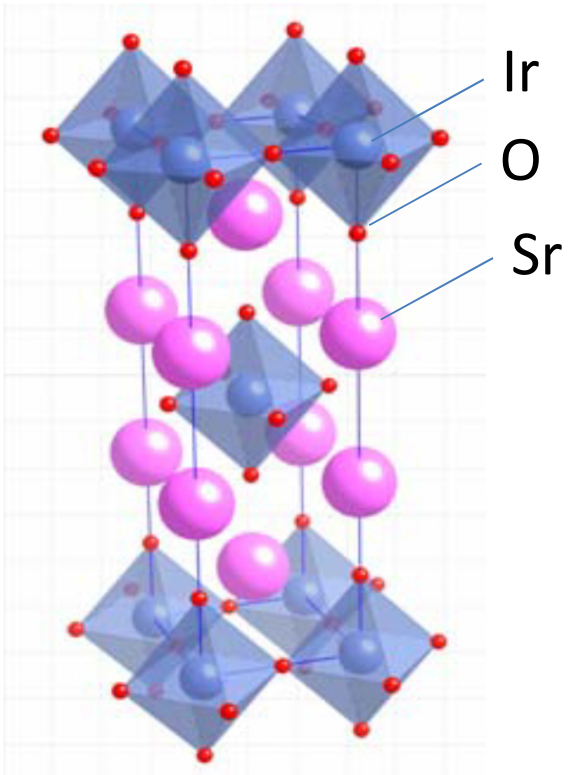
Les composés iridates Sr_2IrO_4 : ressemblances et différences avec les cuprates

Véronique Brouet
Laboratoire de Physique des Solides d'Orsay



$Ir^{4+} = 5d^5$

History

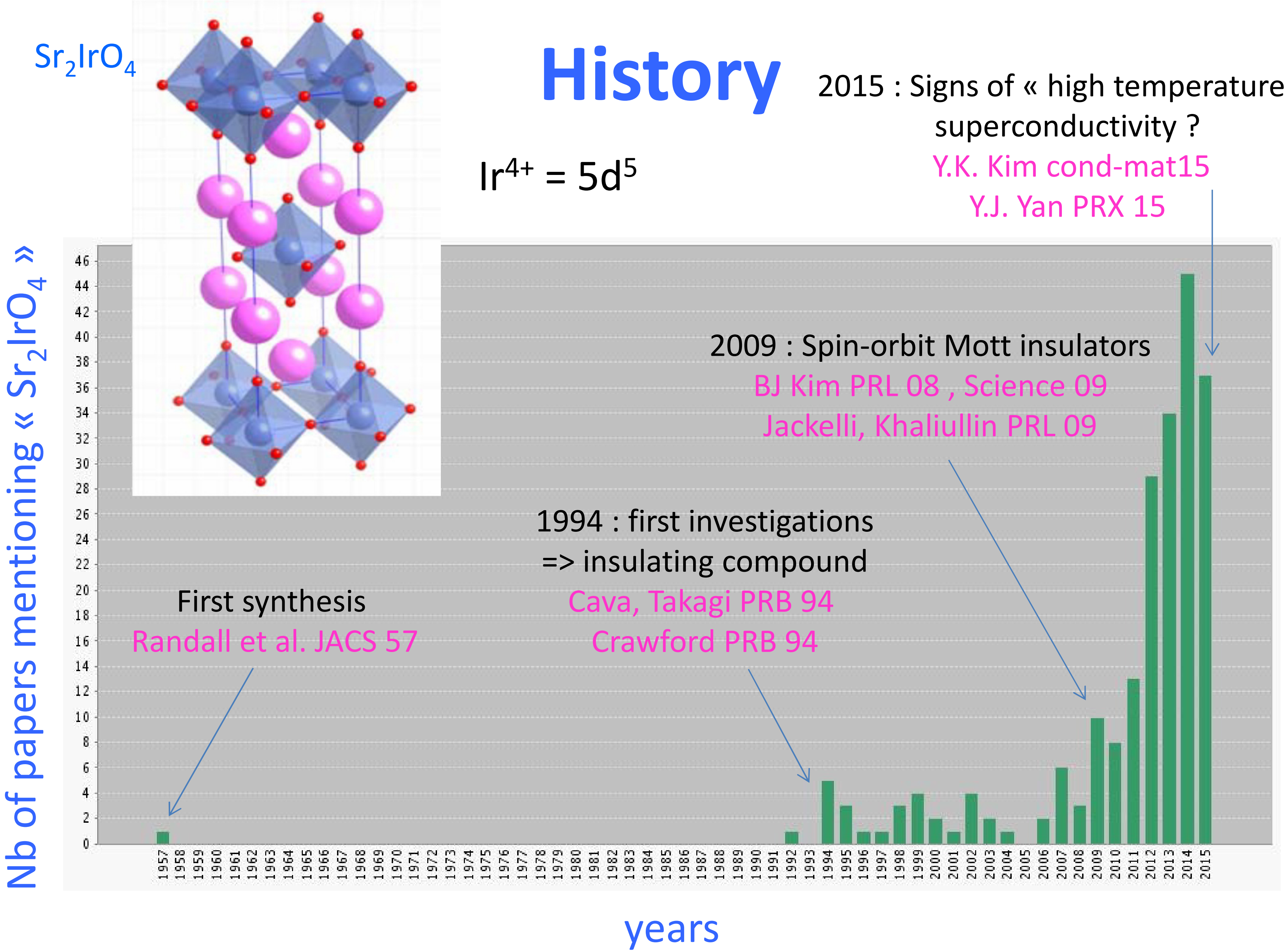
Sr_2IrO_4

$Ir^{4+} = 5d^5$

2015 : Signs of « high temperature » superconductivity ?

Y.K. Kim cond-mat15

Y.J. Yan PRX 15



Outline

The insulating state

- What is a « Spin-Orbit Mott » insulator ?
- Theoretical and experimental study (by ARPES) of the electronic structure
- How close are these systems from a metal-insulator transition ?

The « metallic » state

- « Bad metals » can be obtained by chemical doping,
  for example Sr/La or Ir/Rh substititions
- ARPES sees a state that is « almost » metallic with no well defined quasiparticles
- Difference with K evaporated samples : larger doping ? Different perturbation from dopant ?

$\Rightarrow$ Photoemission studies (ARPES) at SOLEIL CASSIOPEE beamline

Thanks to A. Louat, J. Mansart, D. Le Boeuf and P.H. Lin (LPS)

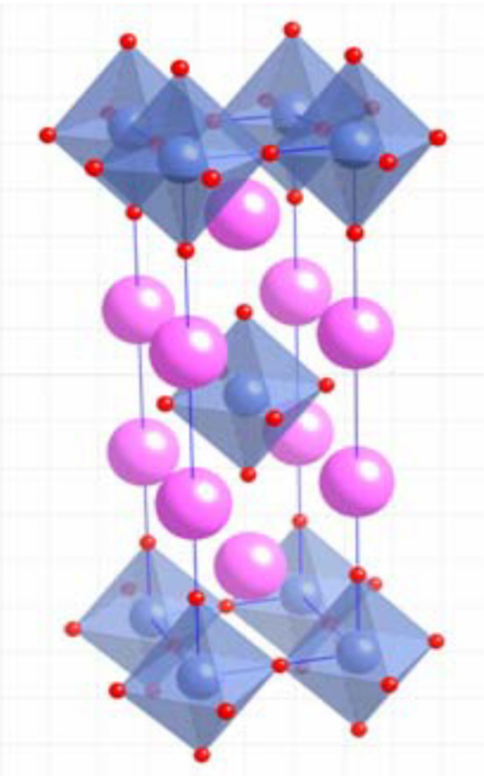
Thanks to P. Le Fèvre, F. Bertran, J. Rault (SOLEIL, CASSIOPEE)

$\Rightarrow$ Crystal growth

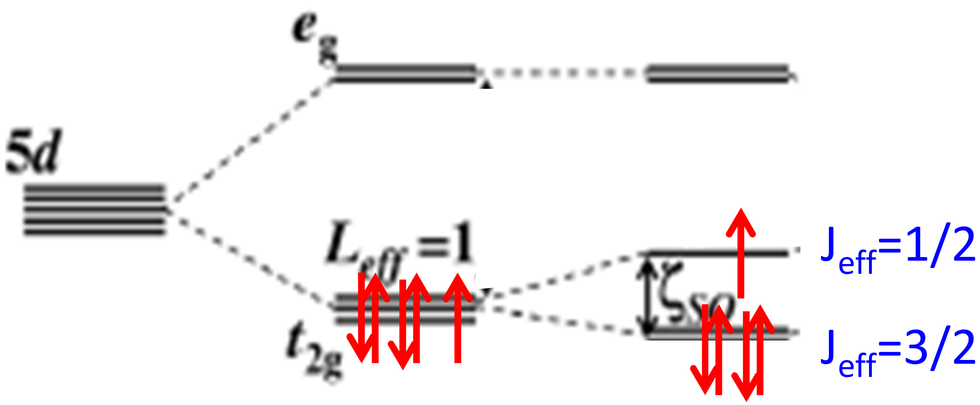
Thanks to I.R. Fisher (Stanford University) and D. Colson (CEA-SPEC)

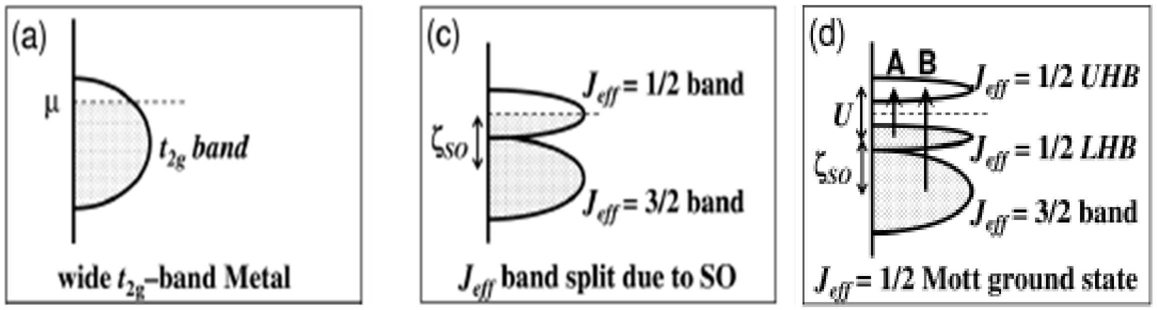
Sr_2IrO_4 : a spin-orbit Mott insulator

Weak correlations are expected for 5d metals. However, the strong spin-orbit splitting reshapes the band structure in a way that favors strong correlations.



Sr_2IrO_4
(simplified structure)





Rather weak correlations

Strong correlations

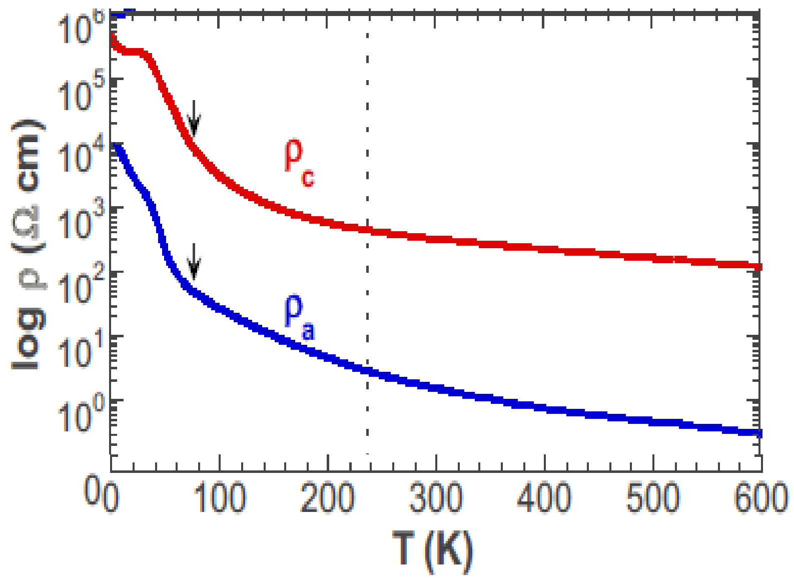
Mott insulator

B.J. Kim et al. PRL 2008

Analogy with cuprates => superconducting if doped ?? *Wang, Senthil PRL 2011*

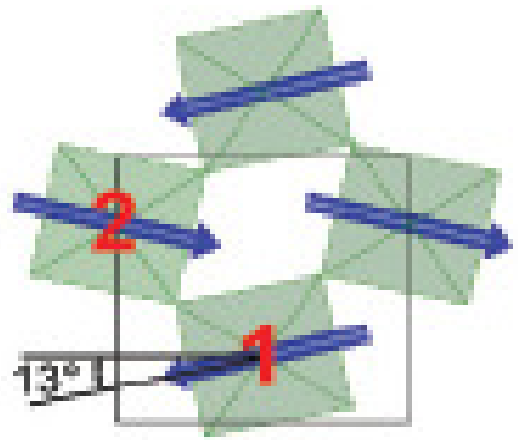
Sr_2IrO_4 : an insulator with AF transition at 240K

Resistivity => insulating below and above T_N



Chikara, G. Cao *et al.* PRB09

Magnetic order below T_N=240K

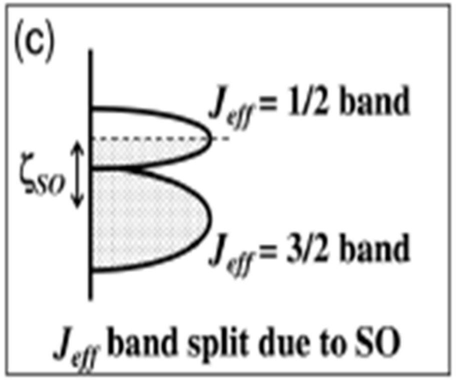


M=0,2μ_B/Ir

Feng Ye, PRB13

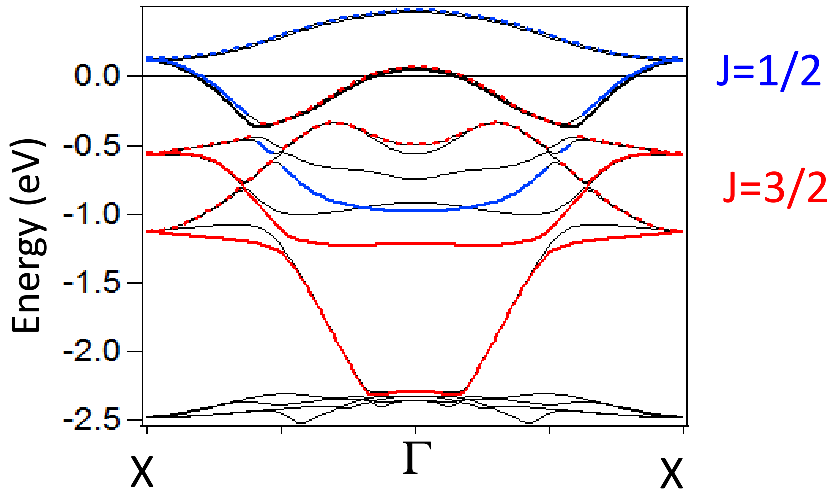
Dhital PRB 13

The insulating state : electronic structure

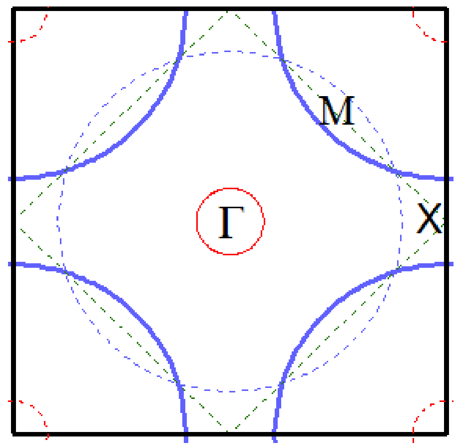


Band structure

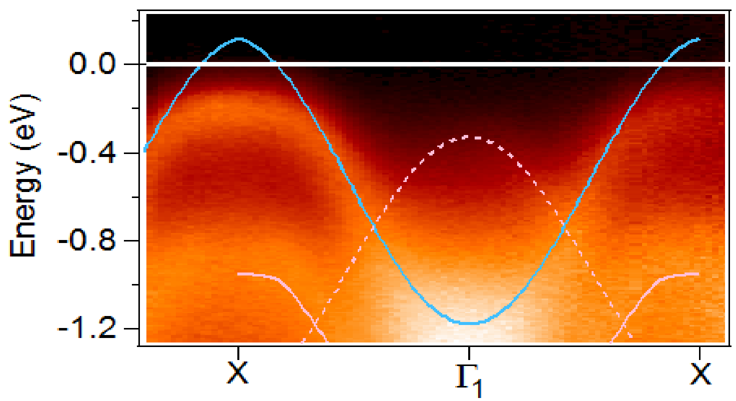
including spin-orbit (done with Wien2k)



Fermi Surface



Dispersion measured by ARPES

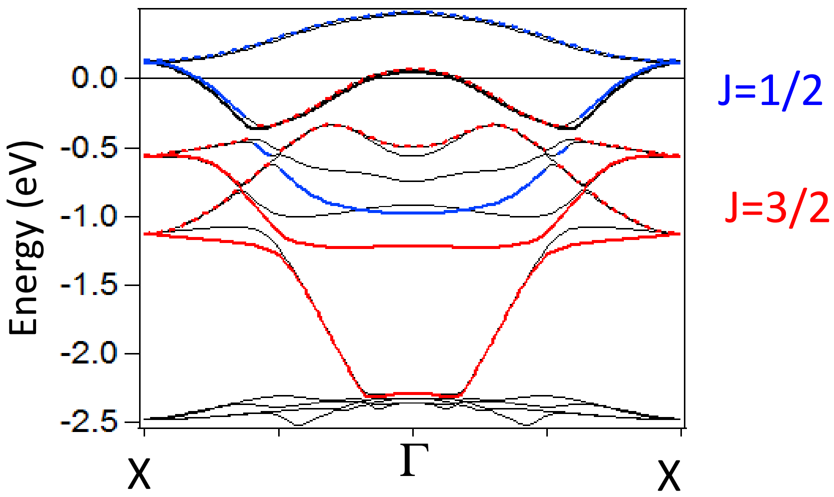


---- J=1/2 band, from band calculation

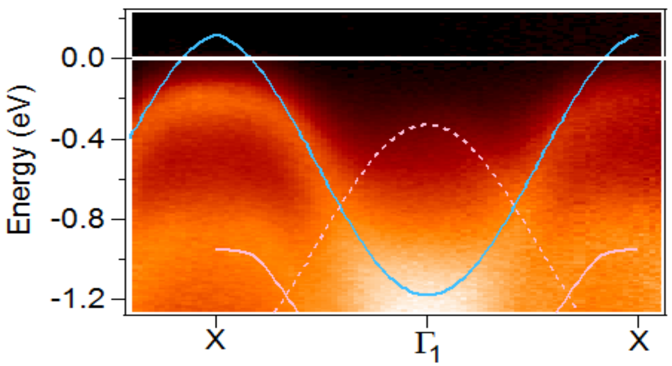
---- J=3/2 bands shifted down by 0,35eV

The insulating state : electronic structure

Band structure



Dispersion measured by ARPES

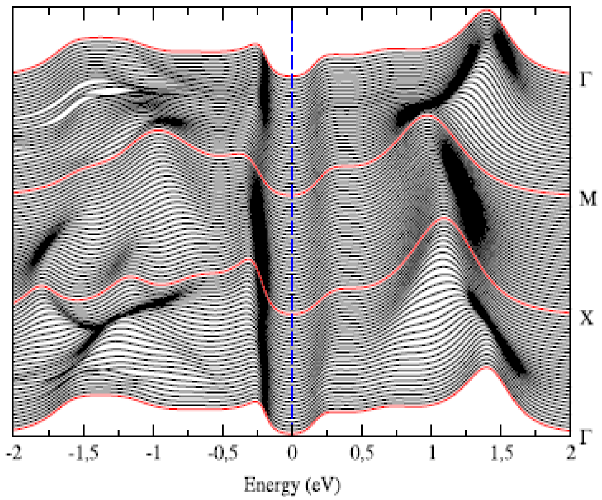


DMFT study

=> Correctly predicts filling of J=3/2 state

=> Correctly predicts opening of a gap in J=1/2 state

(c) Spectral density for jeff=1/2

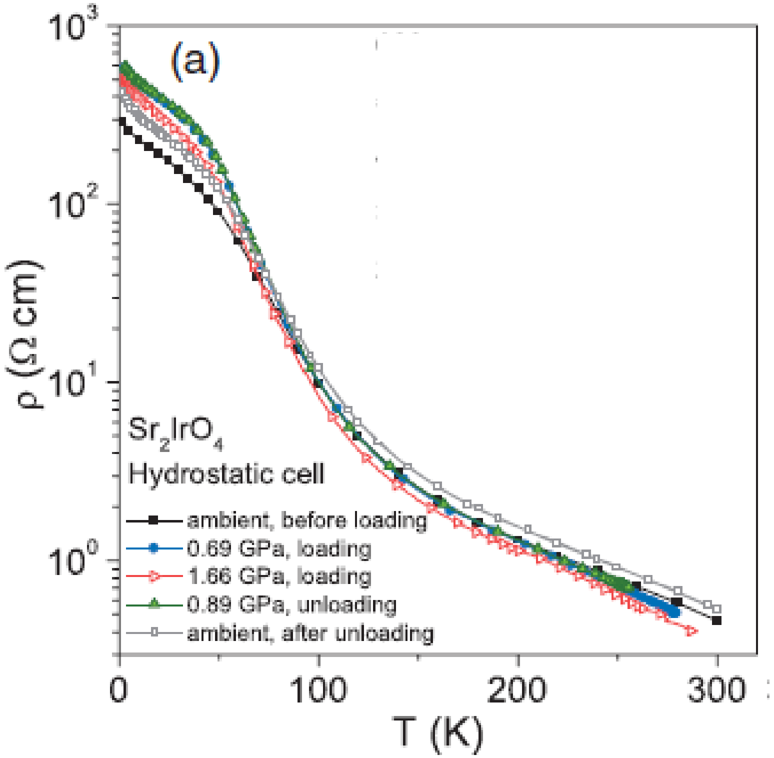


Martins, Biermann *et al.* PRL 11
Arita *et al.*, PRL 11

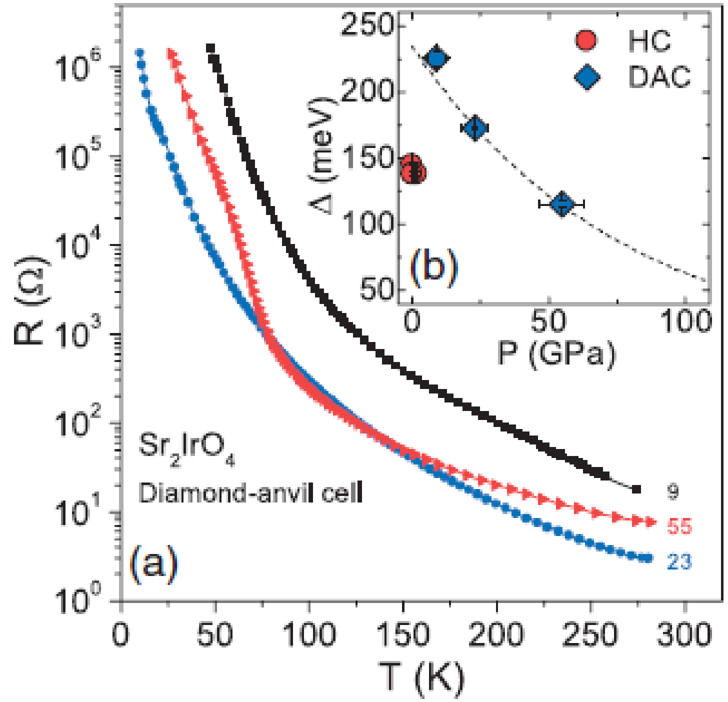
How close are they from the metal-insulator transition ?

It seems difficult to induce a MIT under pressure in Sr_2IrO_4 (up to 55GPa)

Up to 2 GPa



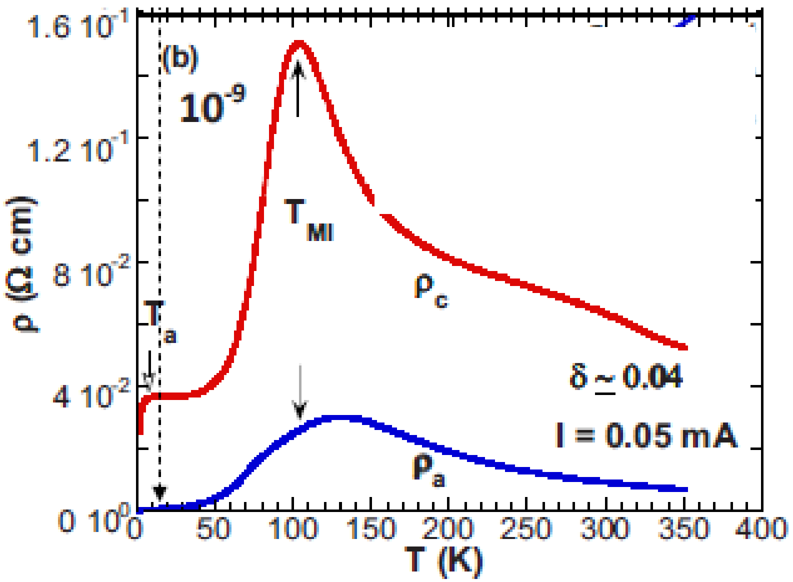
Up to 50 GPa



Zocco *et al.*, J Phys CondMat 2014

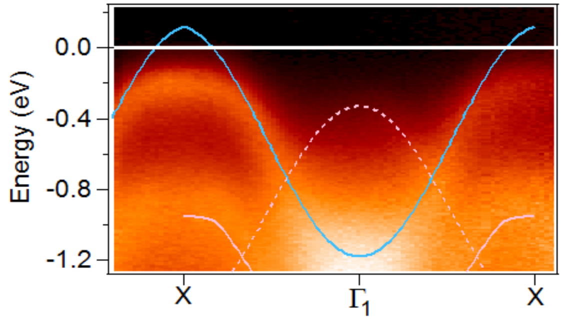
How close are they from the metal-insulator transition ?

A few percent oxygen vacancies is enough to trigger a transition to metallic state

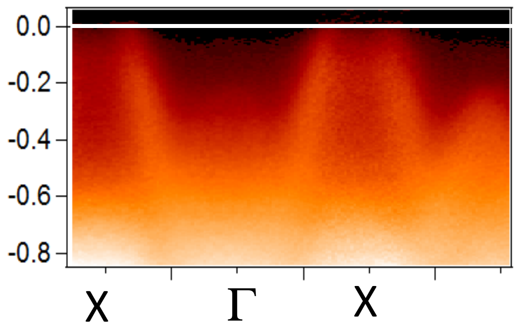


Kornetta, Cao *et al*. PRB 10

ARPES measurements

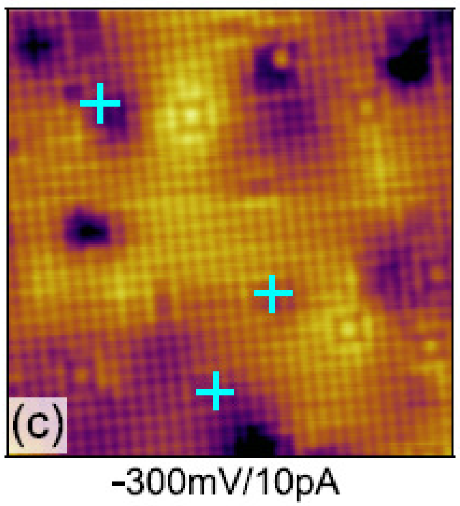


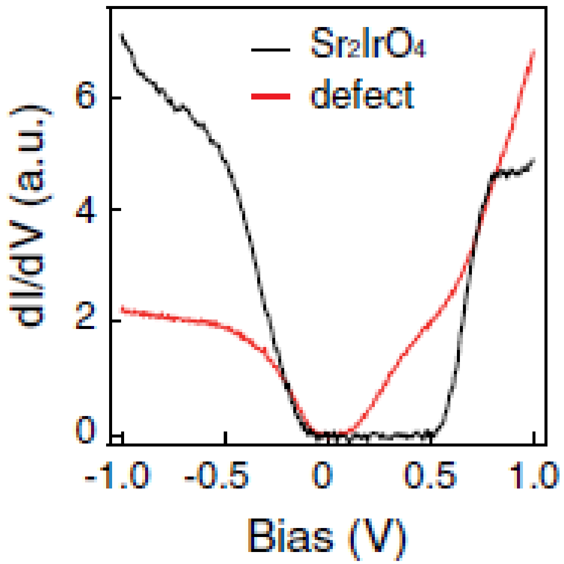
Annealed
In vacuum at 600°C



Defects are very effective to reduce the band gap

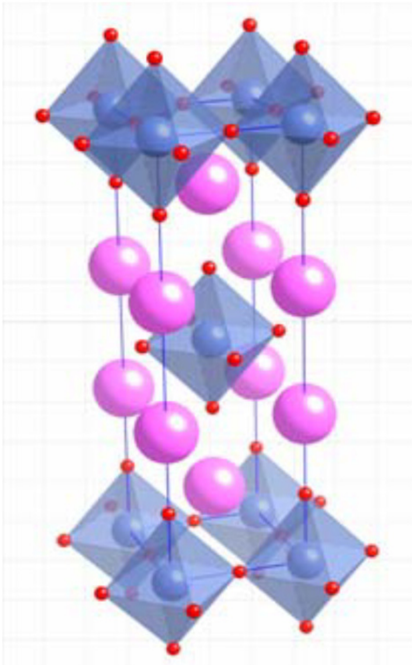
STM measurements





Okada Nature Mat 13 , Dai, PRB12 , Yan PRX 15 …

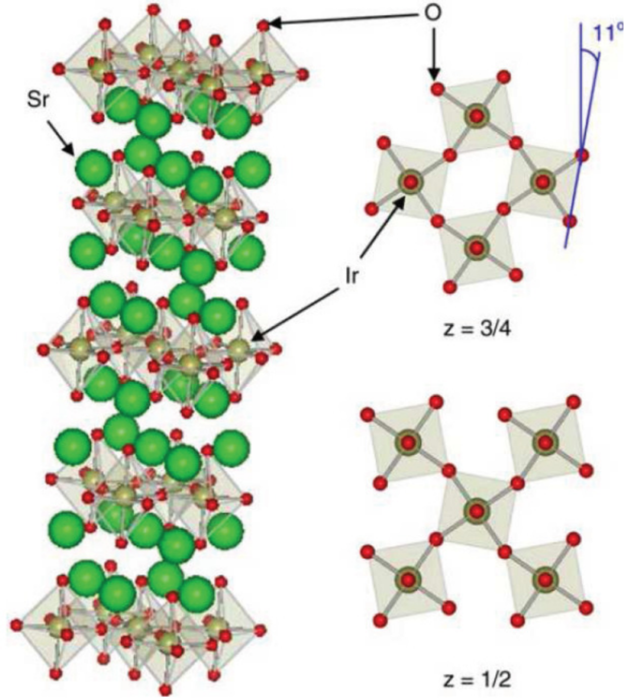
Other important degrees of freedom ?



Ba_2IrO_4

Also insulating

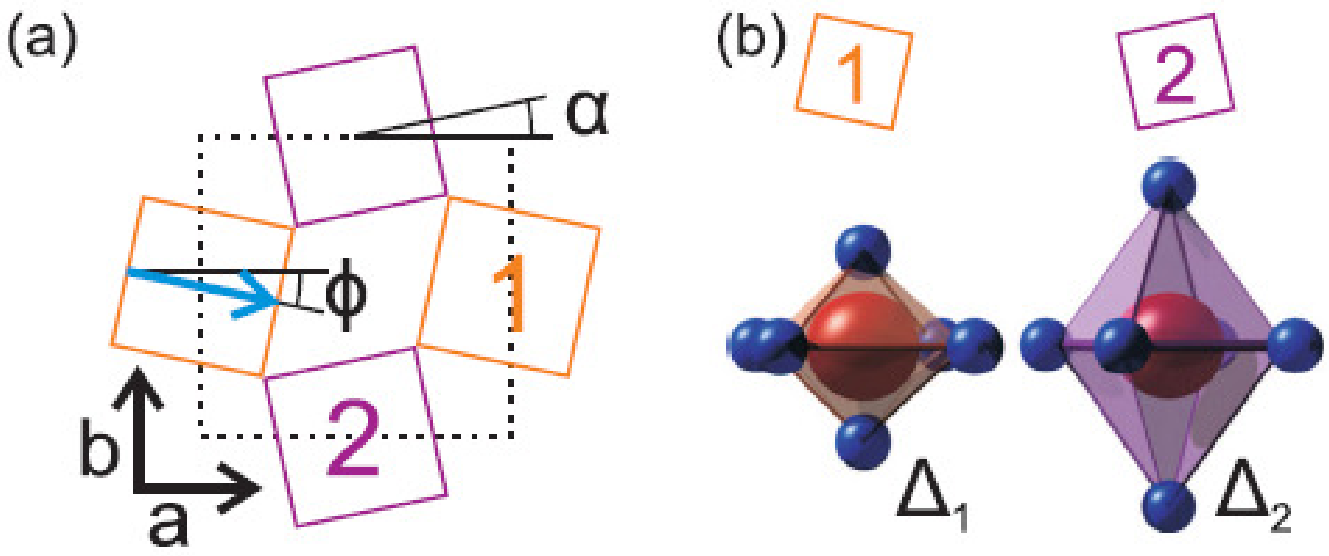
Okabe PRB11



Sr_2IrO_4

$I\,4_1/acd$

Other important degrees of freedom ?



Torchinsky, PRL 15
Ye, Cao et al., cond-mat 15

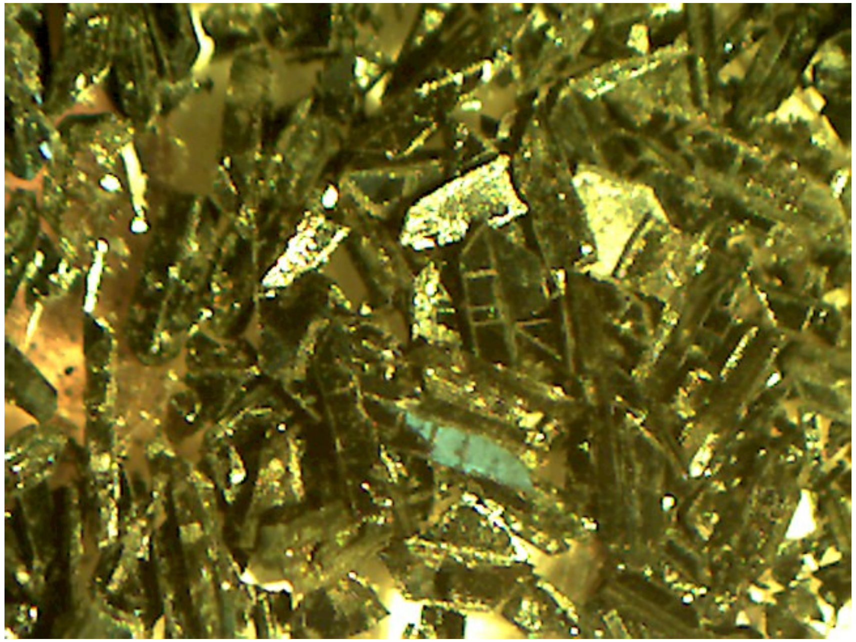
=> 2 inequivalent Ir sites with different oxygen environments

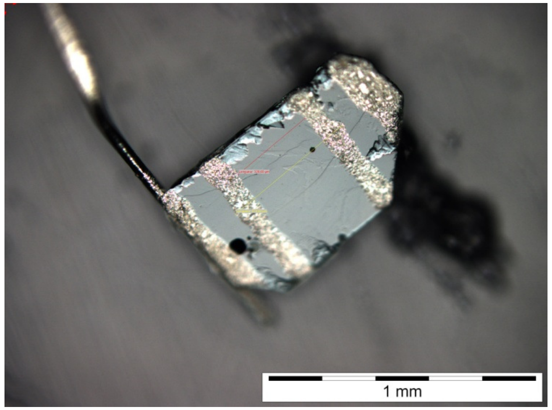
The « metallic » state

doping Sr_2IrO_4…

Samples of Sr_2IrO_4 (home-made !)

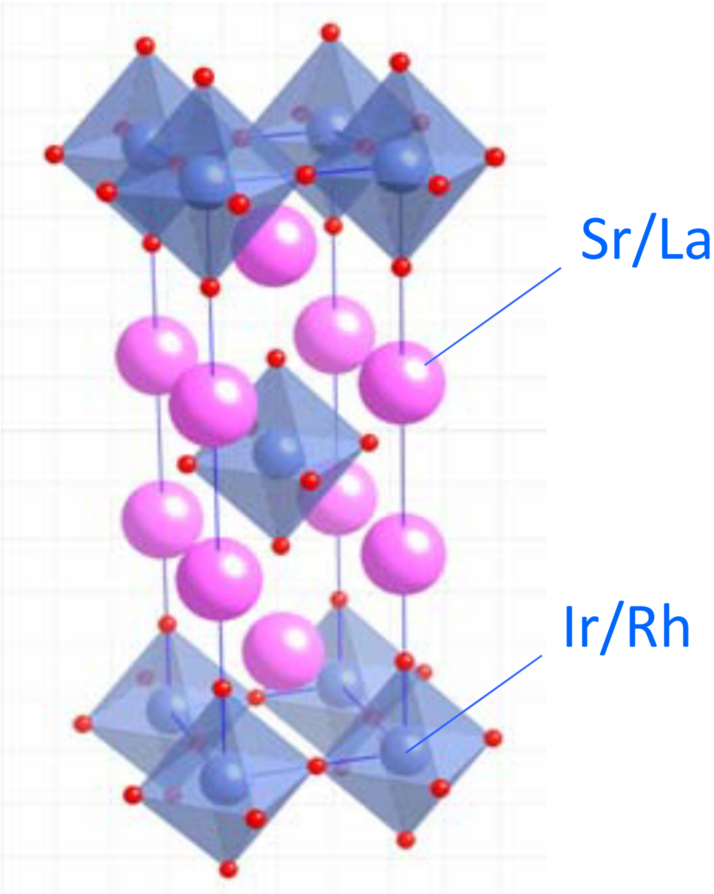
Sr_2IrO_4 : first crystals (October 2013)





Thanks to : I.R. Fisher, Stanford university
D. Colson, CEA-SPEC

Doping by chemical substitutions



Sr/La : electron doping

« clean » out-of-plane substitution, but limited solubility (~4-5%)

Ir/Rh : hole doping

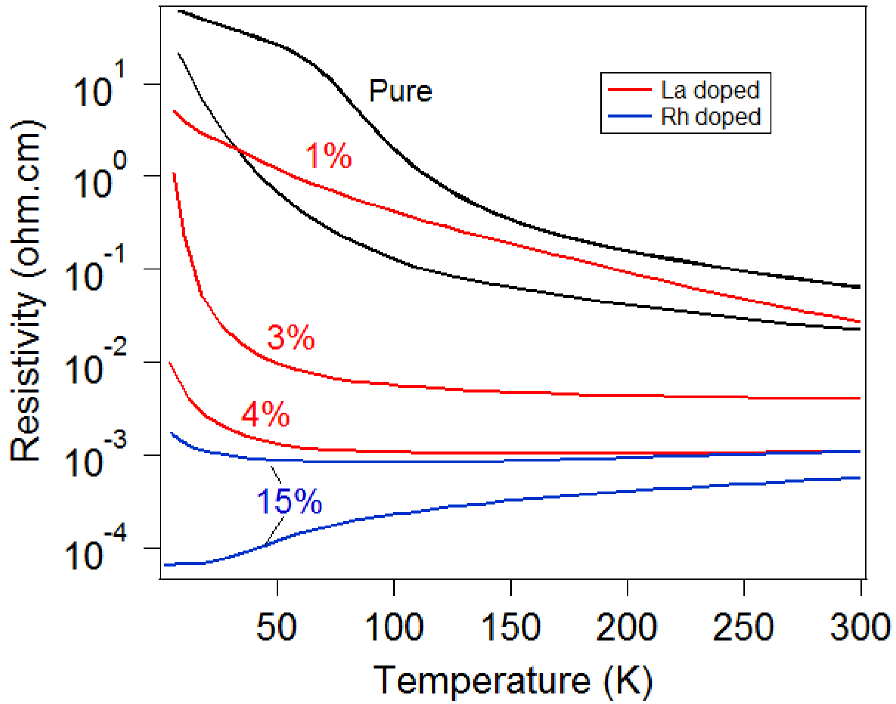
Ir and Rh are isoelectronic
But it seems Rh^{3+} ($4d^6$) is formed, giving $5d^{5-x}$ on Ir sites.

Clancy PRB 14

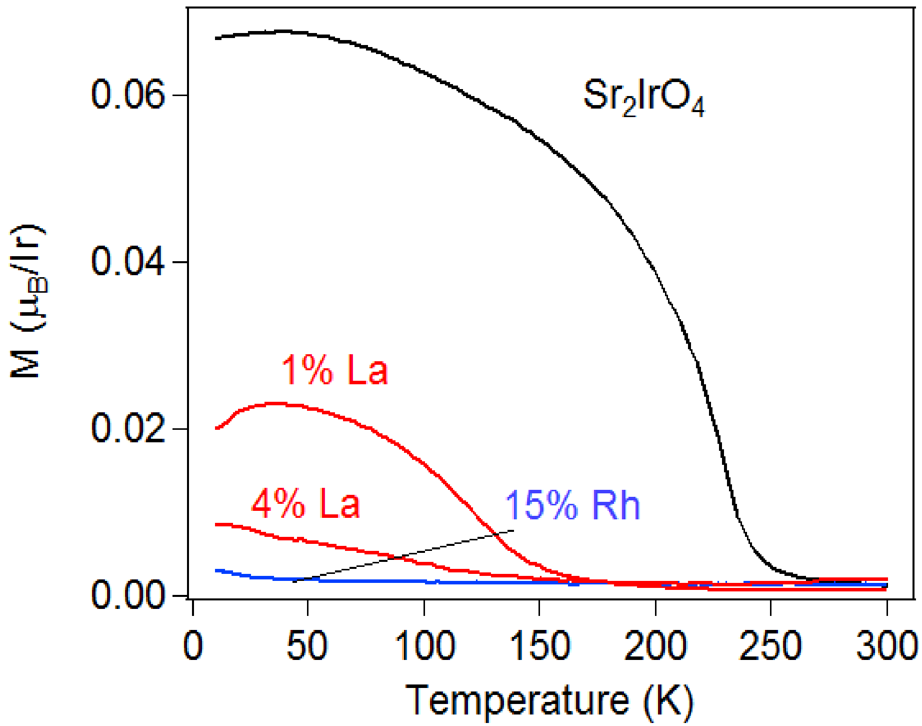
=> Large Rh dopings can be reached but strong perturbation of IrO_2 plane.

Towards a metallic state

Resistivity



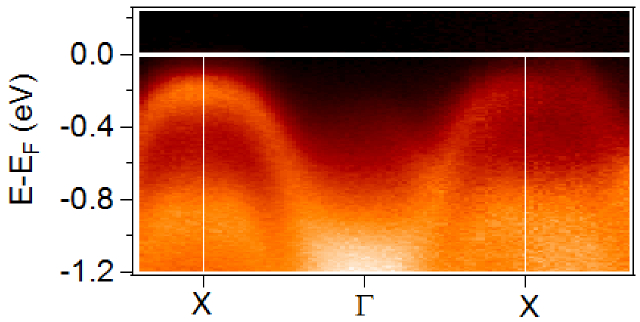
Magnetization (1T)



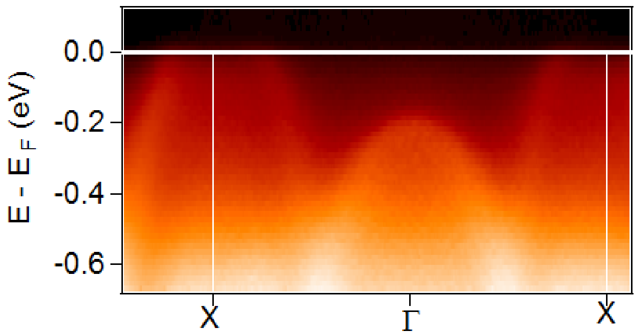
Electronic structure measured by ARPES for Rh doping

Dispersion along ΓX

Pure

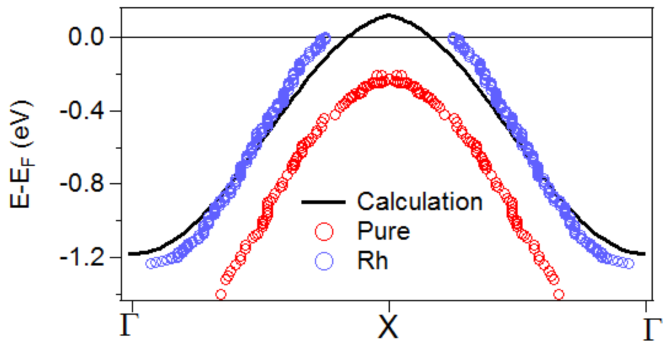


15% Rh

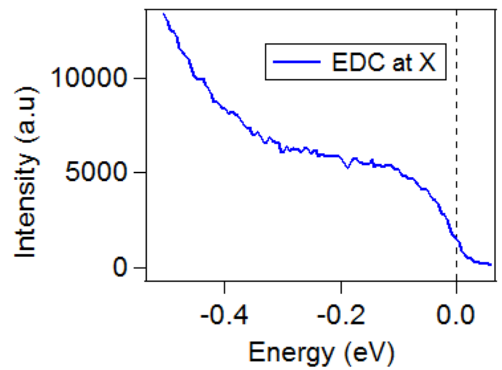


V. Brouet *et al.* PRB 2014

Compared dispersions



EDC at k_F (Rh sample)



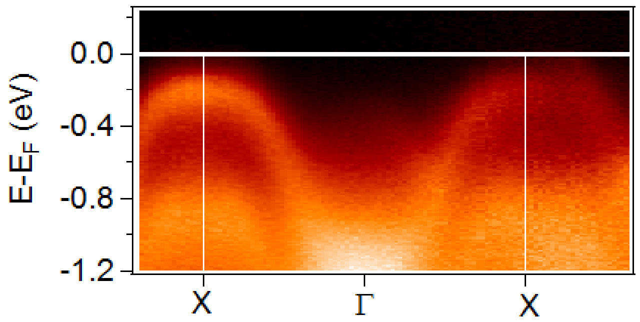
⇒ There is spectral weight at E_F in the Rh sample but no quasiparticles.

⇒ There is no renormalization compared to band calculation.

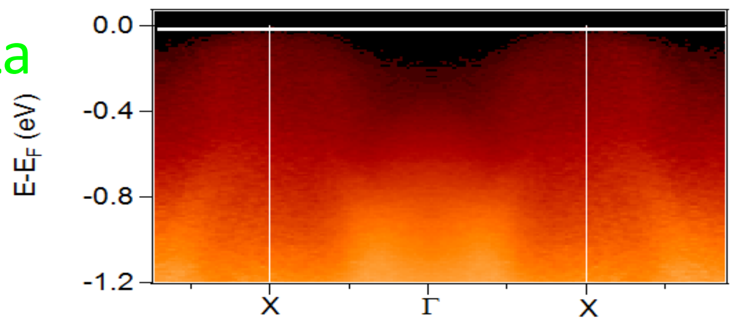
Electronic structure measured by ARPES for La doping

Dispersion along ΓX

Pure

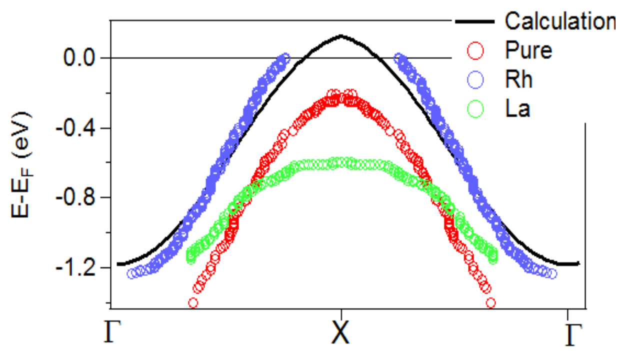


4% La

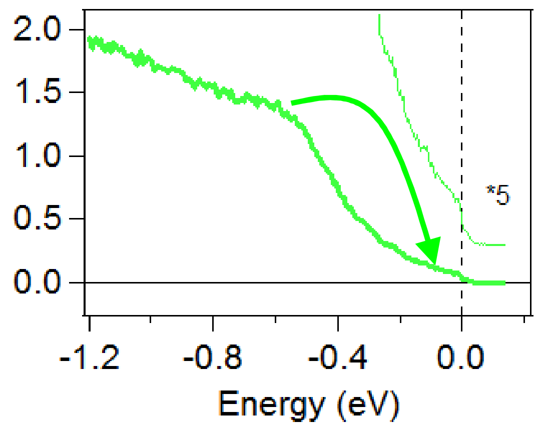


V. Brouet *et al.* PRB 2014

Compared dispersions



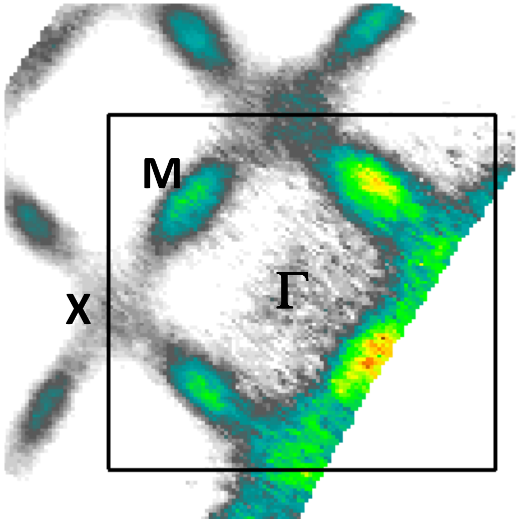
EDC at k_F (La sample)



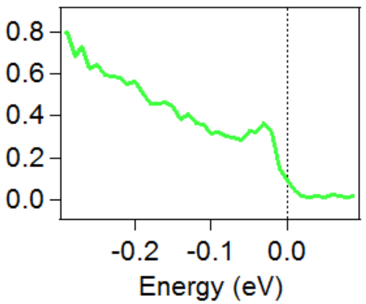
⇒ The bands shift down but weight is transferred inside the gap

Emergence of Fermi Surface in La doped systems

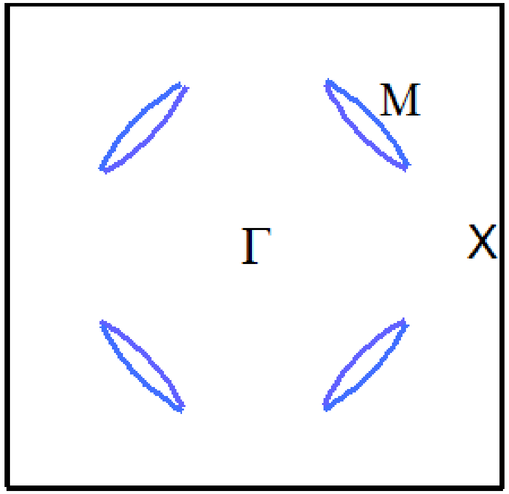
Fermi Surface develops from M points



QP peak at M

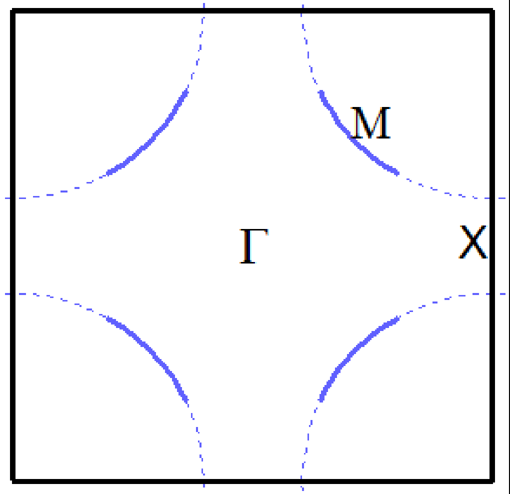


Small pocket at M ?



Small metallic pocket coexist with gap

Fermi arc ?

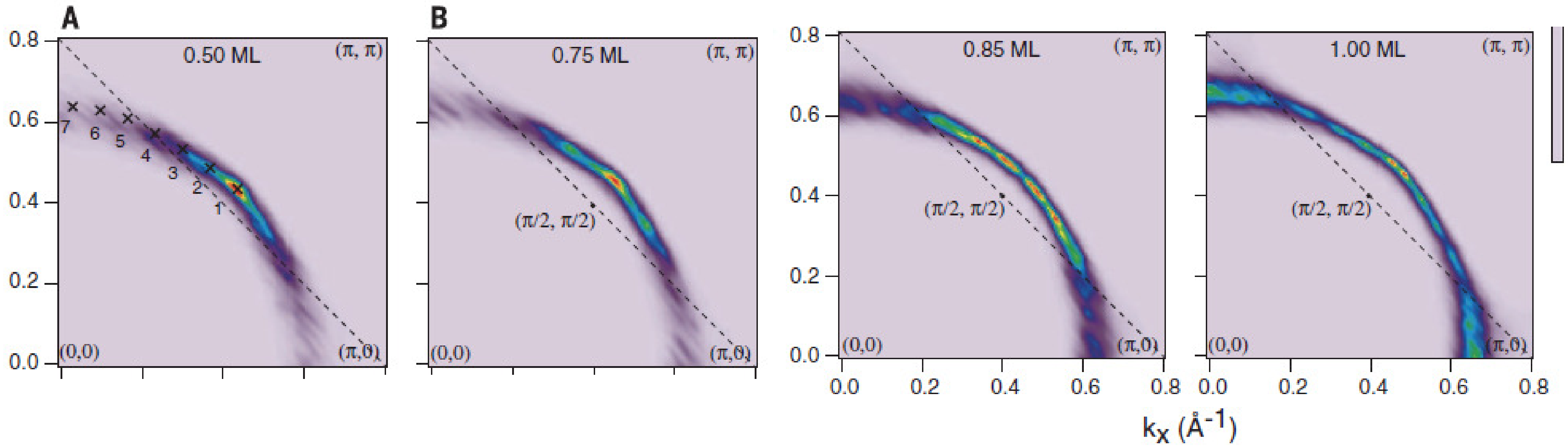


Like cuprates !?

See also : A. De la Torre et al., PRL 2015

Fermi arcs in Sr_2IrO_4 doped by K on surface

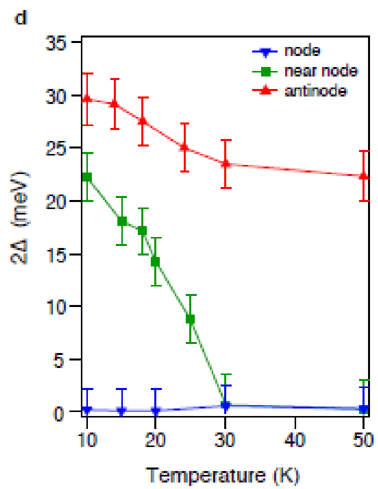
Y.K. Kim *et al.*, Science 14



Anisotropic gap opens below 30K

(ARPES + STM)

Y.K. Kim cond-mat15
Y.J. Yan PRX 15



Larger doping than bulk ?

Different type of doping ?

=> Similar behavior than cuprates ?

Conclusions

- New insulating state emerges from the combination of moderate electronic correlations and strong spin-orbit coupling

- The transition to a good metallic state is difficult, but local perturbations easily suppress the gap locally

- ARPES allows to monitor the appearance of a metallic Fermi Surface. There is no evidence of renormalized band dispersion.

- Perspectives : full properties of doped compounds
  comparasion between chemical and « external » doping

ANR « SOCRATE » : Spin Orbit Coupling in iRidATEs

=> Study of impact of SOC on correlated, magnetic and topological properties

Sample Synthesis : V. Brouet, D. Colson, J.B. Moussy, L. Fruchter, Z.Z. Li
ARPES : V. Brouet
NMR : F. Bert, P. Mendels
Transport : L. Fruchter
Raman : Y. Gallais, A. Sacuto, M.A. Méasson
RIXS : J.P. Rueff, V. Ilakovac
Theory : M. Civelli, M. Rozenberg, M.O. Goerbig, S. Biermann

----- Collaborations welcome -----

------ Post-docs available -----