ARPES study of many-body effects and electronic reconstructions in misfit cobaltates

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CASSIOPEE :
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P. Le Fèvre, F. Bertran

Outline

Na_xCoO_2 and misfit cobaltates

Counter-intutive evolution of the correlation strength with doping

Nature of low energy excitations in cobaltates ?

Study of ARPES lineshapes

=> Consistent with strong correlations (Z = 0.15 at x=0.7).

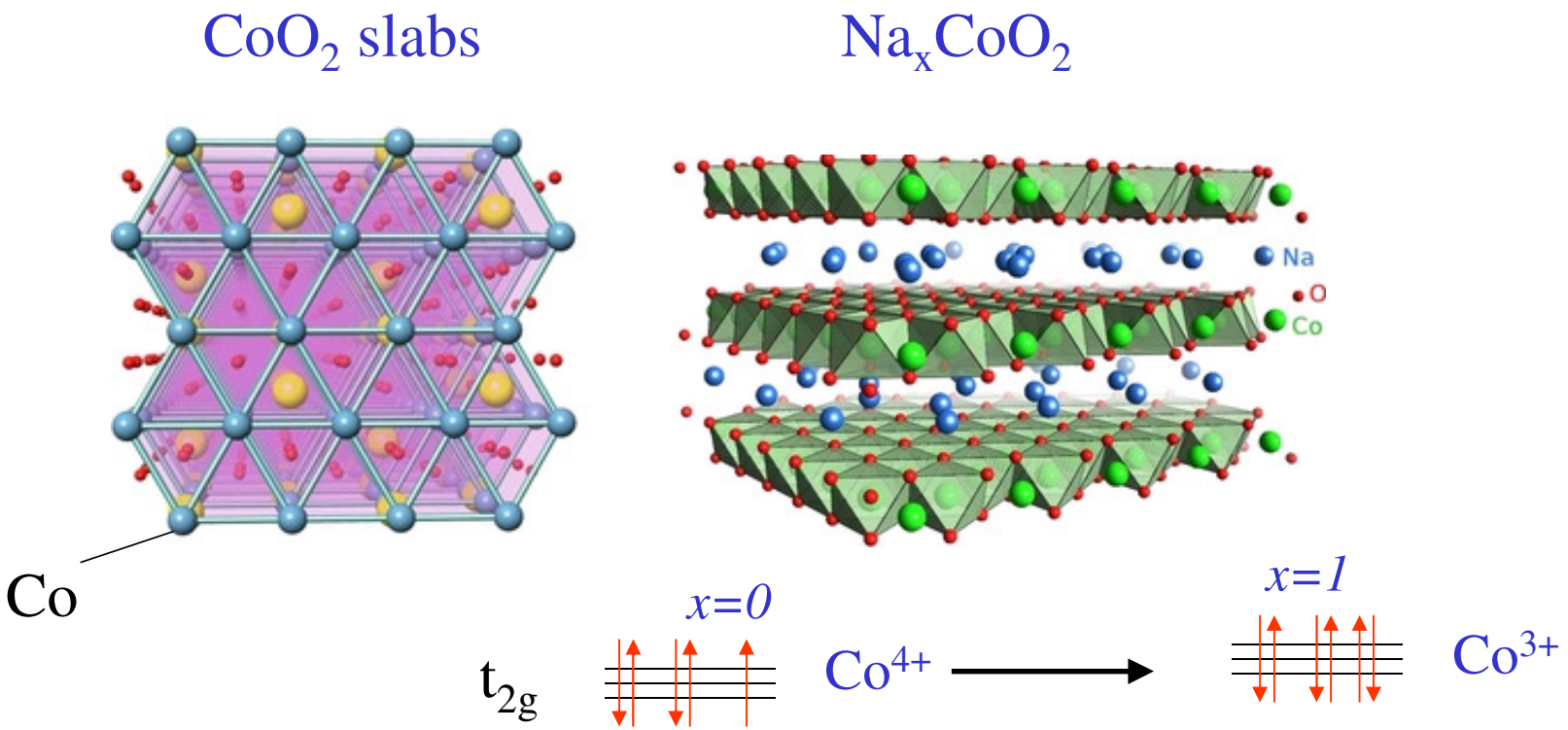
=> Increasing correlations near x=1, towards the band insulator.

Influence of the 3D environment on electronic orderings in CoO_2 planes ?

=> Deviation from the rigid band filling picture at high x

=> Consistent with partial electronic localization induced by the Na or misfit potentials

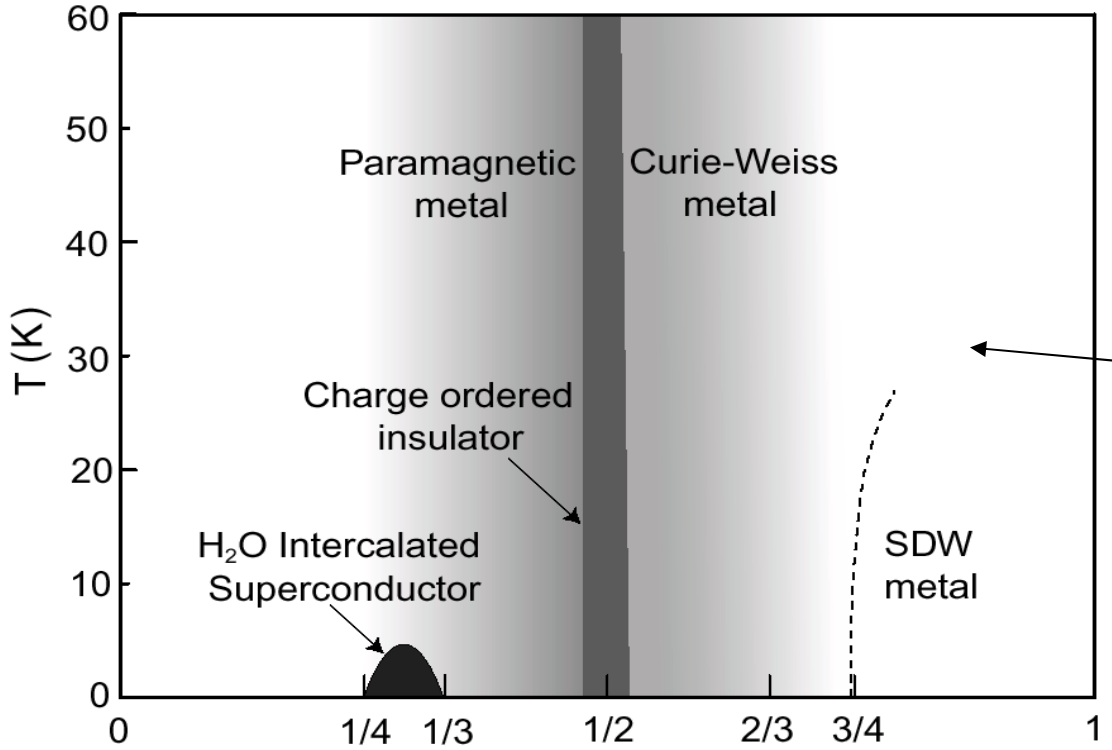
Cobaltates : triangular planes of Co filled by a variable number of electrons



Metallic phases with charge, spin, orbital degrees of freedom…
How do they interact ? Does Na plays a role ?

From Mott insulator to band insulator…

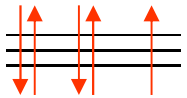
Na_xCoO_2



Foo *et al.*, PRL **92**, 247001 (04)

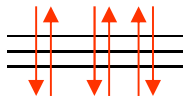
High TEP

t_{2g}



Co^{4+}

Co^{3+}



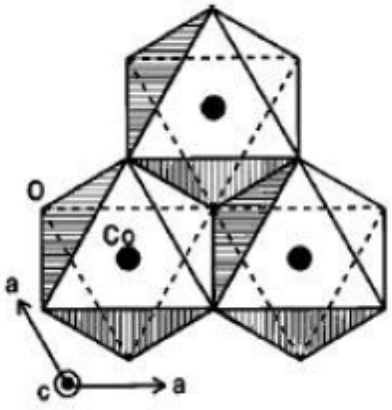
Mott insulator ?

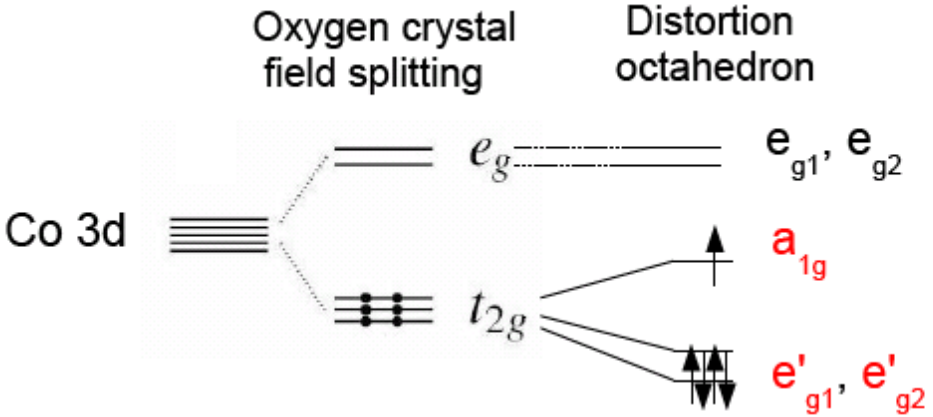
Band insulator

Magnetic correlations seem to appear near the band insulator !

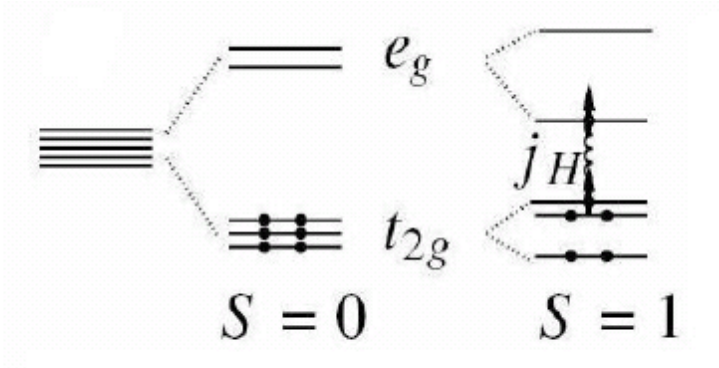
Competing degrees of freedom

Triply degenerate band, hybridization with oxygen, triangular geometry may frustrate AF correlations…





Possibility of coupled spin-orbital-lattice excitations
=> spin-orbital-polarons ?



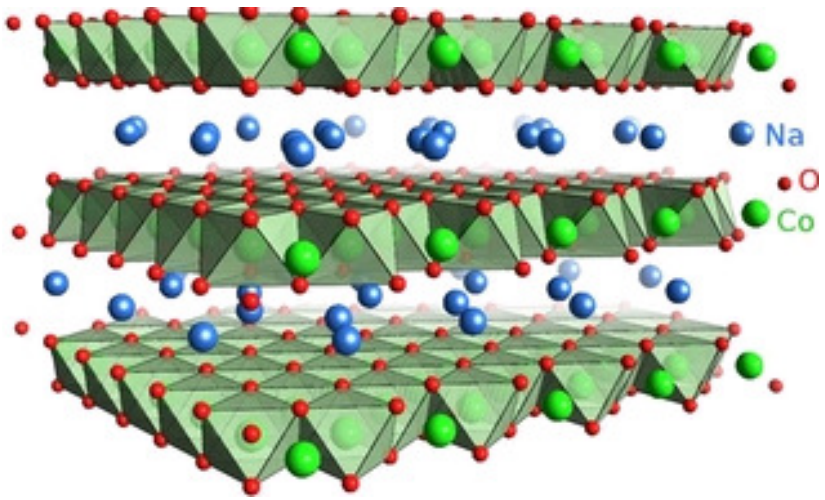
« The low-lying magnetic states of Co^{3+}, accessible for electrons via the intersite hopping, provide an extra dimension in physics of Na_xCoO_2. »

Khaliullin and Chaloupka PRB 77, 104532 (2008)

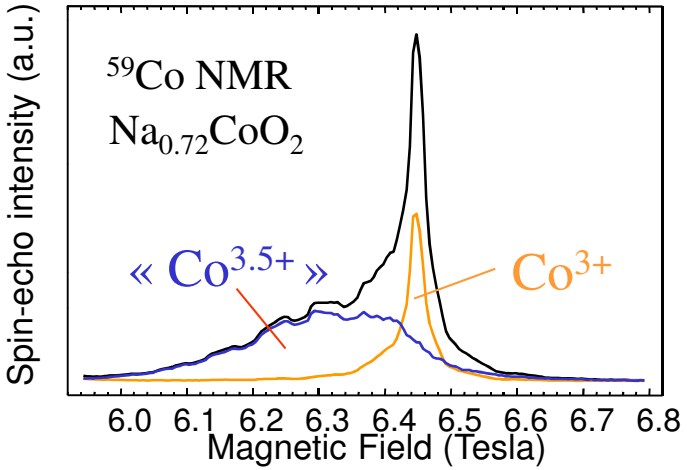
An additional degree of freedom : role of Na ?

Na induced correlations ?

Marianetti and Kotliar
PRL **98**, 176405 (2007)

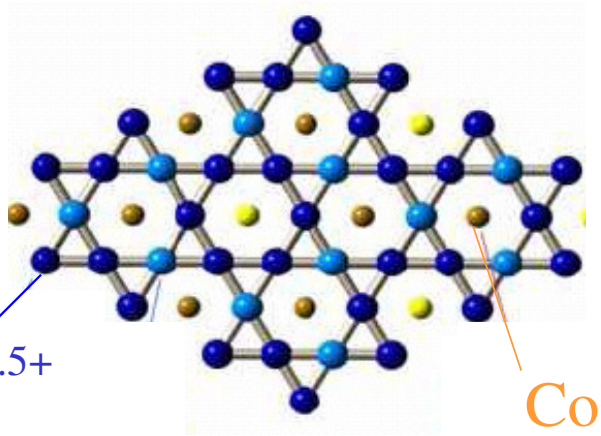


NMR detects inequivalent Co sites at high x



I.R. Mukhamedshin *et al.*, PRL 2005

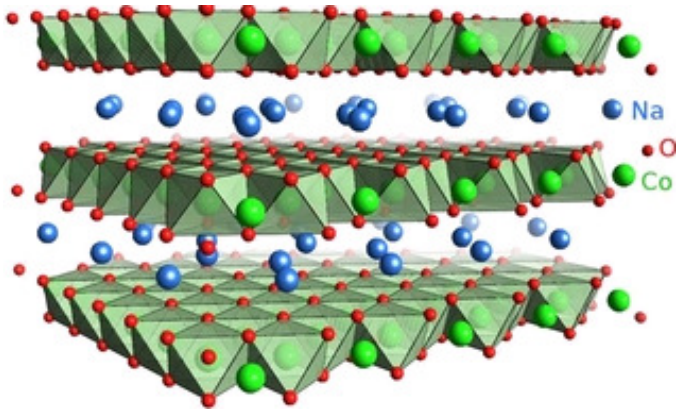
The charge order is induced by Na order



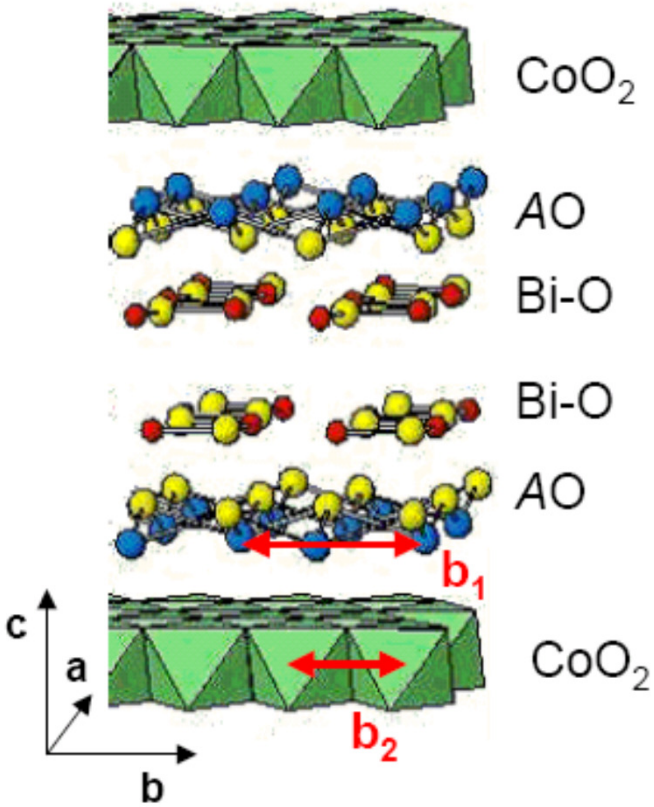
H. Alloul *et al.*, EPL 2009

Two families of cobaltates : Na and misfits

Na_xCoO_2



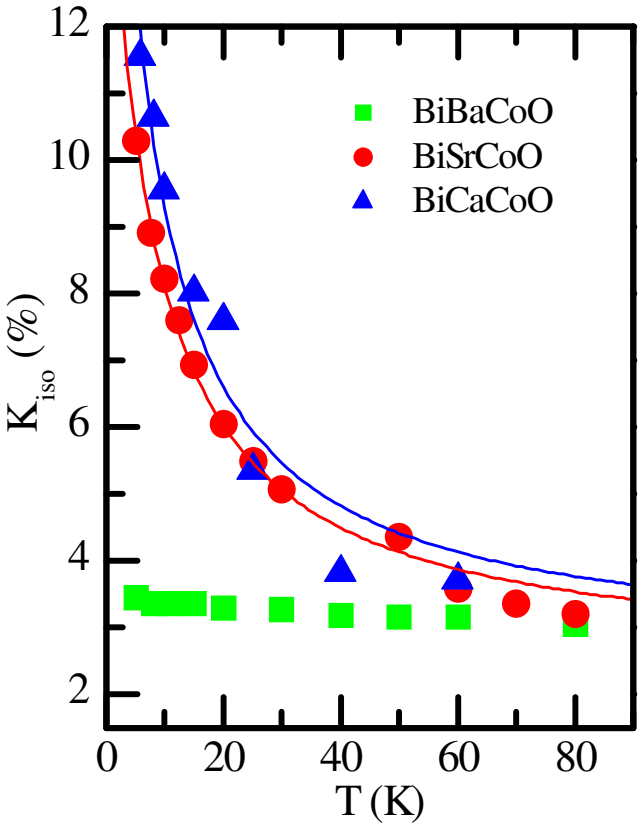
$[Bi_2A_2O_4]\,[CoO_2]_{b1/b2}$



- Charge transfer from Rock-Salt planes to CoO_2 planes
- Doping equivalent to x=0.7-0.9
- Different 3D environment (better surface quality for ARPES)

Electronic properties of misfit cobaltates

Pauli to Curie-Weiss susceptibilities

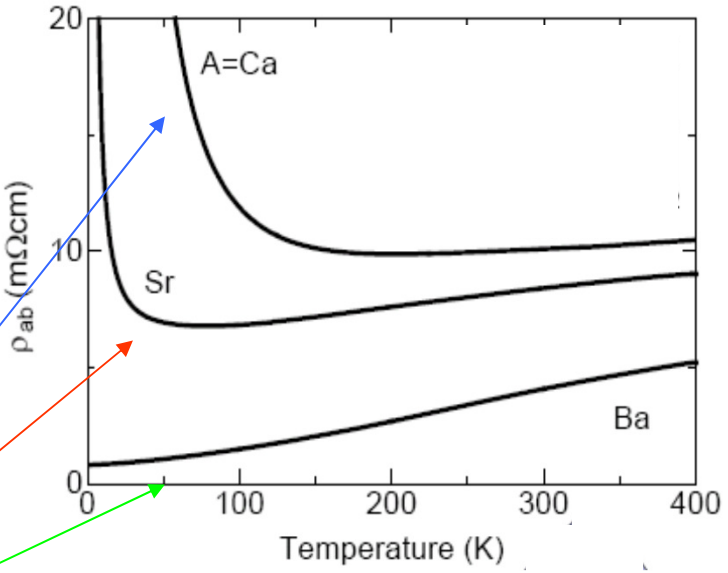


J. Bobroff *et al.* PRB 2007

High TEP values

x=0.85
x=0.75
x=0.7

Resistivity vs Temperature

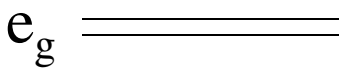


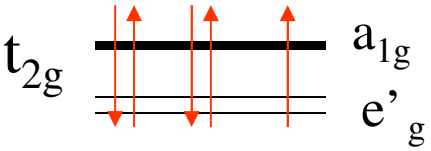
W. Kobayashi *et al.*

Same magnetic interactions
& different charge order / disorder ?

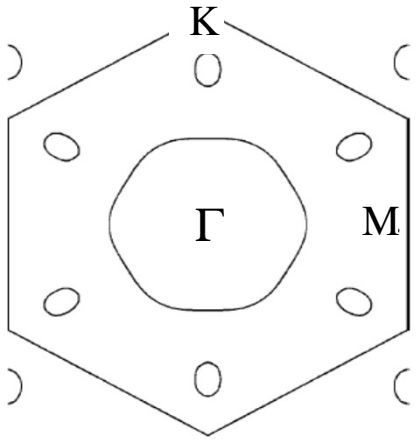
Electronic structure as seen from ARPES

Band structure of a CoO_2 plane (from LDA)



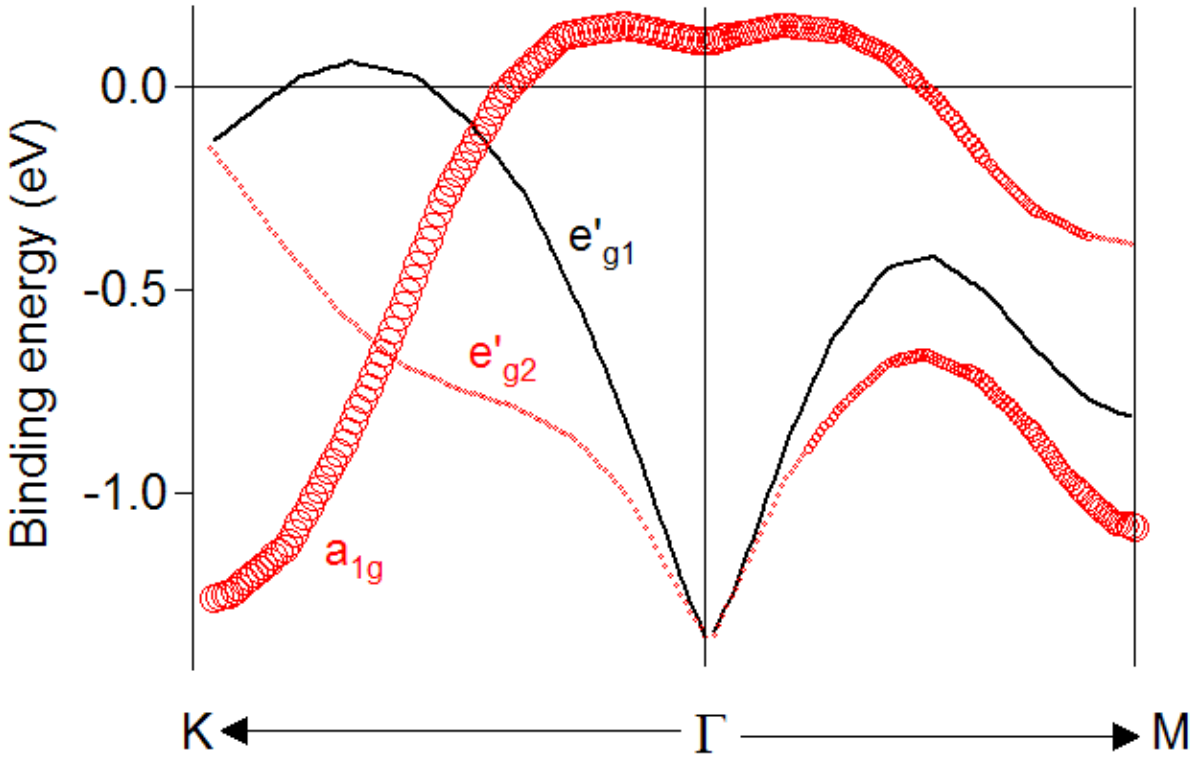


Co^{4+} + *x* electrons
on a triangular lattice



Surface de Fermi

$Na_{0.5}CoO_2$

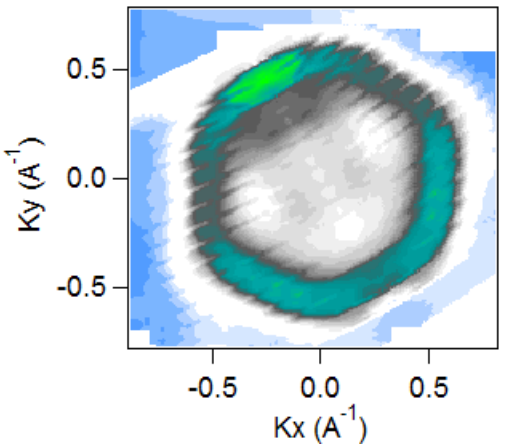


Singh *et al.*, PRB 2000; Lee *et al.*, PRB 2004

Same low energy electronic structure in Na and misfit cobaltates (BiBaCo)

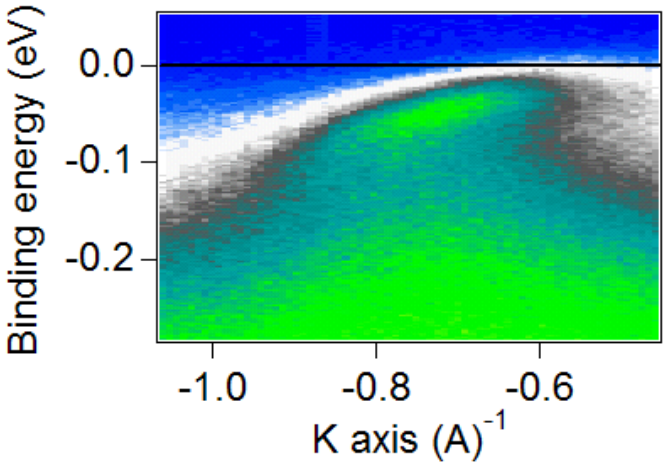
ARPES in Na_xCoO_2 : M.Z. Hasan *et al.*, PRL2004, D. Qian *et al.*, PRL2006
H.B. Yang *et al.*, PRL 2004, 2005

Hexagonal FS from Co a_{1g} band



- No e'$_g$ pockets

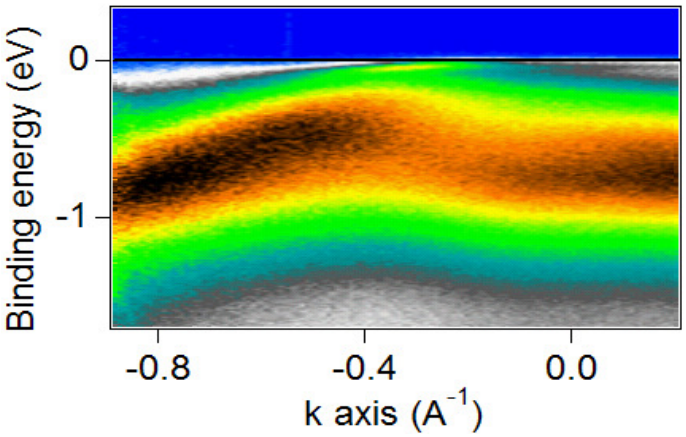
High effective mass



- Narrow band near the Fermi level

$V_F = 0.3 eV.Å$

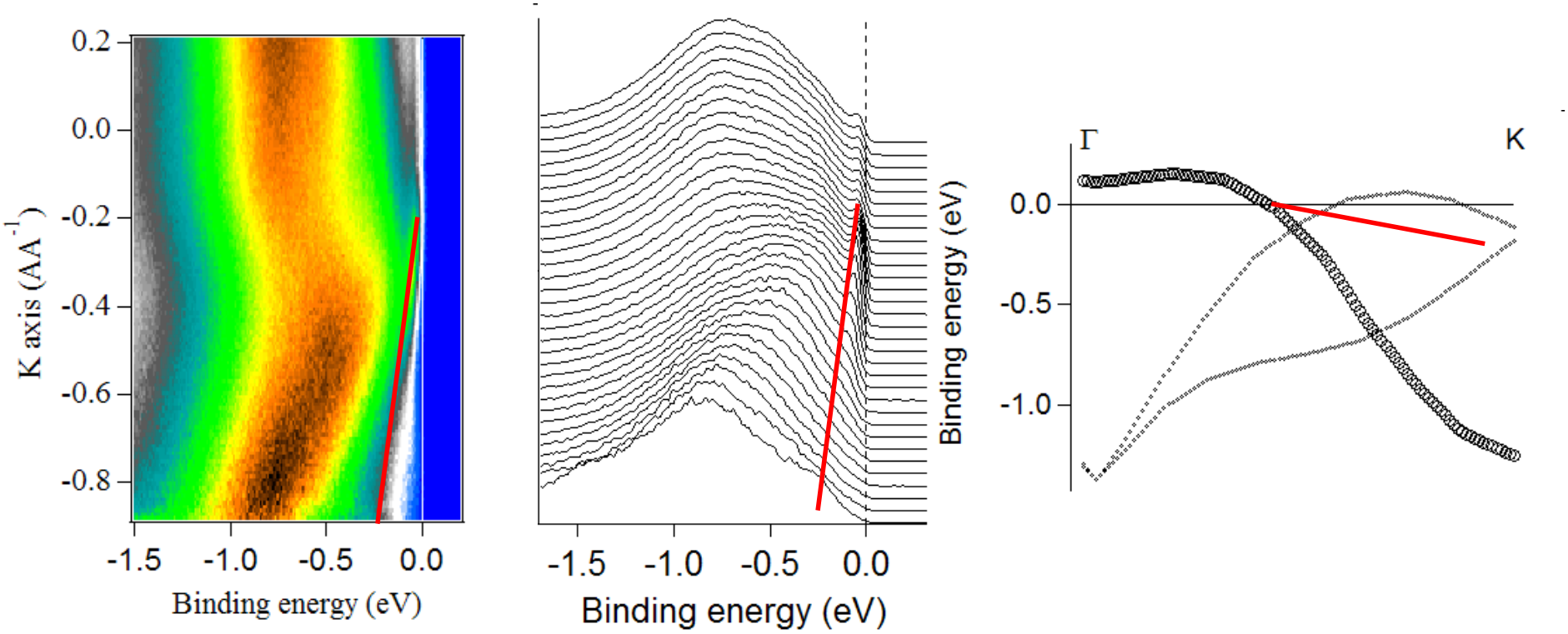
Peculiar lineshape



- Two dispersing components

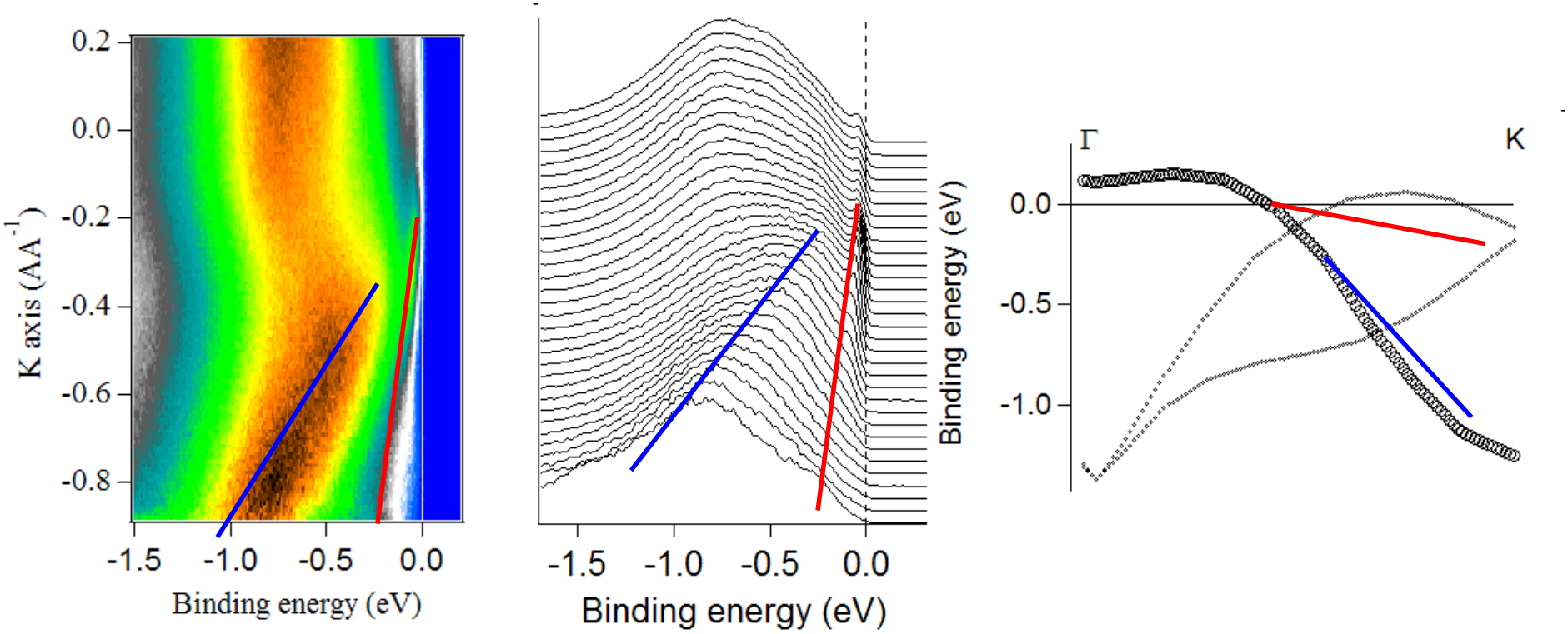
V. Brouet et al., PRB2007

How to interpret the lineshape in BiBaCo ?



- Strongly renormalized a_{1g} band

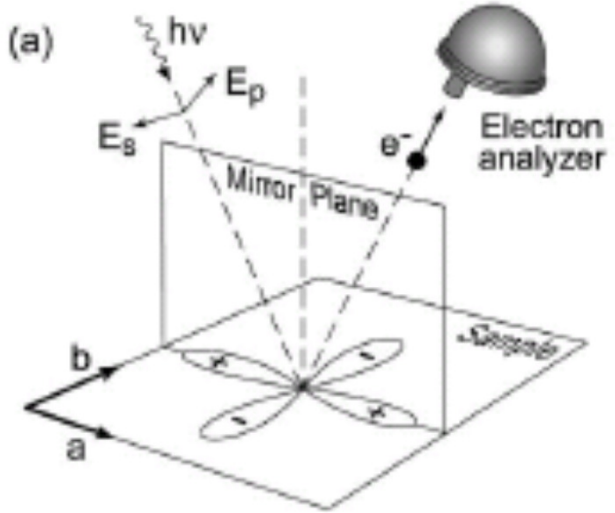
How to interpret the lineshape in BiBaCo ?



- Strongly renormalized a_{1g} band
- Or kink ? (of what origin ?)
- Or interactions between a_{1g} and e'_g bands ? (hybridization gap)

=> Depending on the interpretation : 1.5<m/m<6*

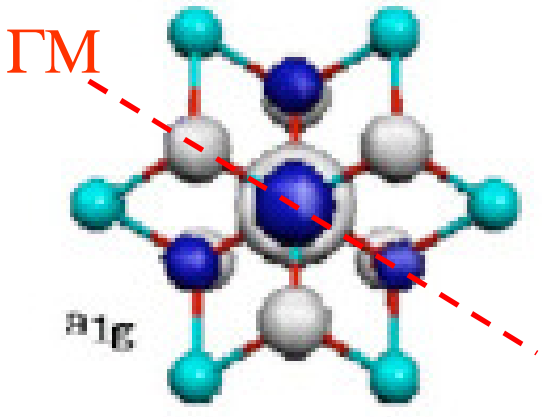
Using light polarization to observe different orbitals



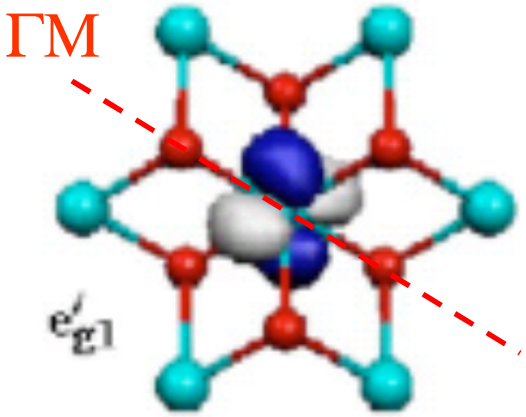
ARPES intensity proportional to :

$$\langle \phi_f^{\mathbf{k}} | \mathbf{A}\cdot\mathbf{p} | \phi_i^{\mathbf{k}} \rangle \begin{cases} \phi_i^{\mathbf{k}} \text{ even} & \langle + | + | + \rangle \Rightarrow \mathbf{A} \text{ even} \\ \phi_i^{\mathbf{k}} \text{ odd} & \langle + | - | - \rangle \Rightarrow \mathbf{A} \text{ odd.} \end{cases}$$

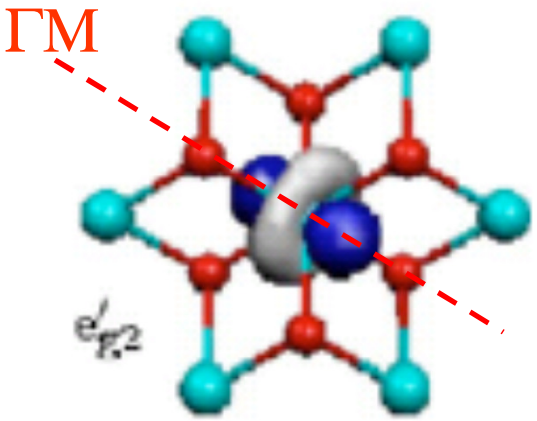
a_{1g} : even



e'_{g1} : odd



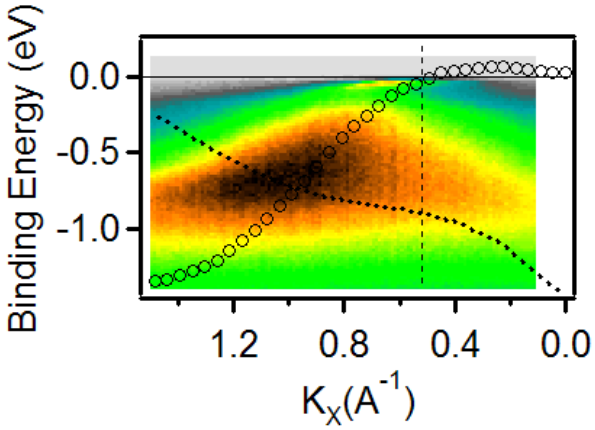
e'_{g2} : even



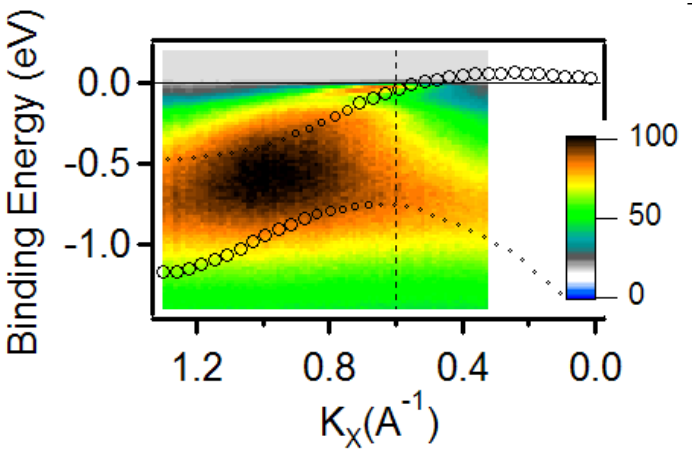
The structure of a_{1g} is not due to interaction with e'_g

Horizontal polarization : even bands $a_{1g} + e'_{g2}$

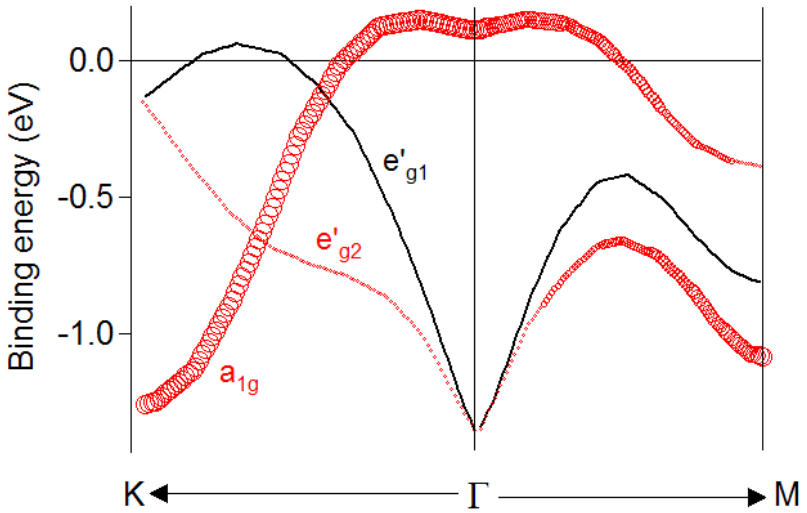
ΓK



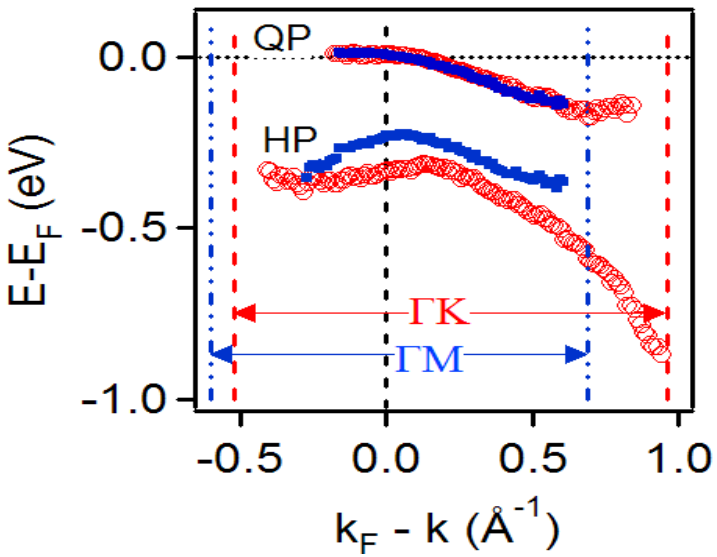
ΓM



LDA bands



Experimental dispersion



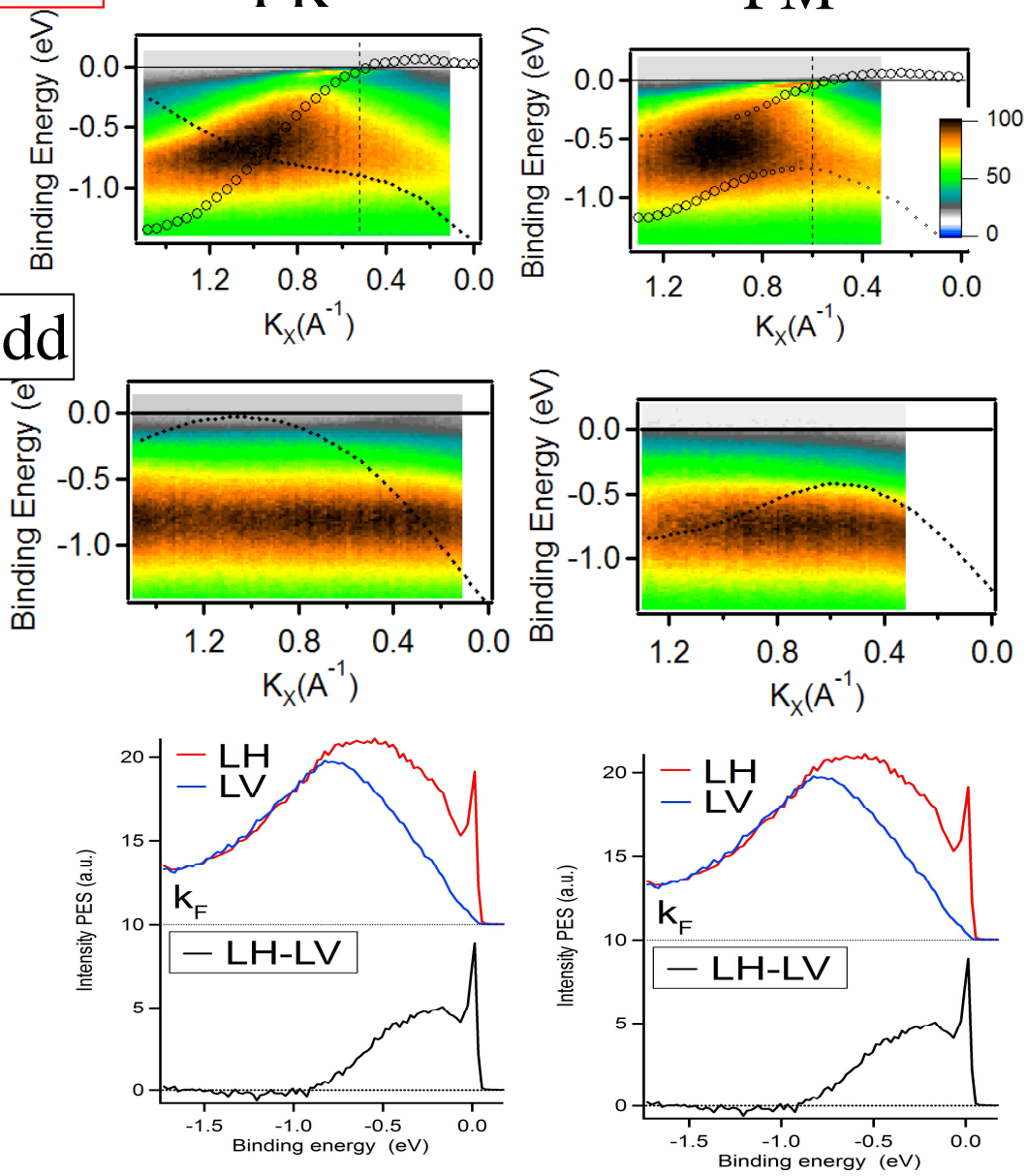
Intrinsic peak-dip-hump structure of a_{1g}

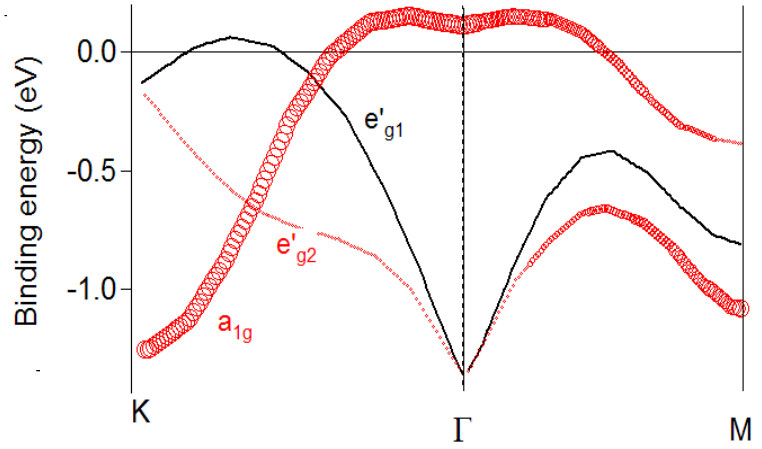
even

odd

ΓK

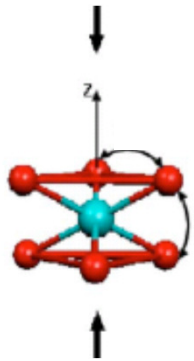
ΓM





a_{1g}/e'_g splitting sensitively depends on the octahedra distortion

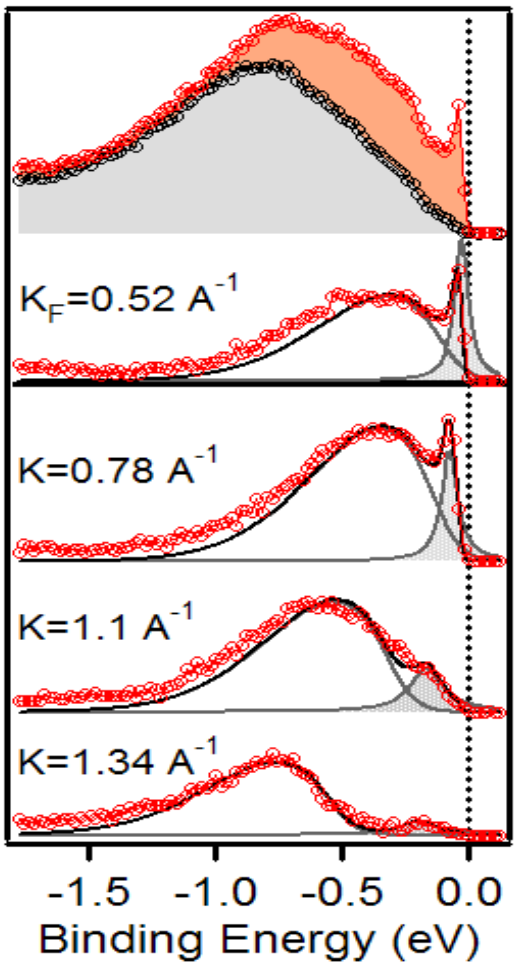
M.B. LePetit, PRB2007



=> Subtracting LV spectrum from LH isolate the PDH of a_{1g}

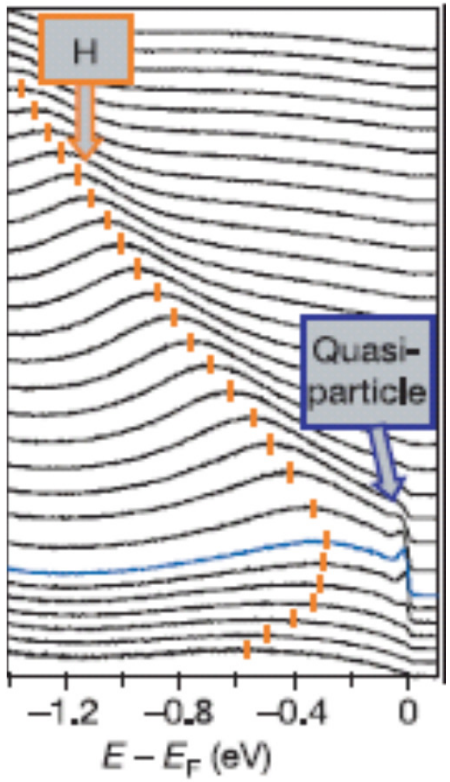
Intrinsic peak-dip-hump structure of a_{1g}

BiBaCo



Manganites

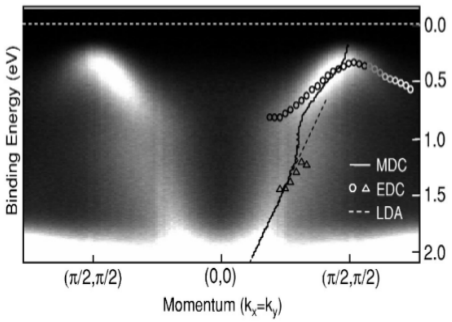
$La_{1.2}Sr_{1.8}Mn_2O_7$



N. Mannella *et al.*,
Nature **438**, 474 (2005)

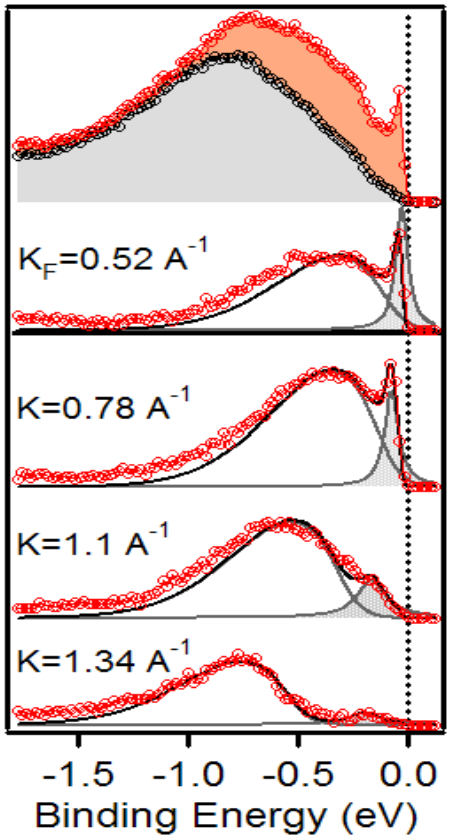
« Waterfall » in cuprates

$Ca_2CuO_2Cl_2$

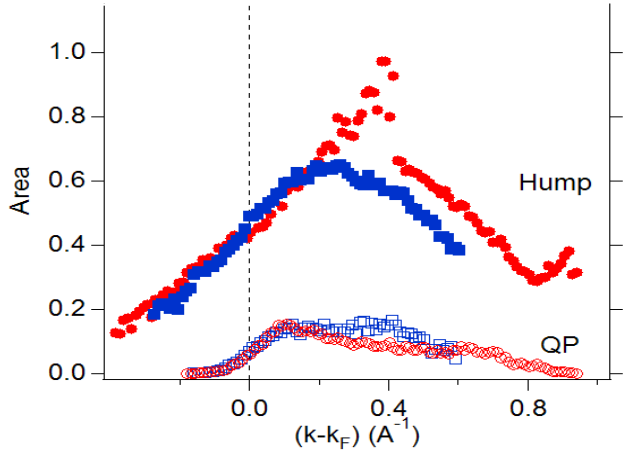


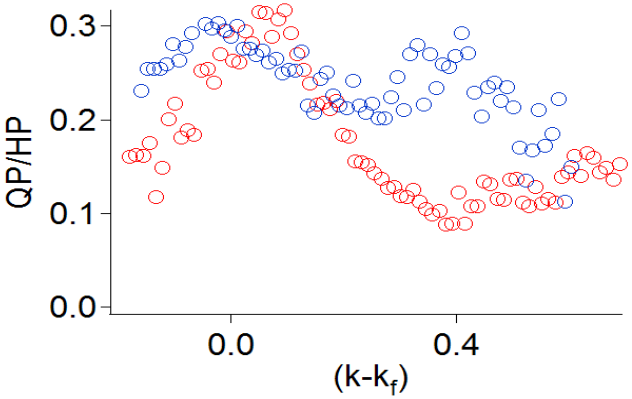
F. Ronning et al. PRB 2005

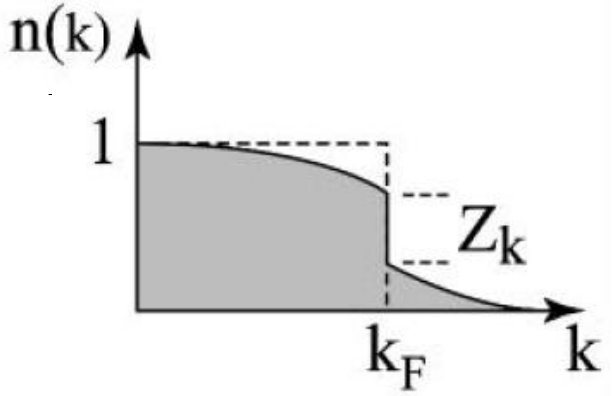
The distribution of spectral weight imply strong many-body effects



Area vs k







=> Z=0.15±0.05

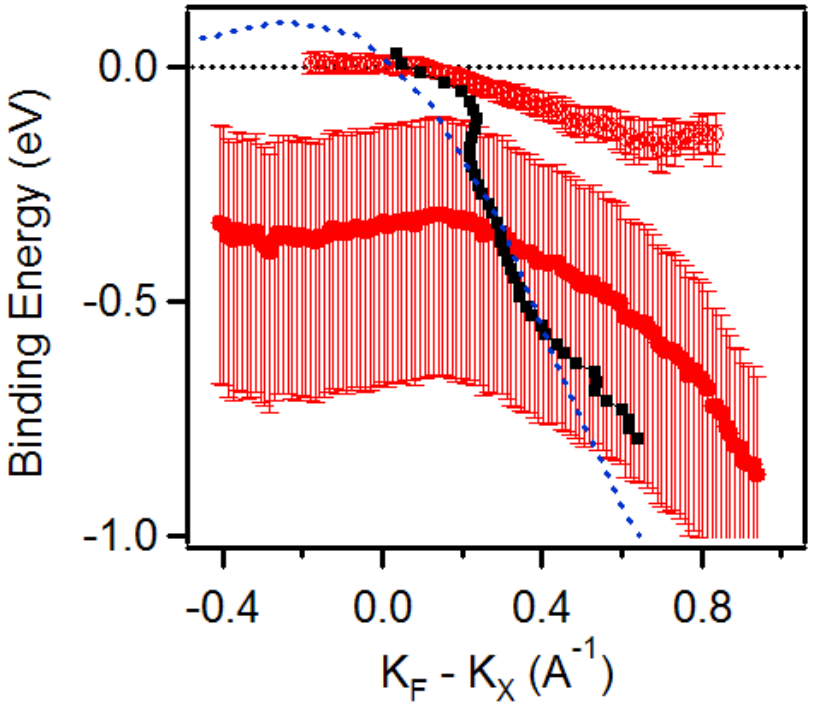
Z * (LDA bandwidth) = 0.2eV

=> 0.2eV is the QP energy scale

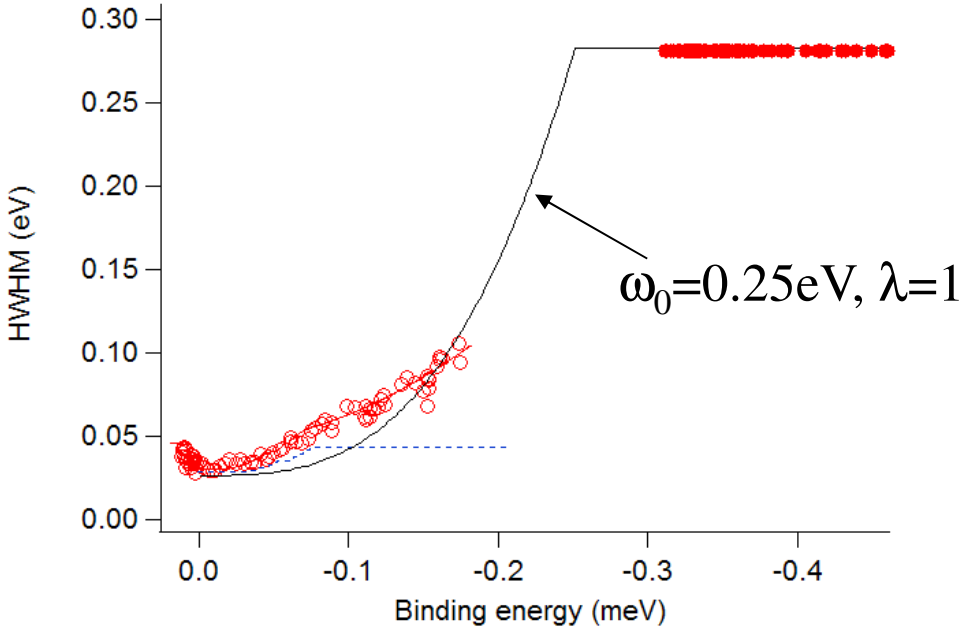
A. Nicolaou *et al.*, PRL 2010

In this case, spectral weight information is more direct than self-energy fits

Dispersion - $\Sigma'(\omega)$



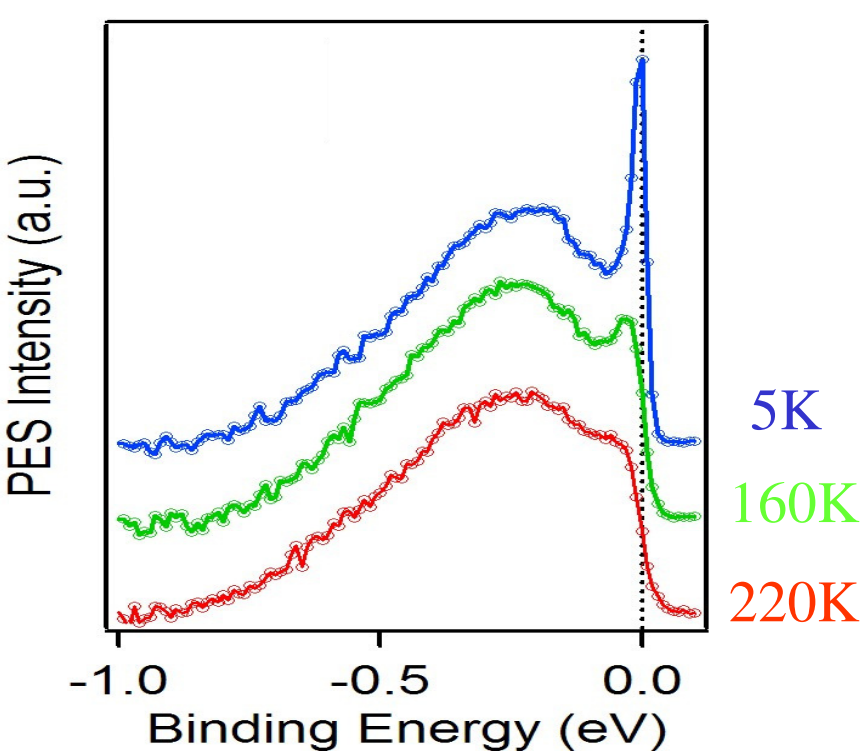
Width - $\Sigma''(\omega)$

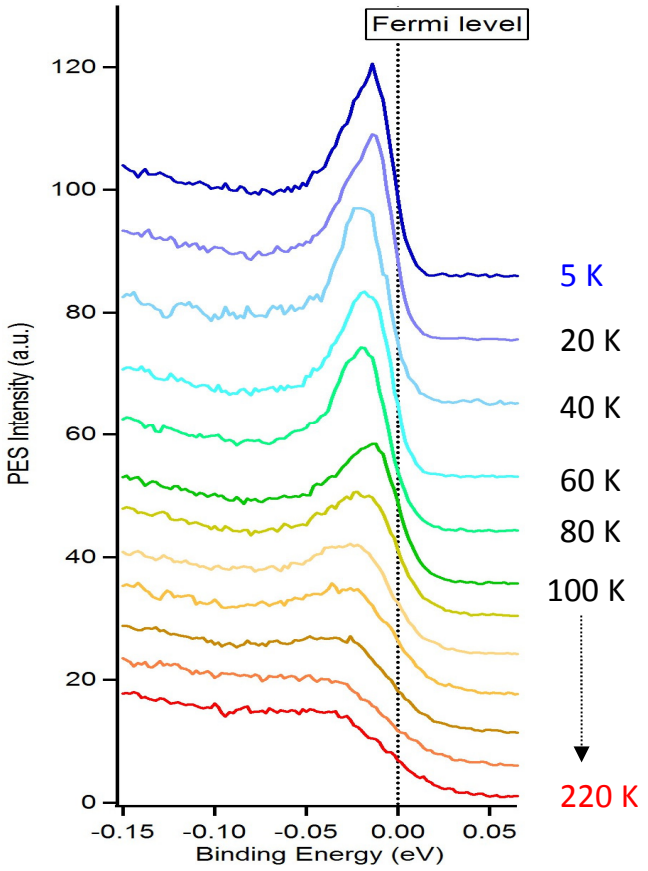


Typical fits of width increase and dispersion renormalization fail to reproduce the HP weight at E_F

A. Nicolaou *et al.*, PRL 2010

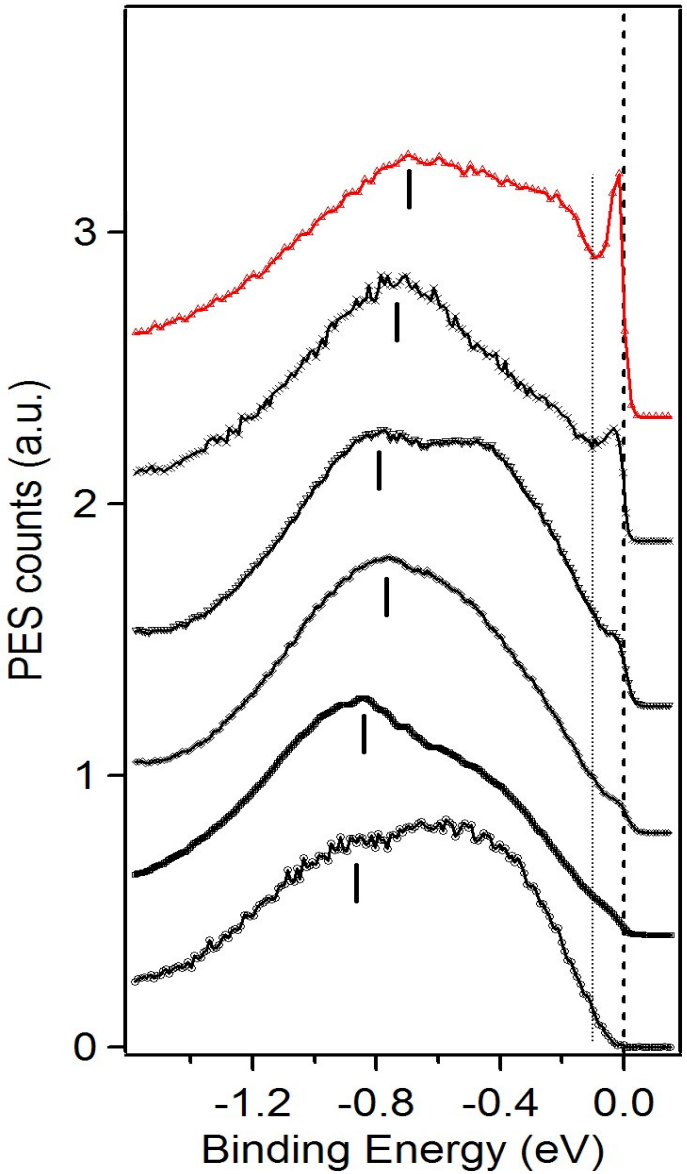
The QP « disappears » at high temperature





Typical behavior of a strongly correlated system

The QP « disappears » when doping increases



BiBaCo
x=0.71, m=2

CaCoO
x=0.75, m=1.6

BiSrCo, Pb doped

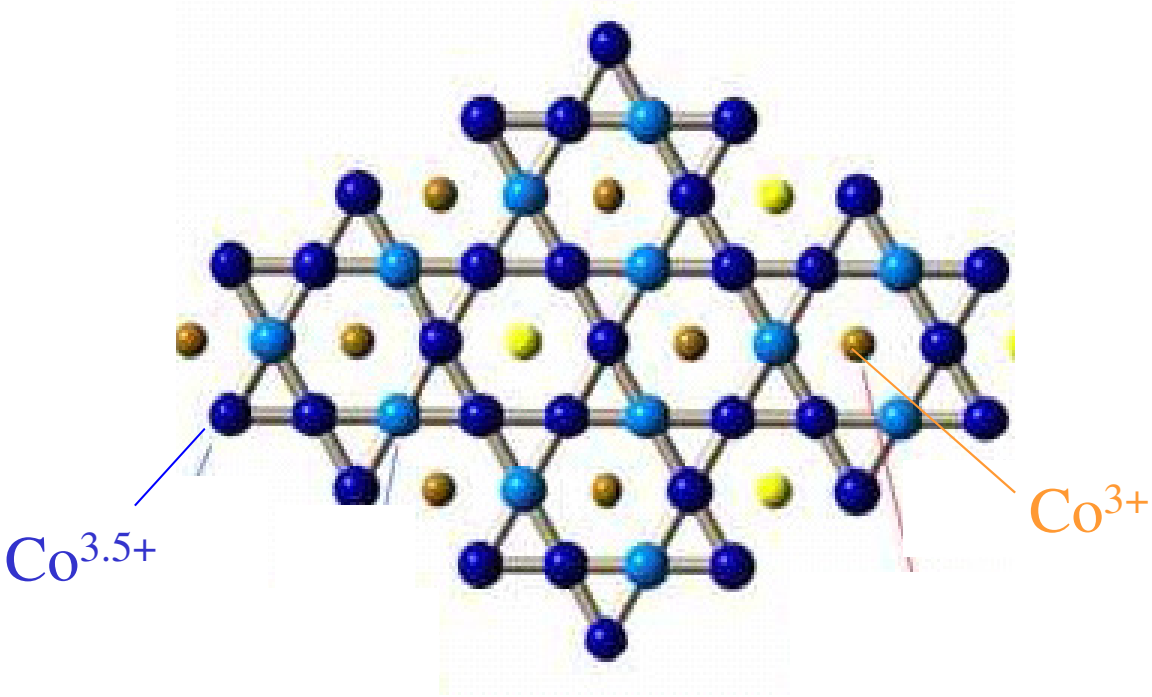
BiSrCo
x=0.77, m=1.82

BiCaCo
x=0.85, m=1.7

x increases towards band insulator

- The correlations seem to increase near the band insulator.
- Why are there strong correlations in this limit ?
  - => Polaronic lineshape ?
  - => Electronic orderings ?

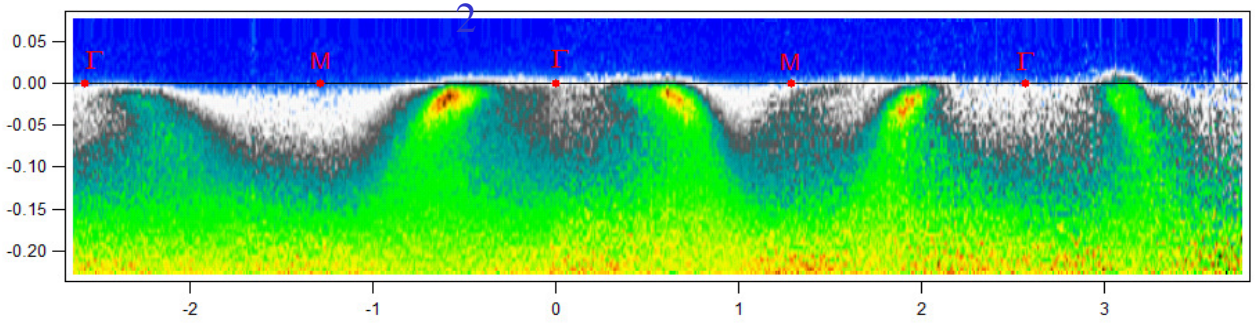
Electronic orderings at high dopings ?

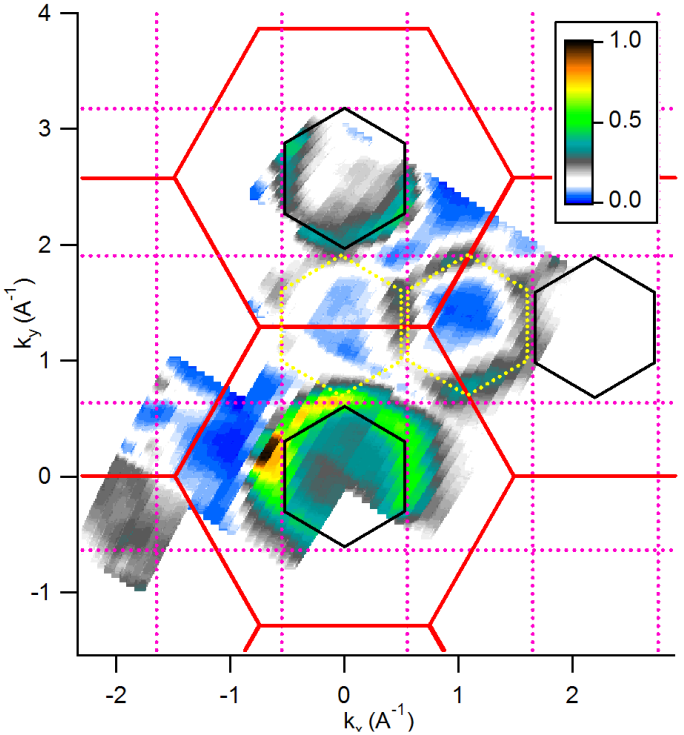


H. Alloul *et al.*, EPL 2009

Misfit cobaltates : Evidence for coupling between Rock-Salt and CoO_2 planes

$[Bi_2Ba_2O_4]_2CoO_2$

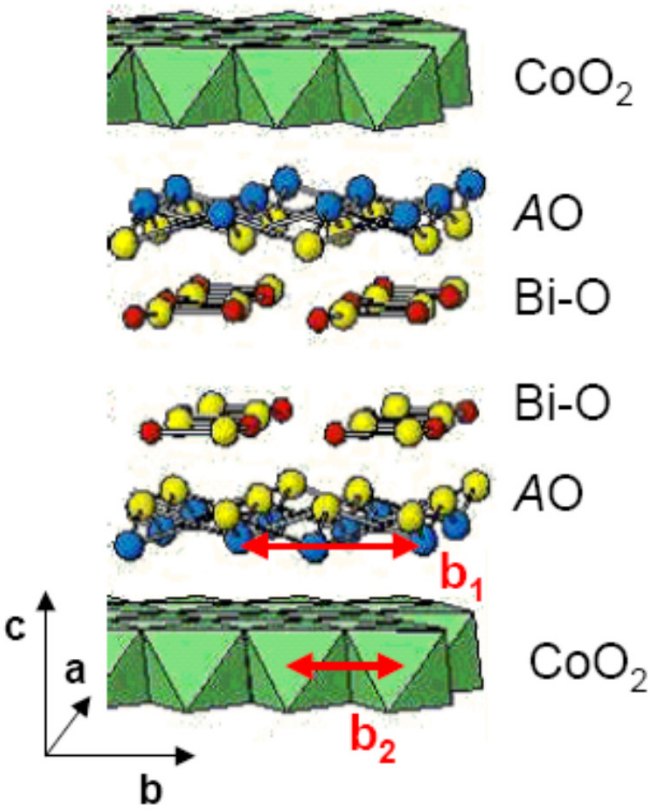


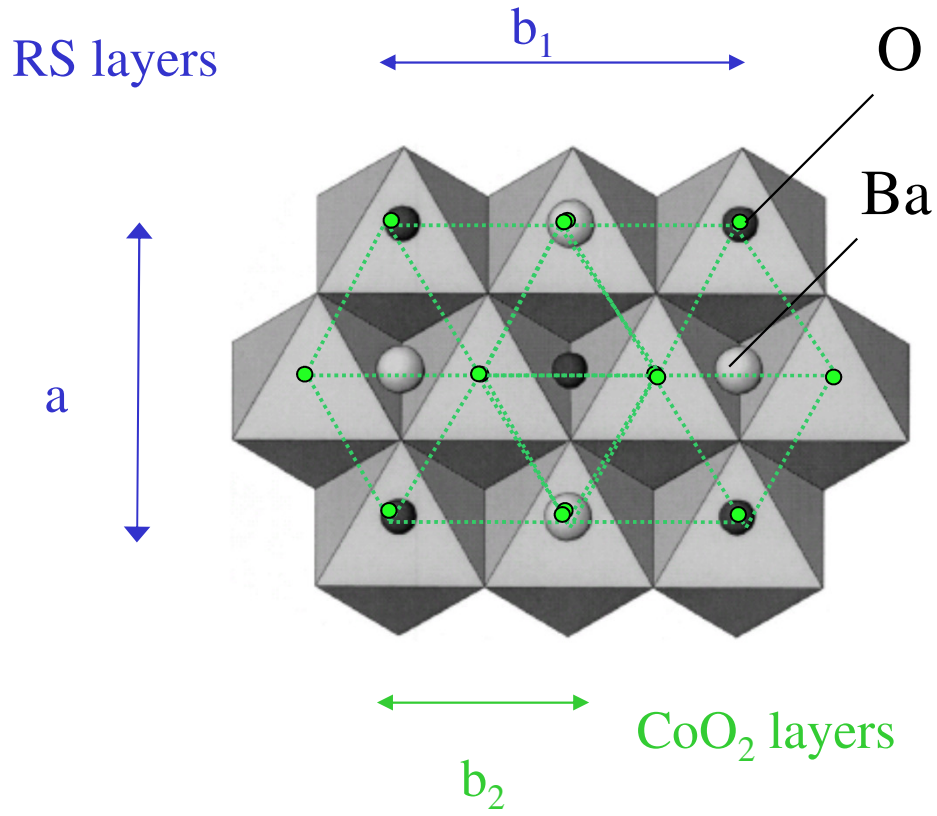


=> Replica appear with RS periodicity

What is the effect of the RS potential on the electronic motion in the CoO_2 plane ?

Rock-Salt structure



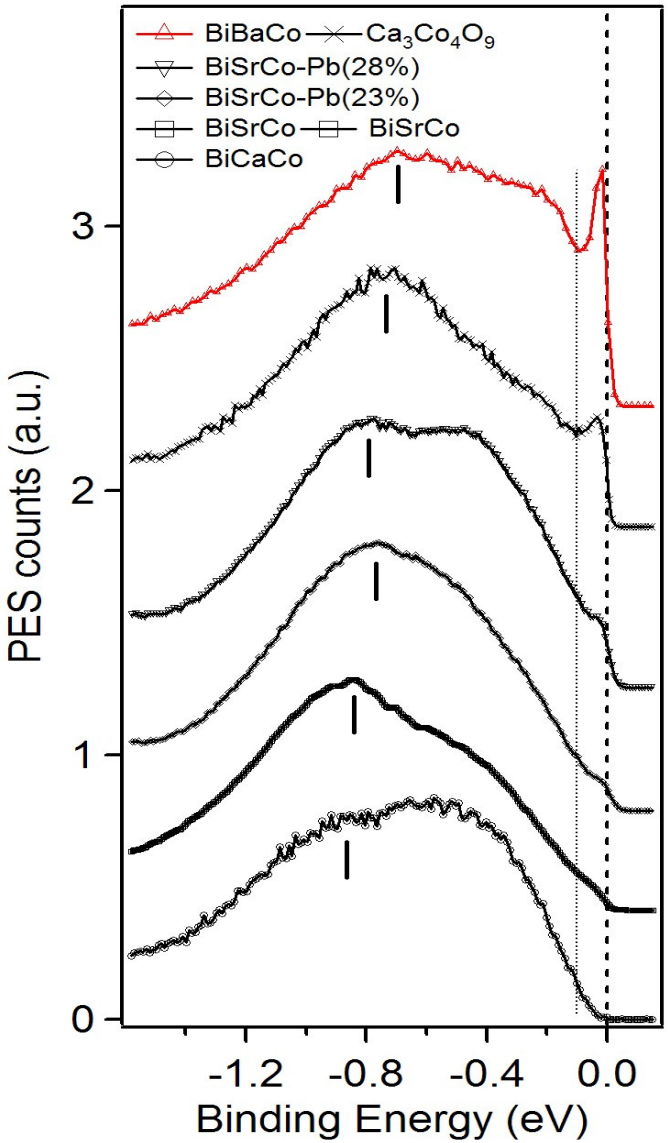


Inequivalent Co sites with respect to Ba^{2+} positions.

=> Situation may be analogous to Na_xCoO_2

=> Co^{3+} may form directly below a Ba^{2+}

The number of metallic holes in the band can be deduced from the FS area



BiBaCo
x=0.71, m=2

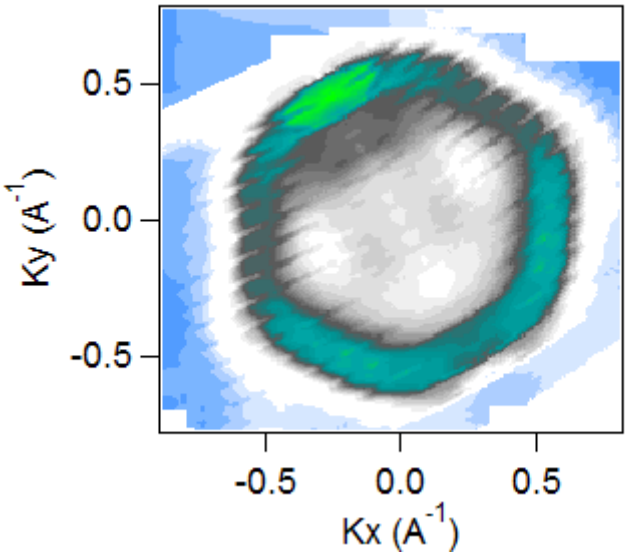
CaCoO
x=0.75, m=1.6

BiSrCo, Pb doped

BiSrCo
x=0.77, m=1.82

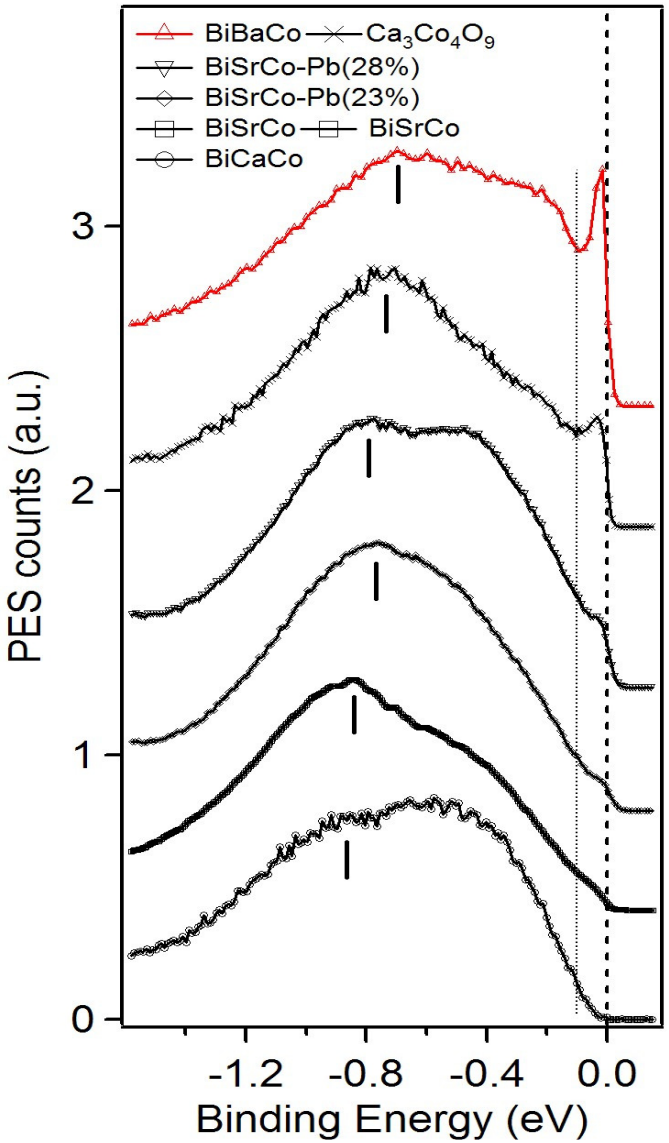
BiCaCo
x=0.85, m=1.7

Fermi Surface of BiBaCo



… k_F=0.6 => x=0.7

The number of metallic holes in the band can be deduced from the FS area



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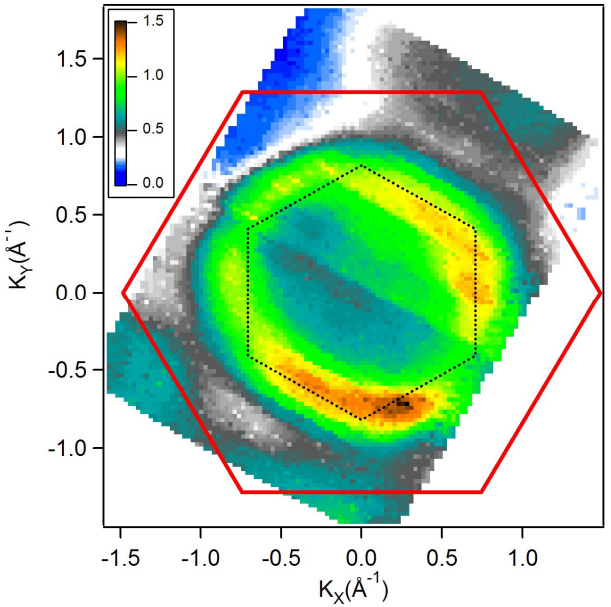
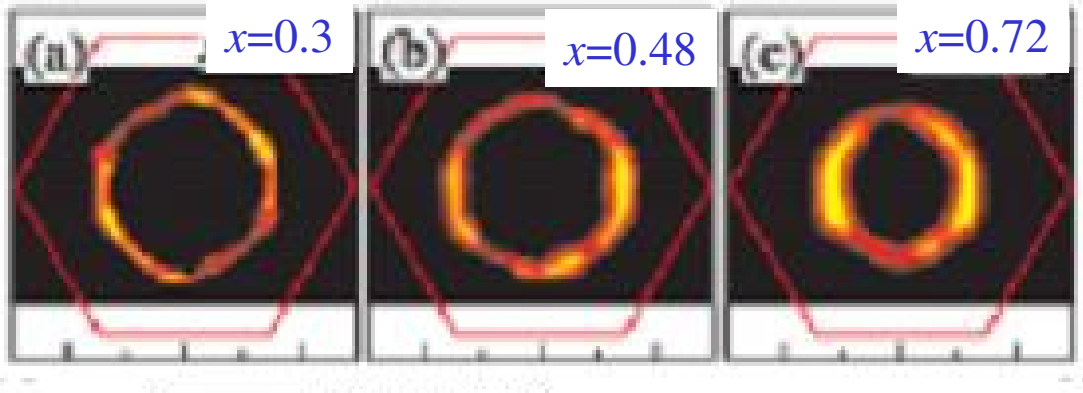
Fermi Surface of CaCoO



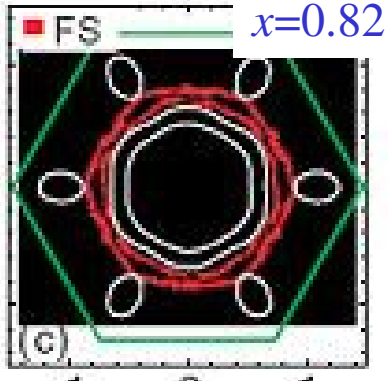
… larger than in BiBaCo
k_F=0.75 instead of k_F=0.6
=> x=0.5

Deviation from Luttinger theorem in cobaltates

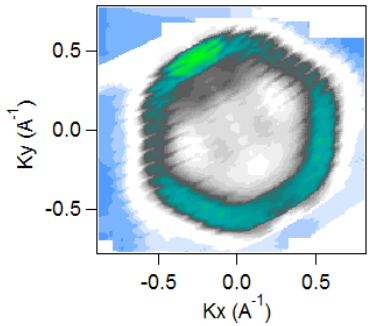
Yang, Ding *et al.*



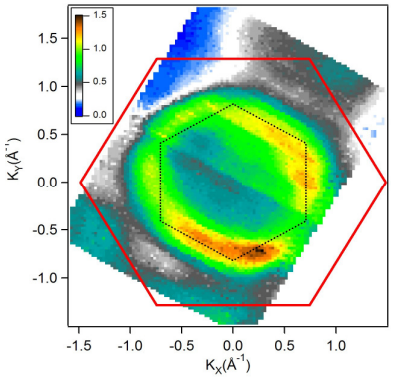
Qian, Hasan *et al.*

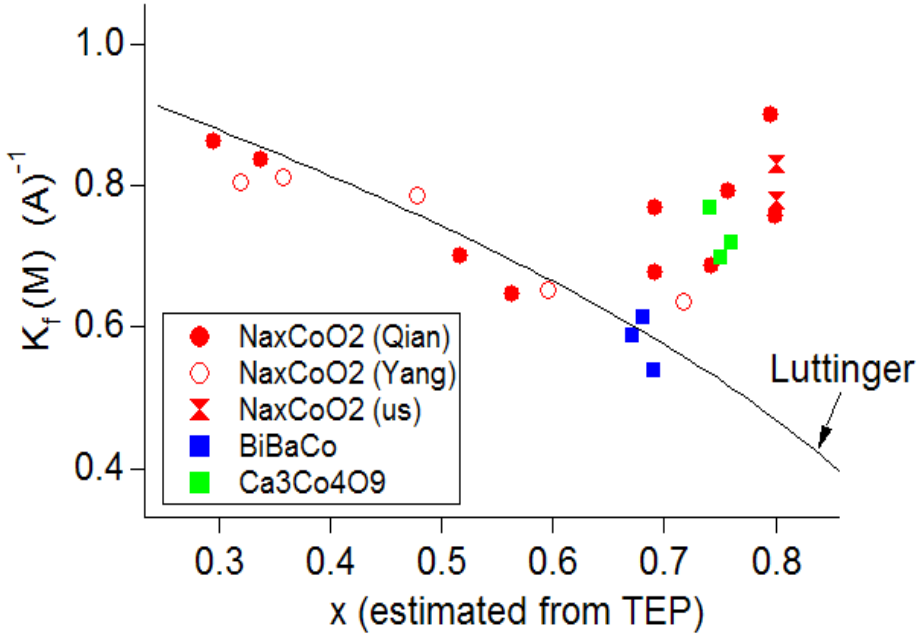


BiBaCo, x=0.7



CaCoO, x=0.75

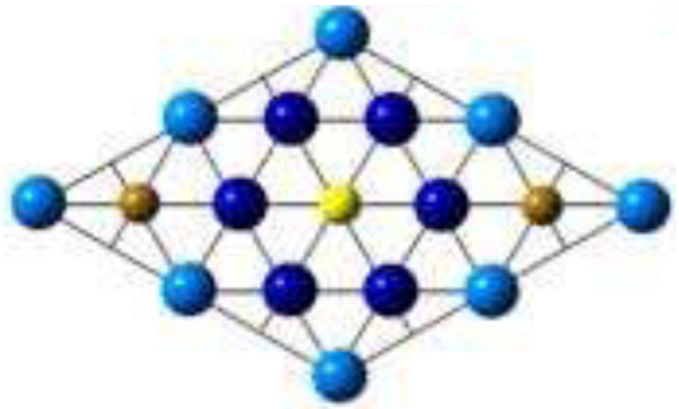




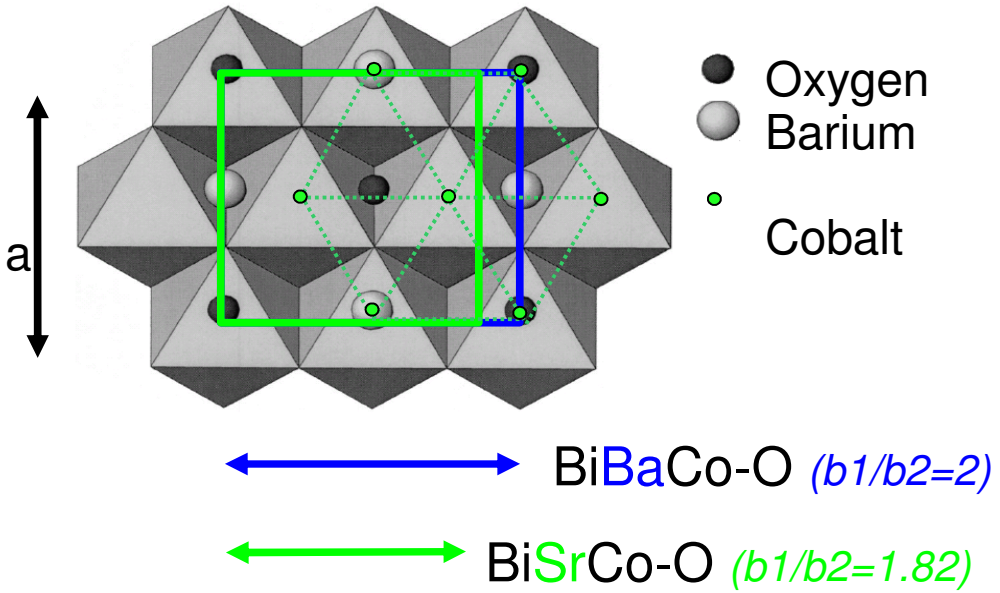
- Deviation from the rigid band filling at high *x*.
- More holes than expected = consistent with presence of Co^{3+}.

Localization with structure depending on the potential inprinted by neighboring planes

$Na_{2/3}CoO_2$
=> Kagomé



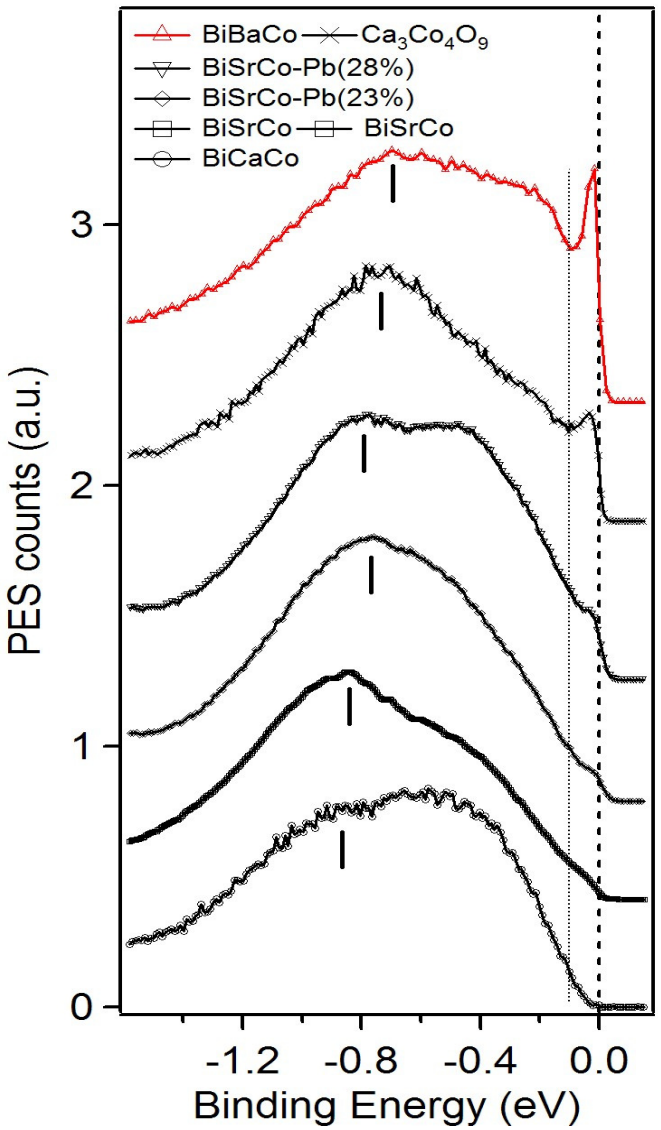
Misfits => « striped » structures



Different metallic structure may explain different evolution of metallicity

A. Nicolaou et al., EPL 2010

New electronic orderings ?



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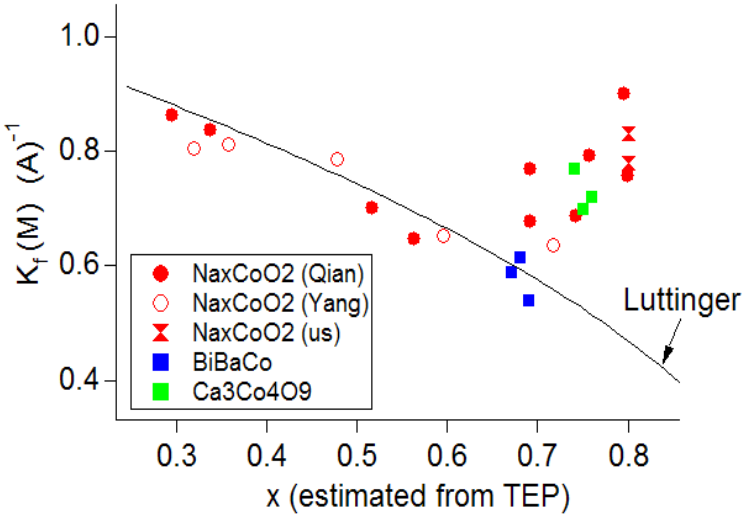

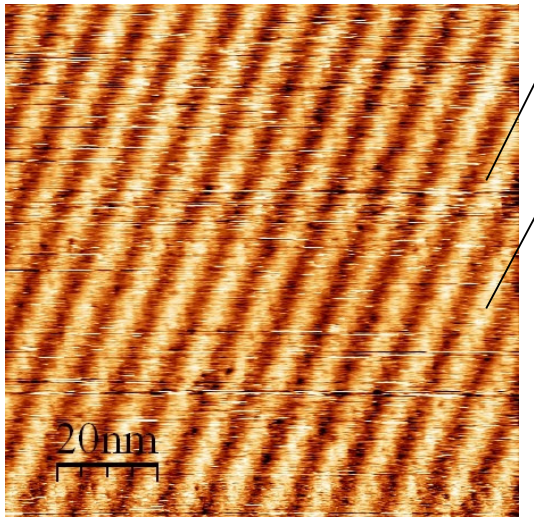

80Å

STM, coll. Soleil.

Conclusions

- Misfit cobaltates offer an alternative opportunity to study CoO_2 slabs. $Na_{0.7}CoO_2$ and BiBaCo show a very similar electronic structure.

- Excitations have a strong many-body character (« peak-dip-hump » structure).
=> *The QP energy scale is 0.2eV.*

- There is a systematic deviation from Luttinger theorem, suggesting inhomogeneous charge order in CoO_2 plane. Its periodicity might depend on the intercalated structure.
=> *Role on CW susceptibilities and high TEP ?*