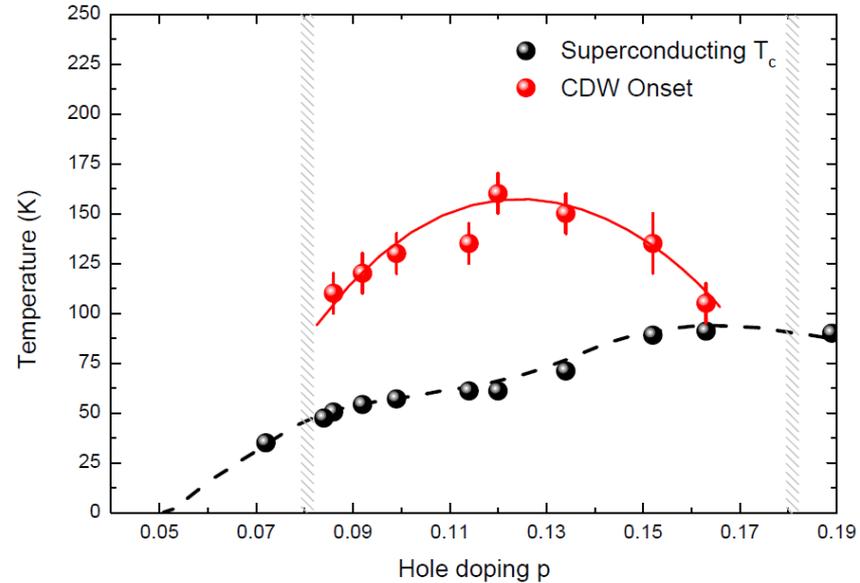
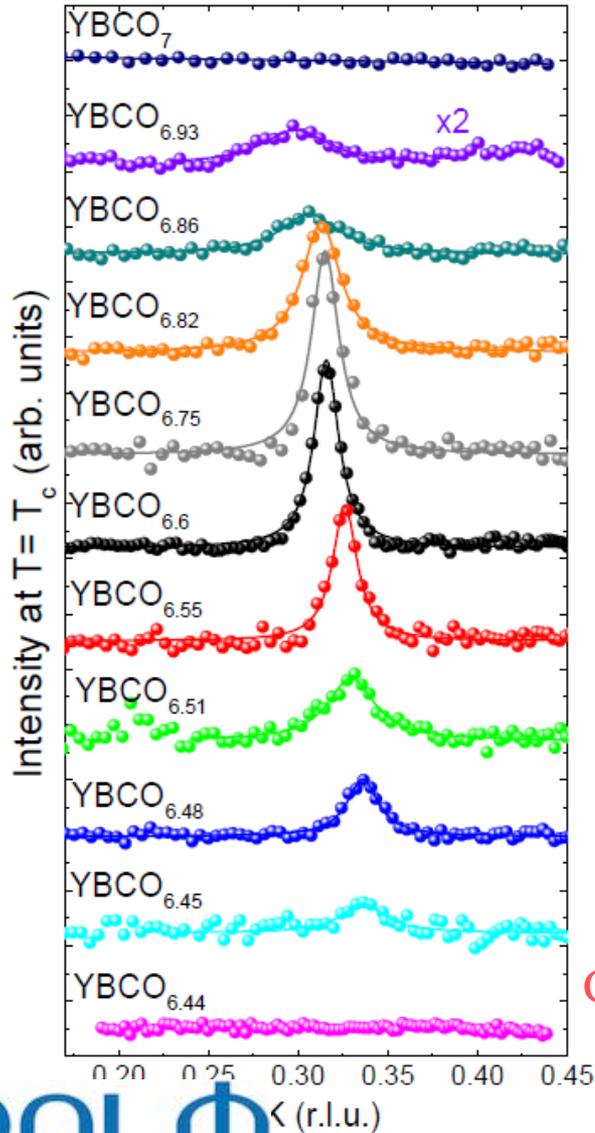
Sound velocity below 60K
Thermodynamic transition

Leboeuf et al. Nat.Phys. **9** 79 (2013)



CDW order in YBCO: Incidence of chain oxygen order?

RIXS (Le Tacon- Keimer)

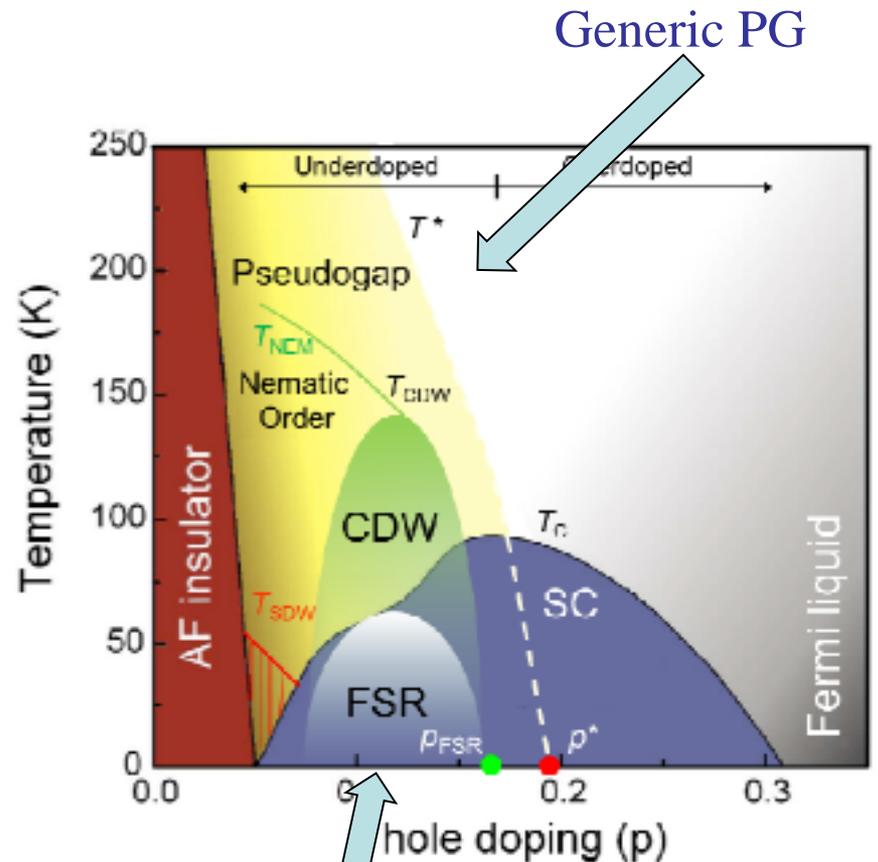
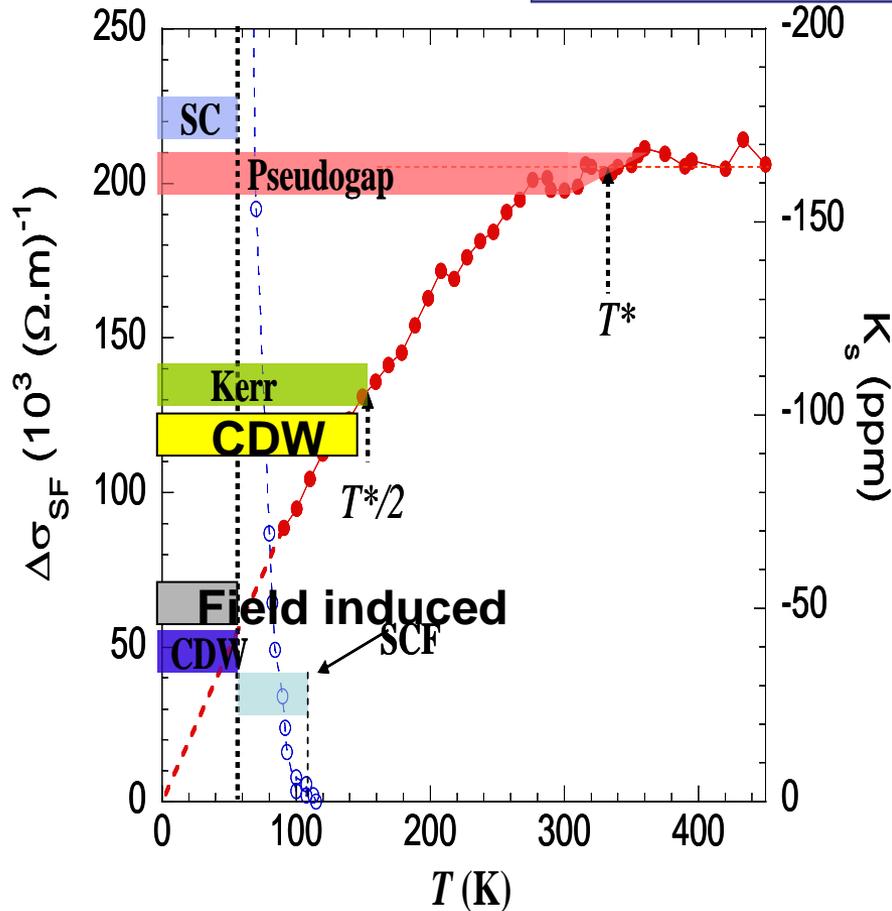


- CDW for doping levels $0.08 < p < 0.16$
- ξ and intensity max around $p \sim 0.12$
- δ_{CDW} **decreases** with increasing doping (FS related ?)

**$T_{CDW}(n_h)$ is dome like contrary to T^*
CDW are not the pseudogap
but occur in the pseudogap phase**

Charge peaks in underdoped YBCO, Bi2201, Bi2212, Hg1201
with comparable but distinct d_{CDW}

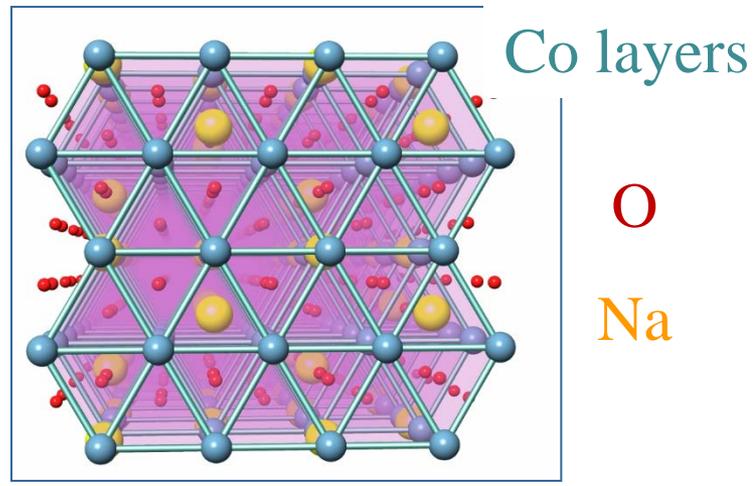
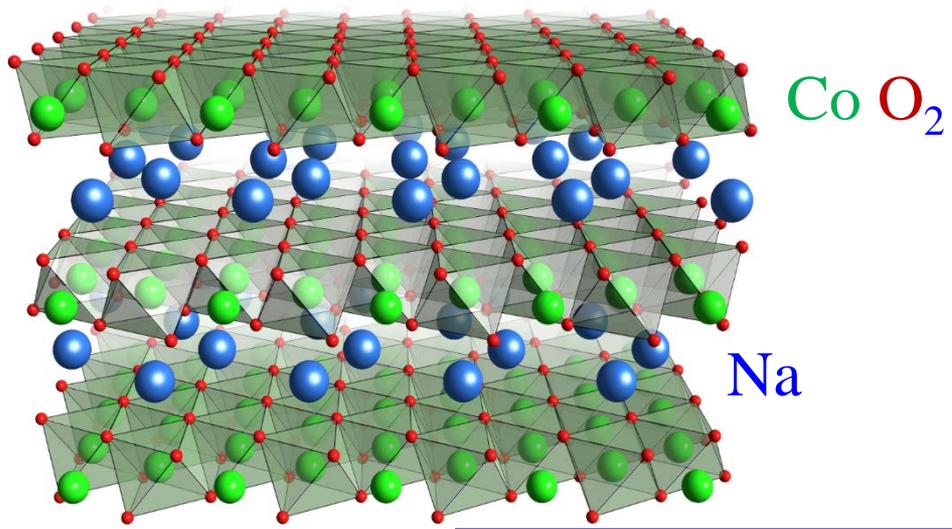
Ordered States and Pseudogap



Most of the pseudogap has been effective when CDW become detectable

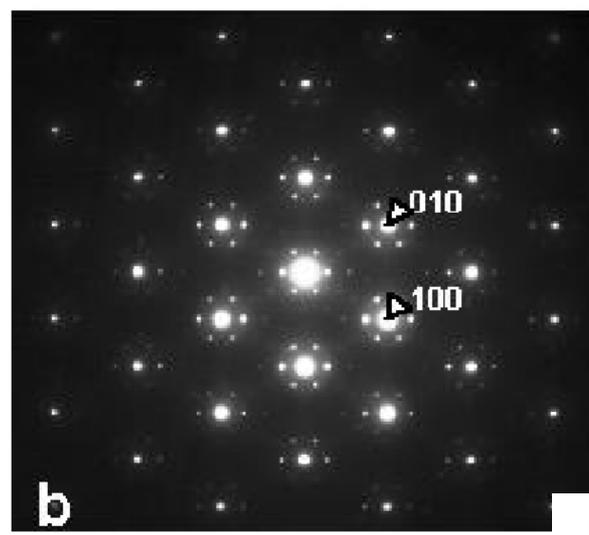
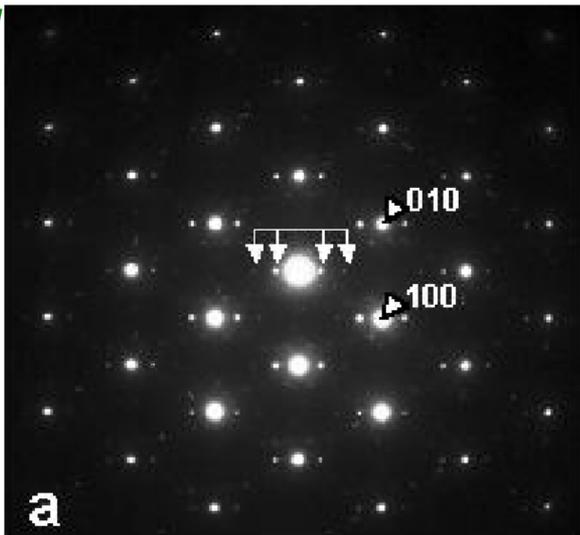
CDW order at low T around some dopings
System dependent: governed by dopant order?

Sodium Cobaltates Na_xCoO_2 : doped triangular lattices



TEM observation of Na ordered states

H.W. Zandbergen et al



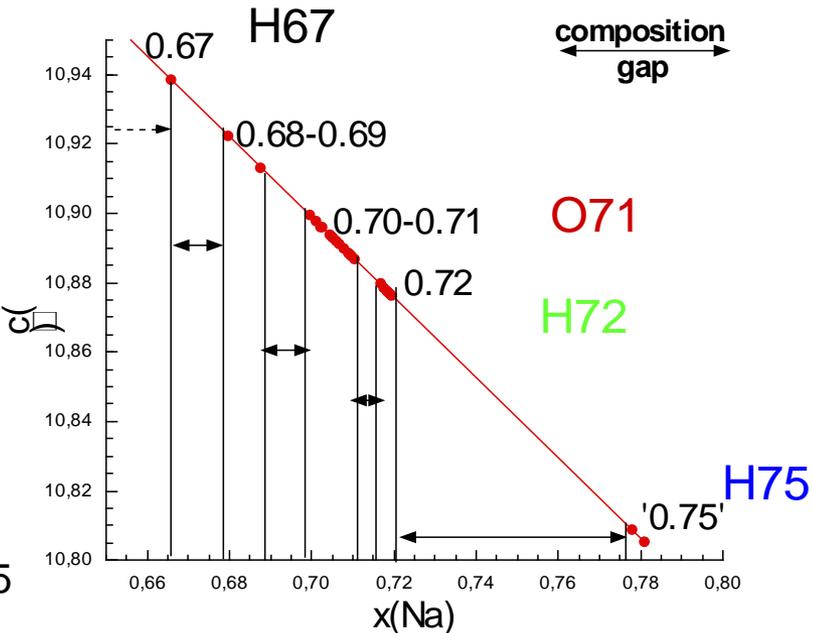
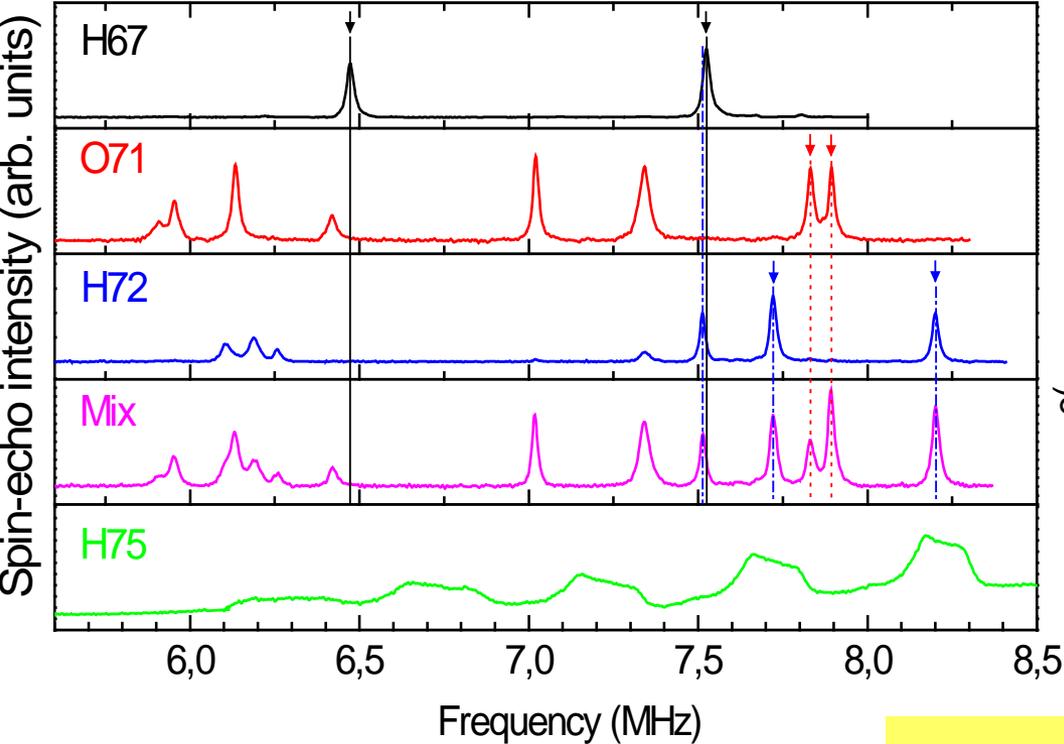
Na ordered phases for $0.67 < x \leq 0.77$

^{59}Co NQR T=4.2K

Powder x ray diffraction

Some limited compositions give stable phases

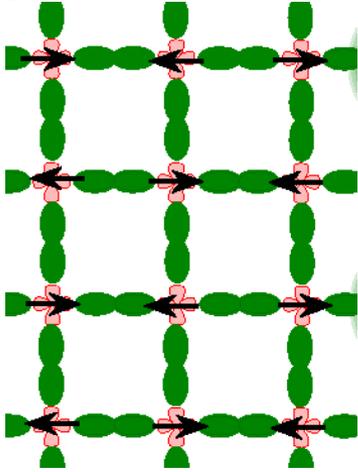
Platova et al, 2010



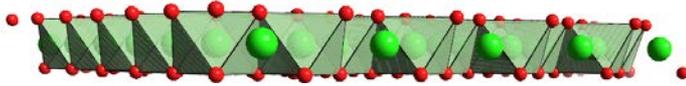
Composition gap = mixture of phases

What one would like theoretically?

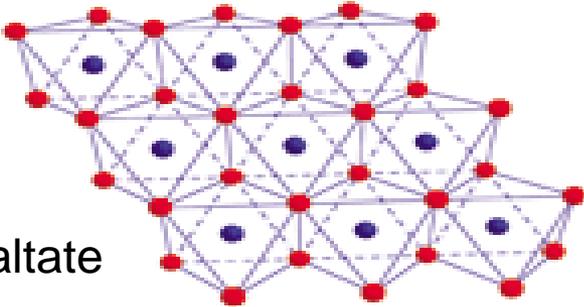
cuprate



A single square lattice CuO_2 plane ?

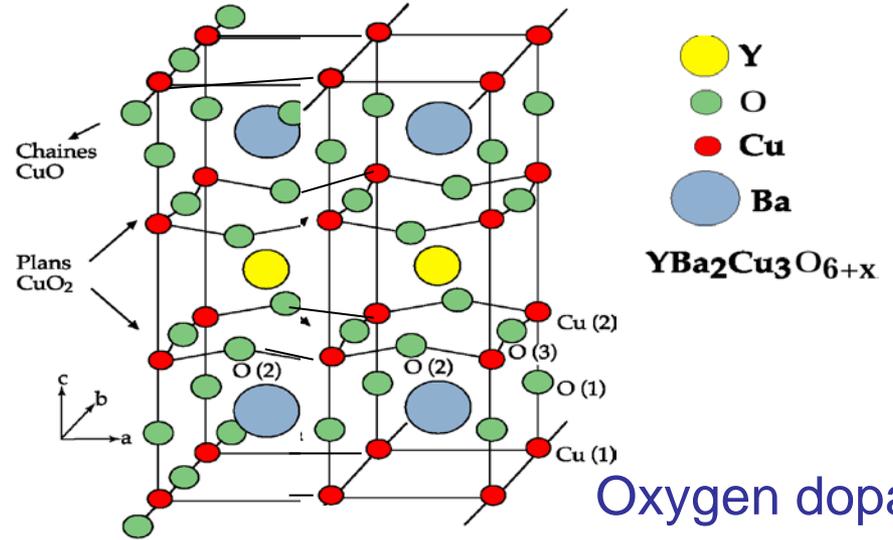


Cobaltate



A single CoO_2 triangular layer ?

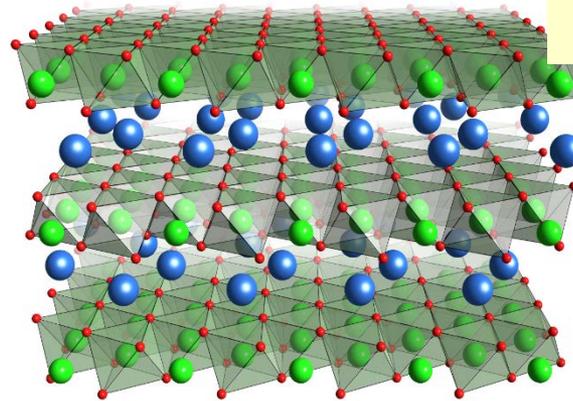
Actual situation!!



Oxygen dopants

between planes

Na dopants

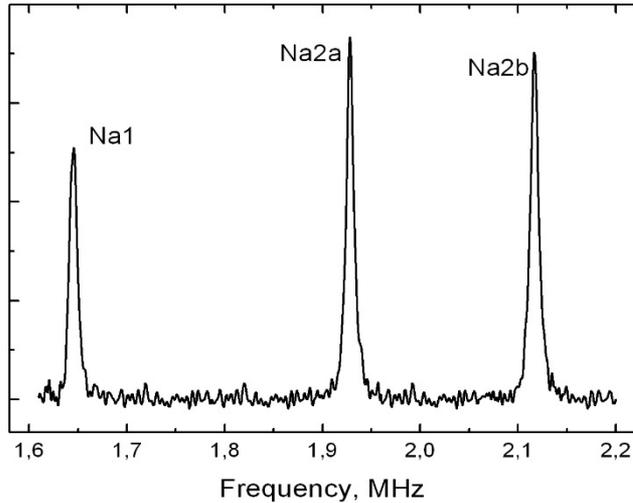
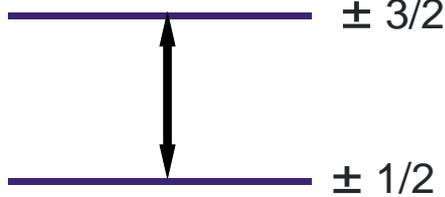


^{23}Na and ^{59}Co NQR for $x=2/3$

Quadrupole hamiltonian
Without applied field

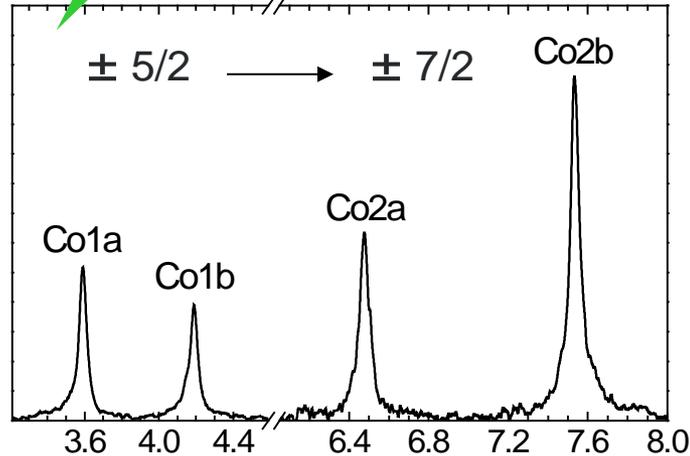
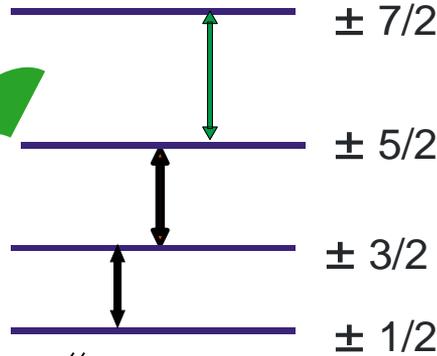
$$\tilde{H}_Q = \frac{h\nu_Q}{6} \left\{ 3I_z^2 - I(I+1) + \eta(I_x^2 + I_y^2) \right\}$$

^{23}Na $I=3/2$

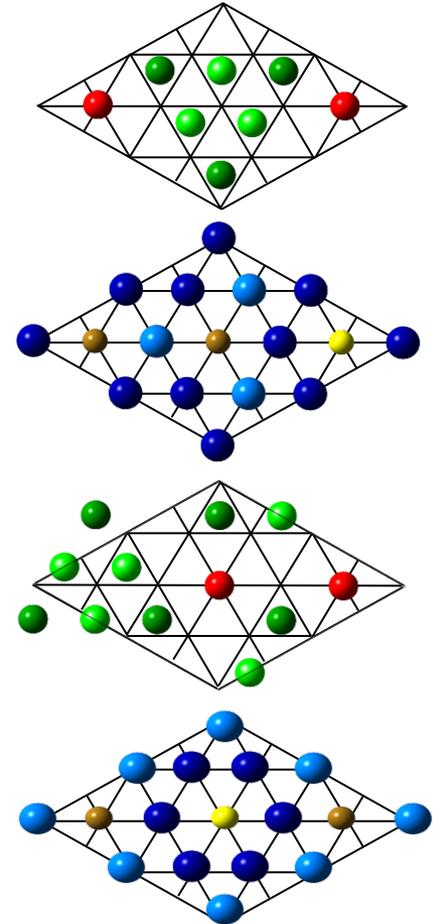


Three Na sites

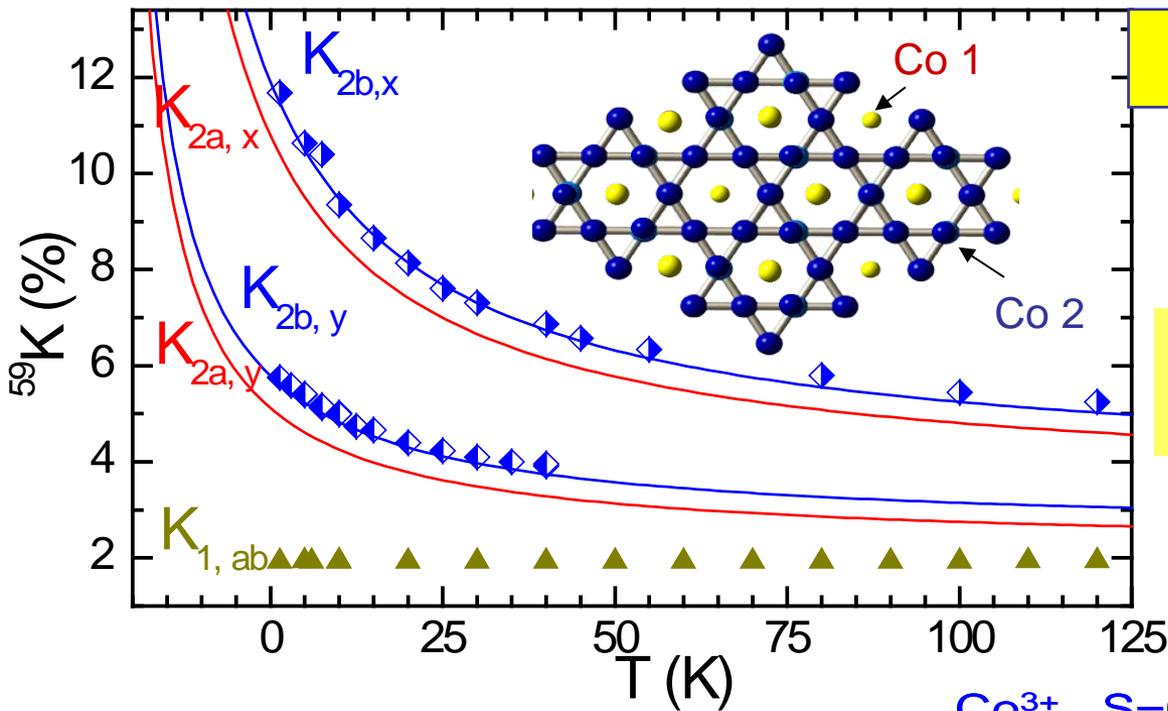
^{59}Co $I=7/2$



Four Co sites



^{59}Co NMR shifts for the four Co sites for $x=2/3$



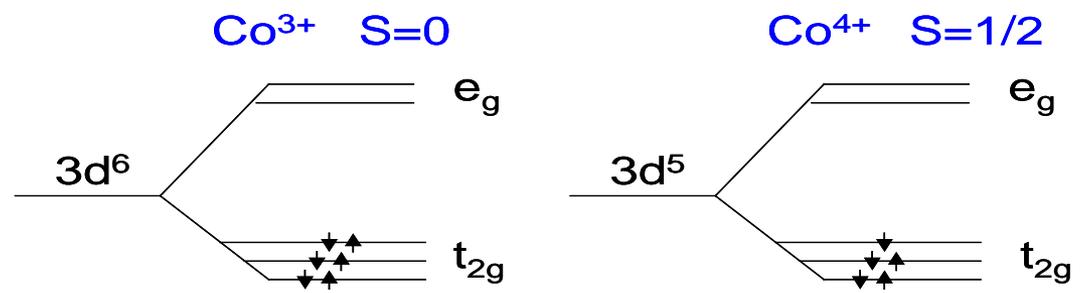
Two distinct electronic properties

Co2 sites display strong paramagnetism

**Co^{3.5+}
Delocalized holes**

Co1 non magnetic **Co³⁺**

High crystal field on the Co ions

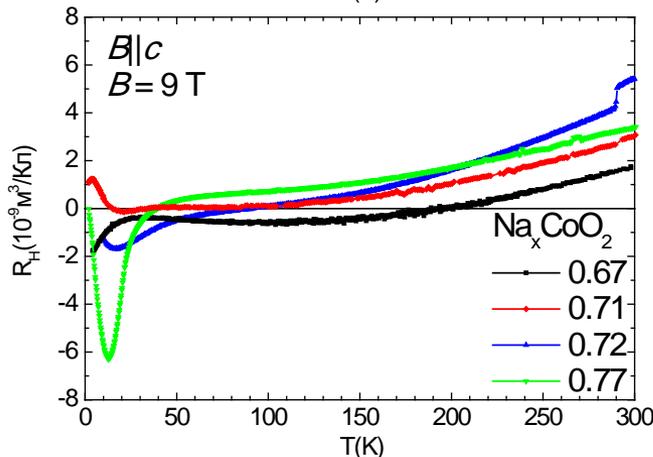
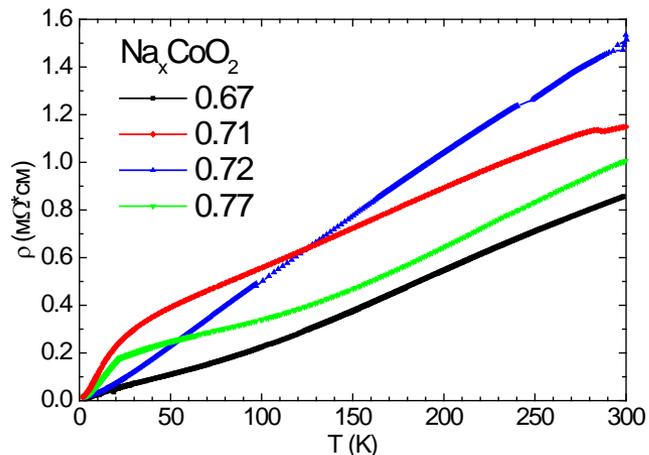


NaCoO₂ band insulator

CoO₂ Mott insulator

Physical properties of the various Na ordered phases

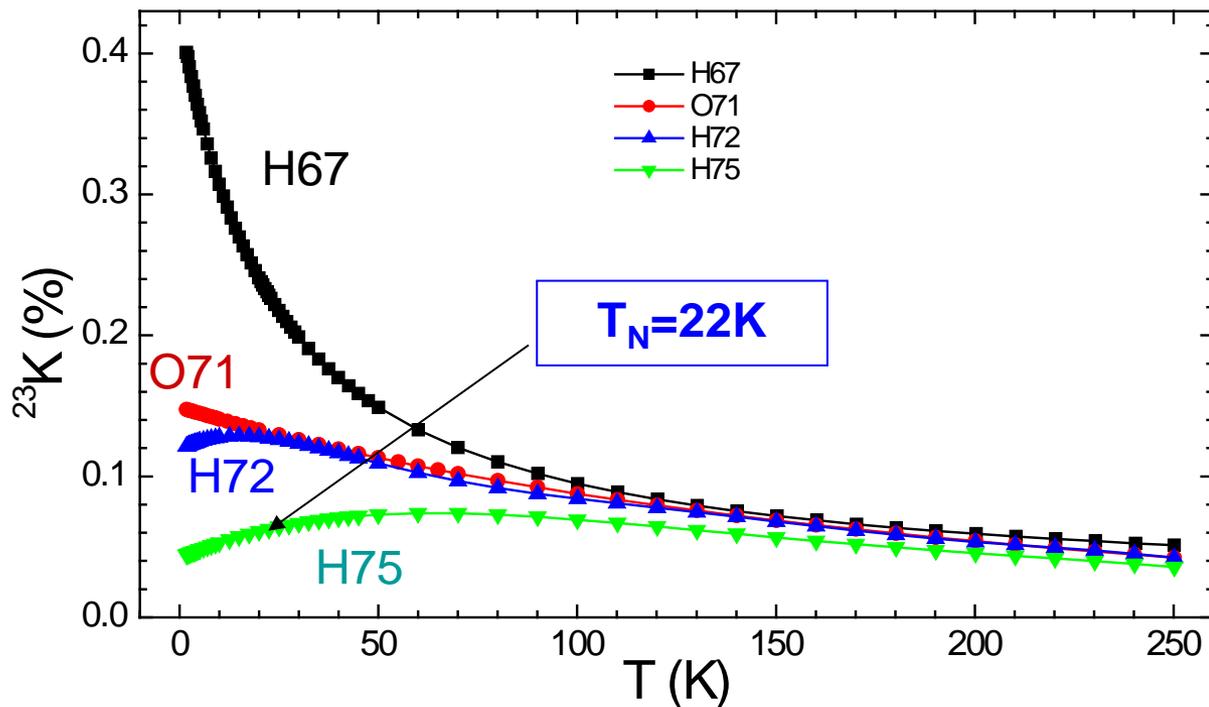
resistivity



Hall effect

H. Alloul, I. Mukhamedshin et al, EPL 2008

^{23}Na NIR shift = spin susceptibility of the Co plane

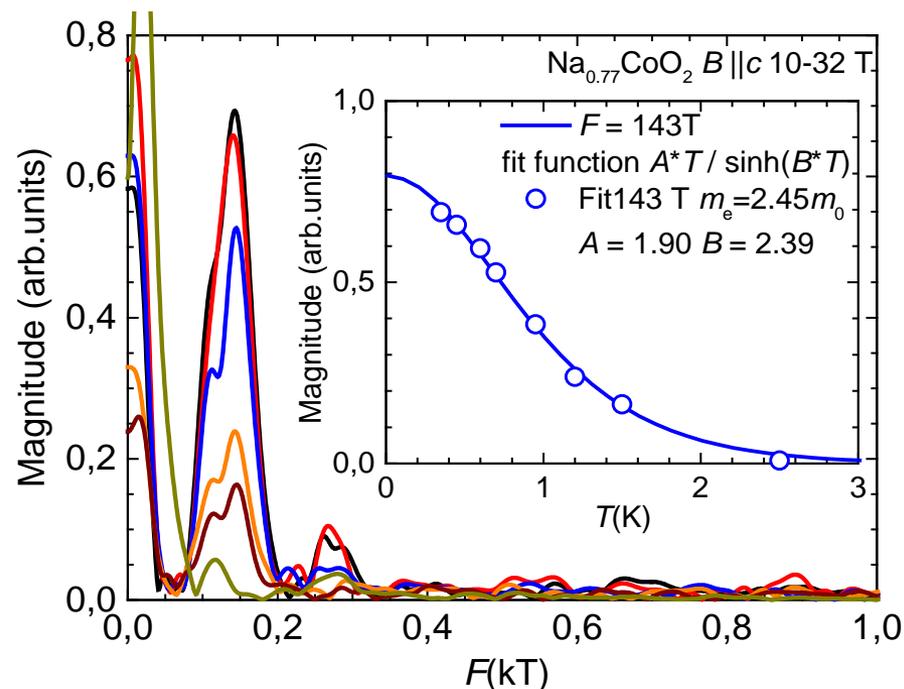
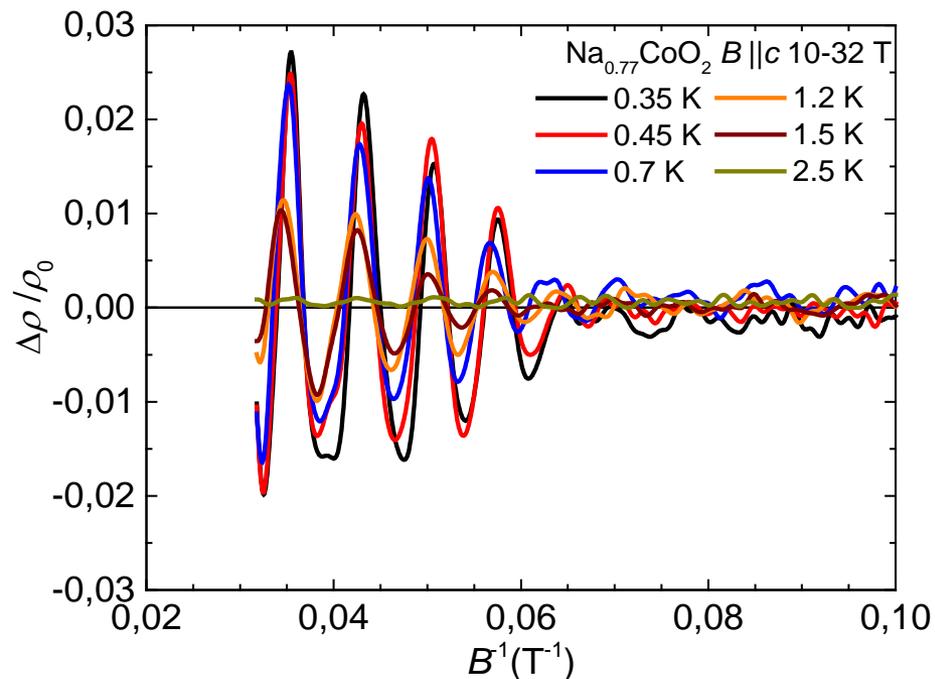


Similar electronic properties above 100K

Very different ground states

Electronic reconstruction associated with Na order

Quantum oscillations seen in the R(H) experiments



Preliminary unpublished data (Maglab+Toulouse)
Electronic reconstruction associated with Na order

Correlated quantum matter: Mott transition, unconventional superconductivity,... charge order

- *Pressure induced Mott transition in Cs_3C_{60}*

1st order 3D Insulator- SC Mott transition/JTD
 Singlet s wave SC with increasing gap
 up to the Mott transition / no pseudogap

- *The high T_c cuprates :*

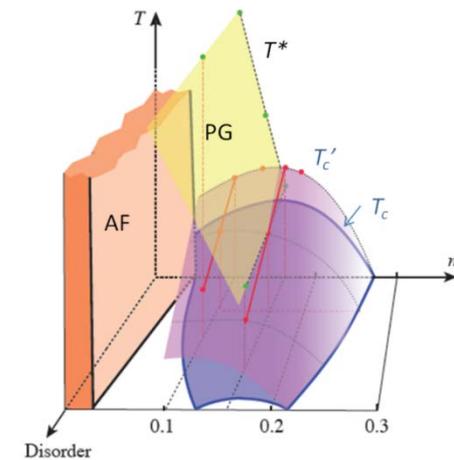
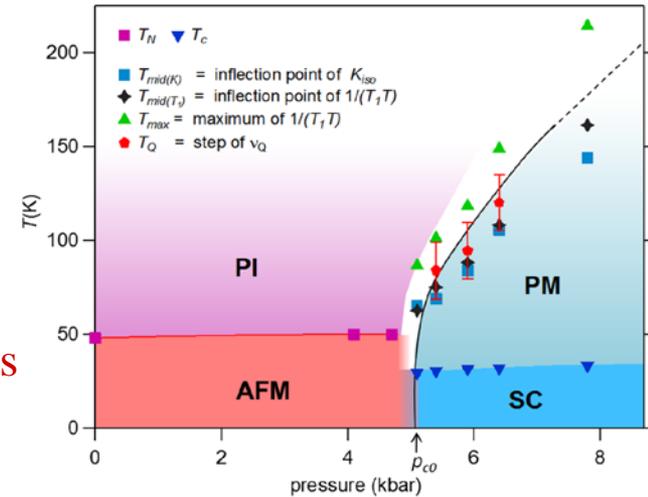
Importance of electronic correlations and Mott physics
 NMR revealed the occurrence of the pseudogap
 Pseudogap is generic and insensitive to disorder
 Non magnetic impurities reveal the magnetic properties

- *SC Fluctuations and controlled disorder*

A preformed pair scenario does not apply
 The PG is not the SC gap
 The phase diagram is disorder dependent

- *CDW orders are not generic and compete with the PG and SC*

Charge order is often generated by dopant order
 Example of Na_xCoO_2 - variety of original metallic ground states



Correlated quantum matter: Mott transition, unconventional superconductivity,... charge order



P. Mendels
NMR- μ SR
(QSL)



J. Bobroff
NMR- HTc/NaCoO
(education -outreach)



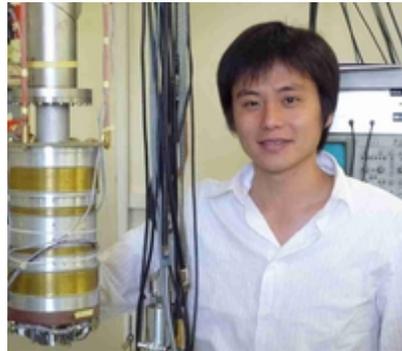
V. Brouet
Fullerites
(ARPES Fe/Ir)



P. Wzietek
1D organics
 Cs_3C_{60}



F. Rullier-Albenque
Transport HT_c/Fe
(SPEC /CEA Saclay)



Y. Ihara Cs_3C_{60}
(Hokaido Japan)



I. Mukhamedshin



A. Dooglav



G. Lang (ESPCI)

(Na_xCoO_2) (Kazan FU)

Matter Summer School-IES Cargese, Corsica, France 5th – 17th august 2019



In this summer school we aim at introducing young researchers in condensed matter physics to the modern concepts and methods used to study strongly correlated electronic systems. Strong correlations are well known to be responsible for the rich behaviors of transition metal oxides, from non conventional superconductivity to Mott insulators, often with interesting magnetic properties, like quantum spin liquid ground states for special lattice geometries. The interplay between spin, charge degrees of freedom and topology is key to understand this wealth of unconventional behaviors. Beyond oxides, strong correlations have been recently proposed as an emergent phenomenon in graphene bi-layers, providing a renewed view on strong correlations.

The school will cover these various aspects of strong correlations in condensed matter from basic courses to examples from current research topics. Relevant theory, numerical methods and experimental techniques will be introduced.

Organization

-Fabrice Bert
(U. Paris-Saclay, France)
-Mark-Oliver Goerbig
(U. Paris-Saclay, France)
-Rajiv Singh (UC Davies, USA)

Topics

-Unconventional superconductivity
-Quantum spin liquids and RVB physics
-Topological matter
-Hubbard model on the triangular lattice
-Strong correlations in graphene bi-layers

Confirmed Main Lecturers

Piers Colman (Rutgers, USA)
Leon Balents (UC Santa Barbara, USA)
Jean-Noël Fuchs (LPTMC, UPMC)
Lucile Savary (ENS Lyon)
Giovanni Sordi (Royal Holloway UL, UK)



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21/12/2018