The studies of electronic structure of strongly correlated materials by the combination of HAXPES and other techniques

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(RIKEN/SPring-8, Excited Order Research team)

HAXPES2009
20-22/May/2009

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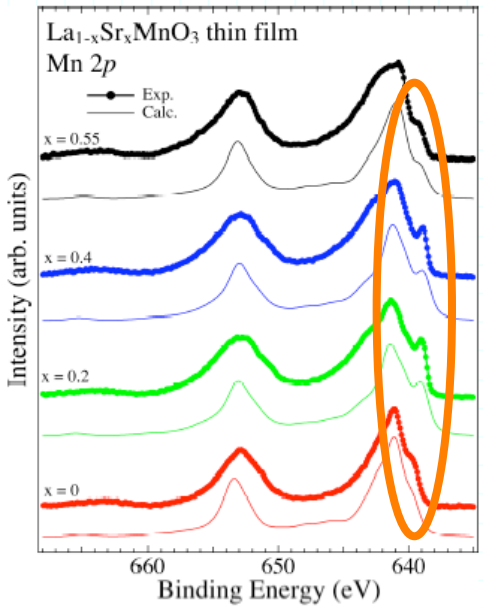
- Introduction
- NiO
- Magnéli phase Ti_4O_7
- Summary

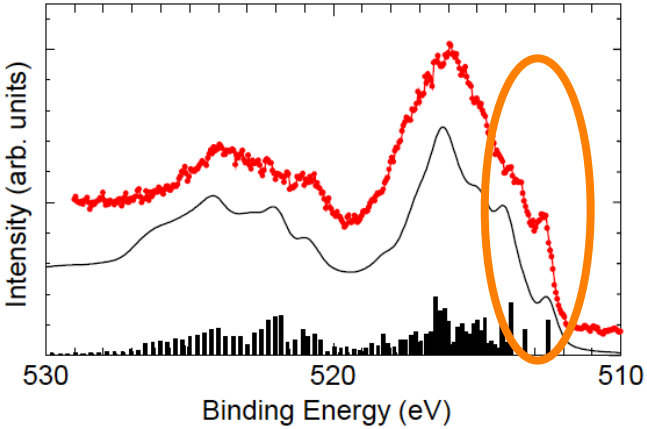
Introduction

$La_{1-x}Sr_xMnO_3$



Horiba *et al.*,
PRL **93** 236401 (2004)

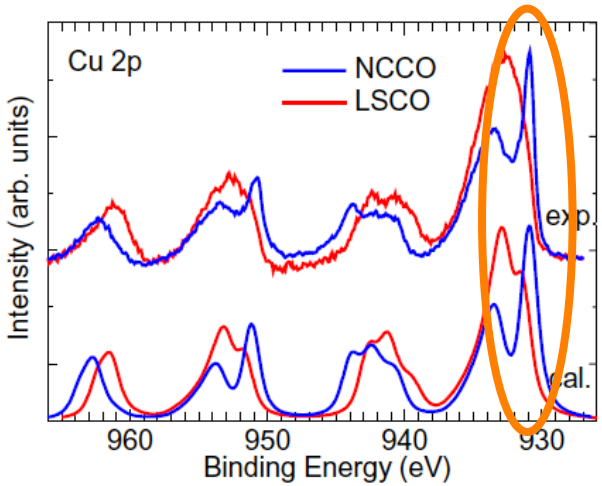
$V_{1.98}Cr_{0.02}O_3$



Taguchi *et al.*,
PRB **71** 155102 (2005)

Kamakura *et al.*,
EPL 68 557 (2004)

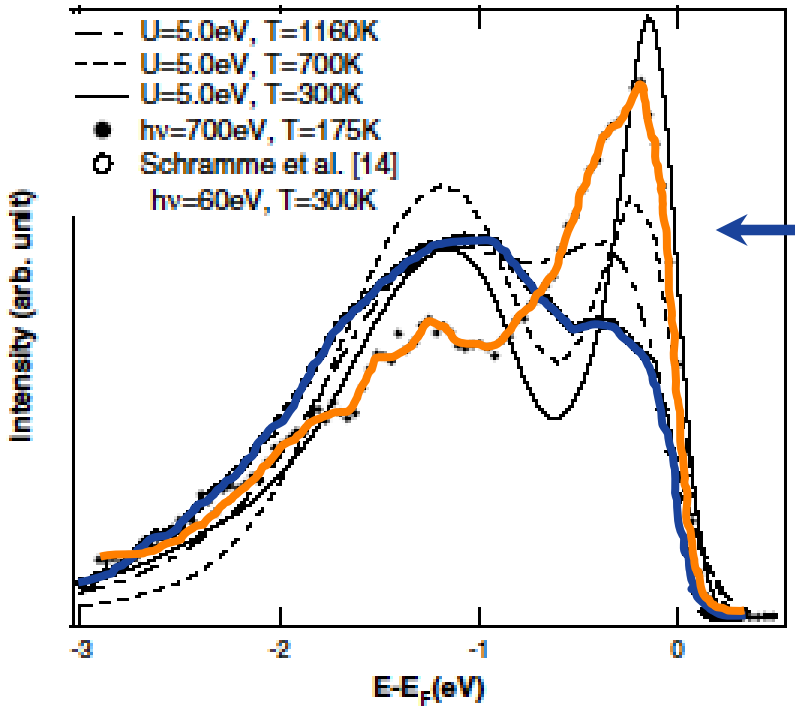
High T_c cuprates



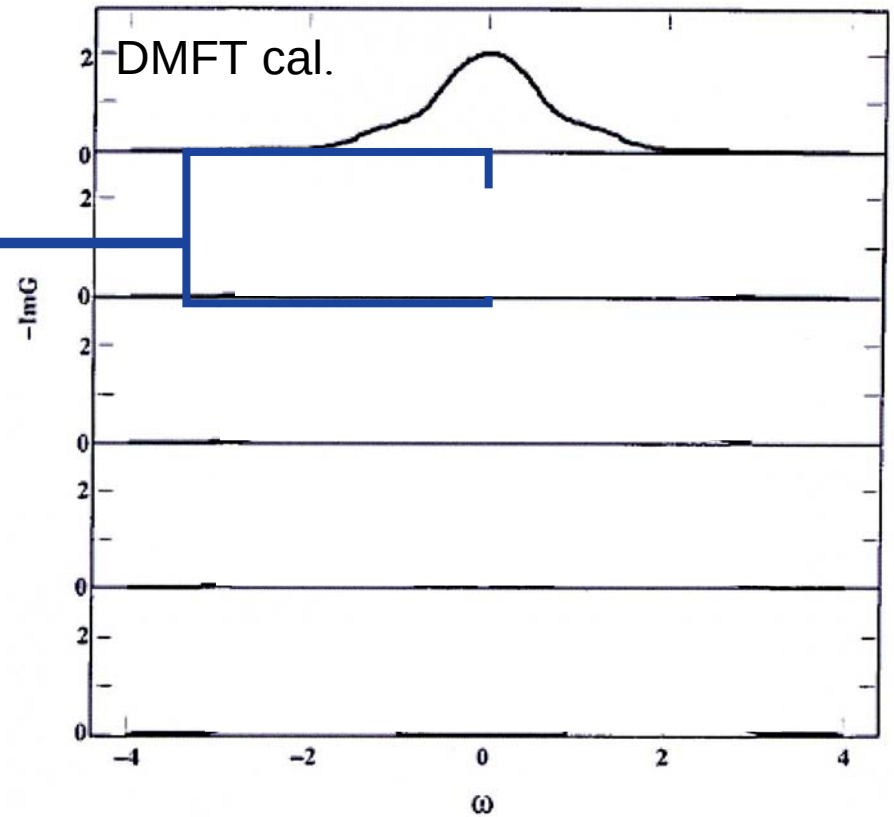
Taguchi *et al.*,
PRL **95** 177002 (2005)

Coherent peak in VB-PES

VB-PES : V_2O_3



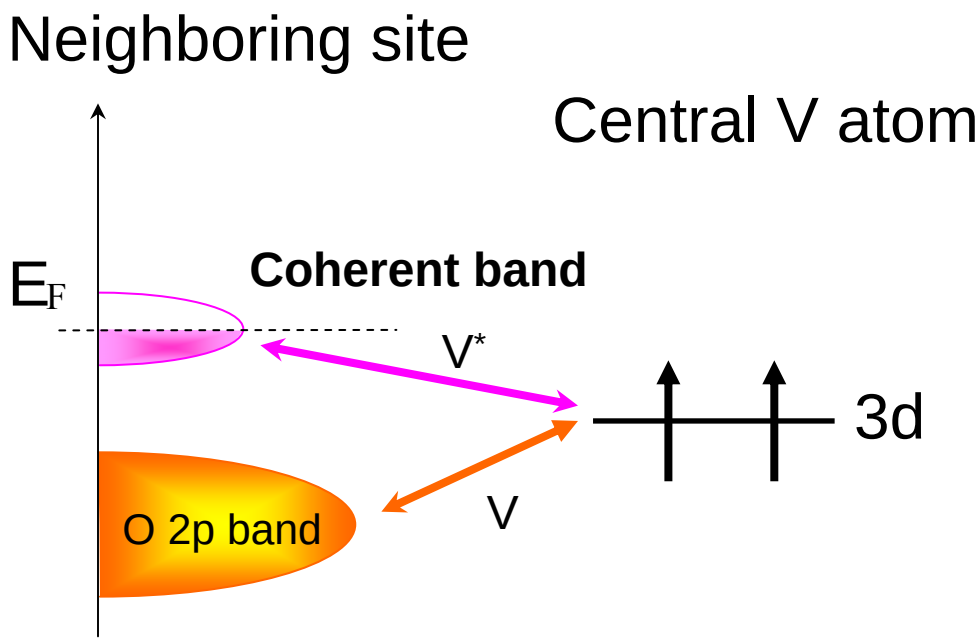
Coherent part



Incoherent part

Mo *et al.* PRL **90**, 186403 (2003)
Zhang *et al.* PRL **70**, 1666 (1993)
Panaccione *et al.* PRL **97** 116401 (2006)
Fujimori's Lecture note

Configuration-interaction (CI) model



1 . Intra-atomic multiplet

2 . Crystal Fields (C_{3v})

3 . Hybridization between O 2p and V 3d orbital

4 . Screening from coherent bands

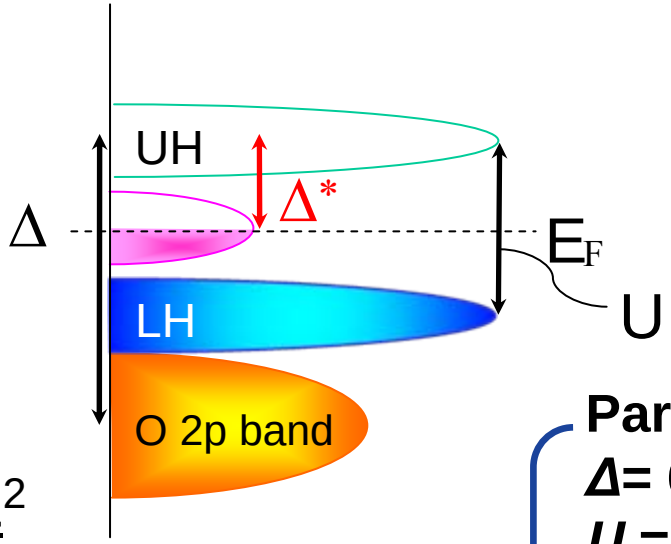
CI model

Ground state : linear combination of 6 configurations

$3d^4\underline{C}^2$

$3d^3\underline{C} \longleftrightarrow 3d^4\underline{L}C$

$3d^2 \longleftrightarrow 3d^3\underline{L} \longleftrightarrow 3d^4\underline{L}^2$



Parameters

***Δ*= 6.0 eV**

***U* = 4.5 eV**

U_{dc} = 6.5 eV

10*Dq* = 1.2 eV

D_{trg} = - 0.05 eV

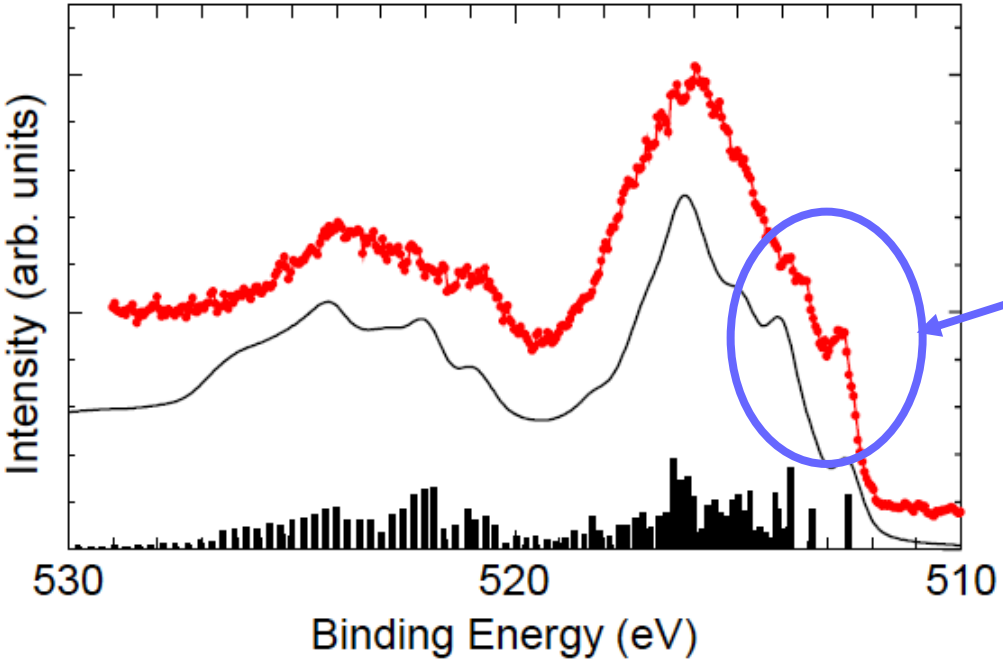
***V* = 2.9 eV**

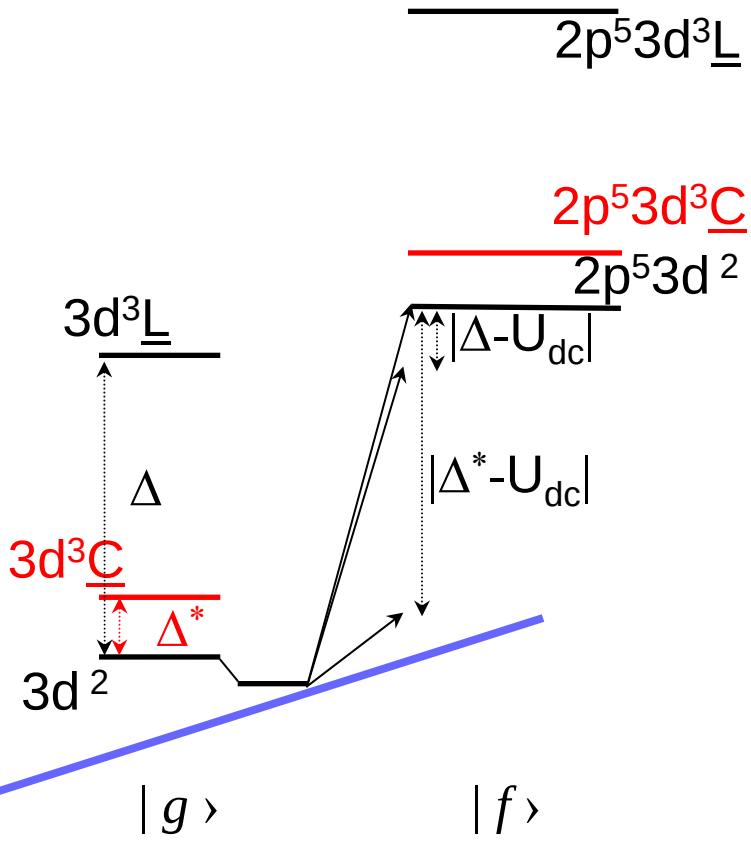
***V** = 0.75 eV**

***Δ** = 0.9 eV**

Rc =0.8, Rv=0.9

Calculation vs. Experiment





Taguchi *et al.*
PRB **71**, 155102 (2005)

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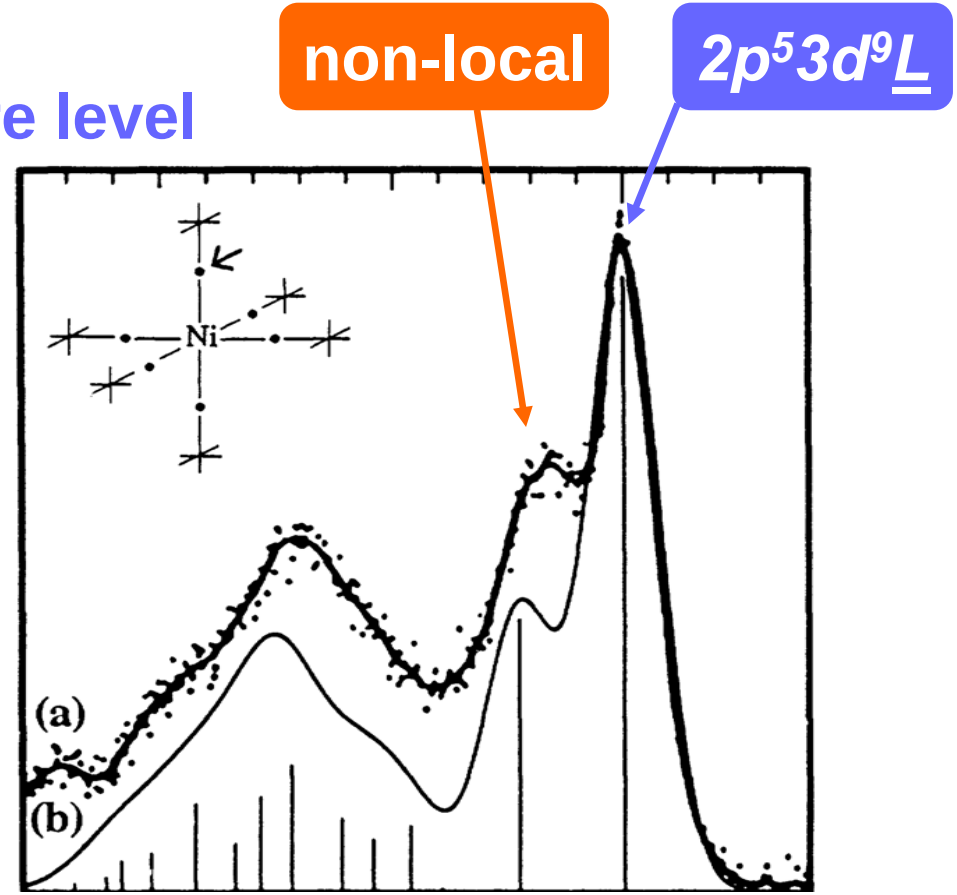
Non-local screening

Ni $2p_{3/2}$ core level



multi-site cluster model

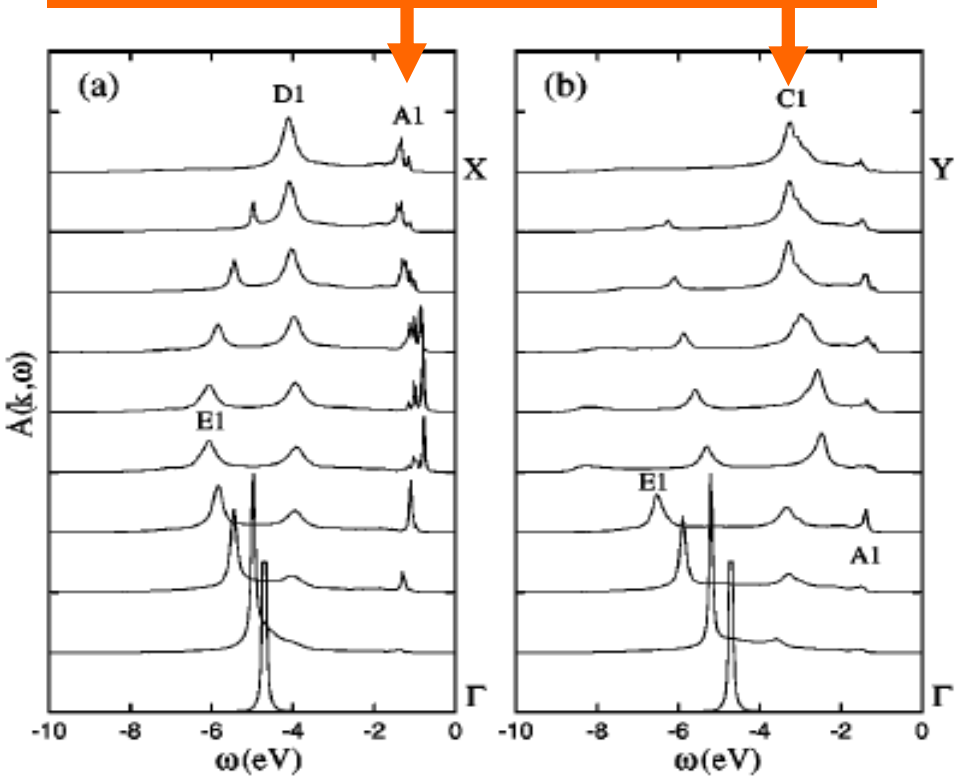
Van Veenendaal *et al*.,
PRL **70** 2459 (1993)

Zhang-Rice doublet bound state

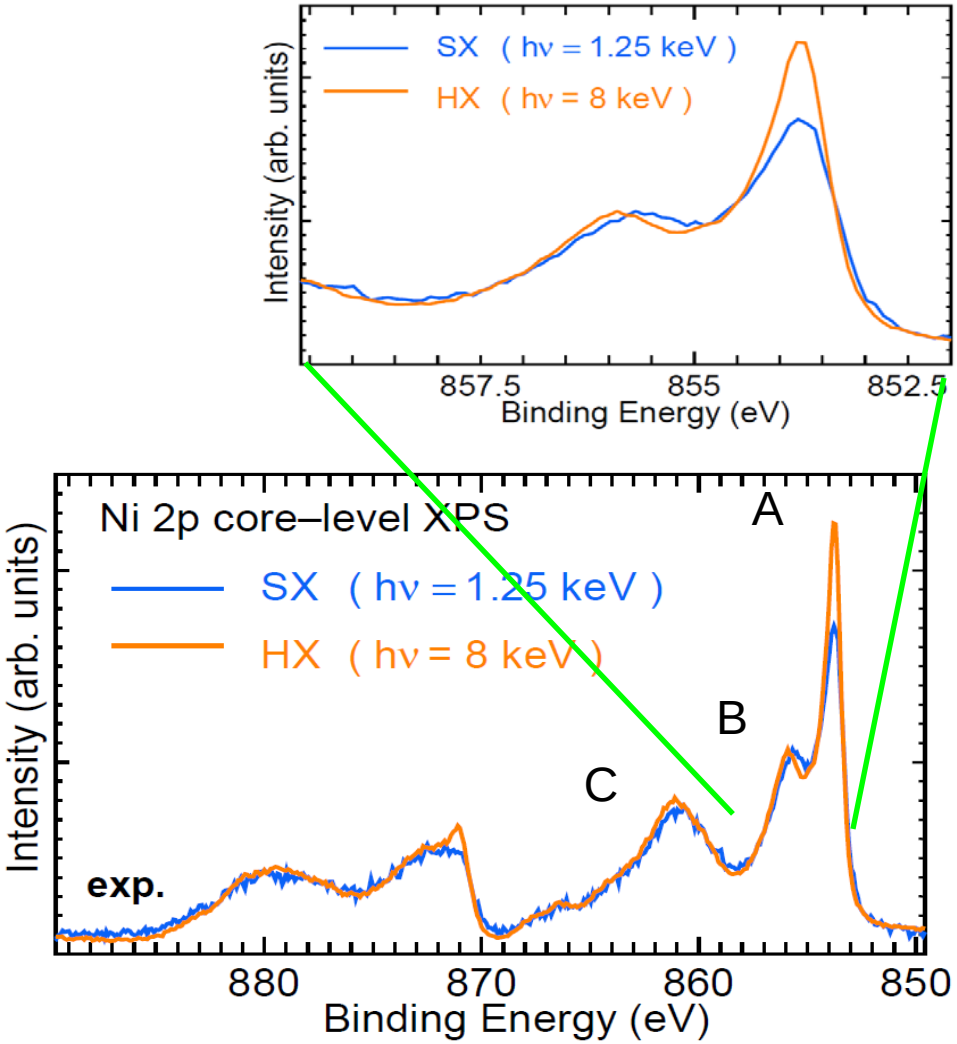
spin-fermion model: Bala *et al*., PRL **72** 2600 (1994)**:** PRB **61** 13573 (2000)

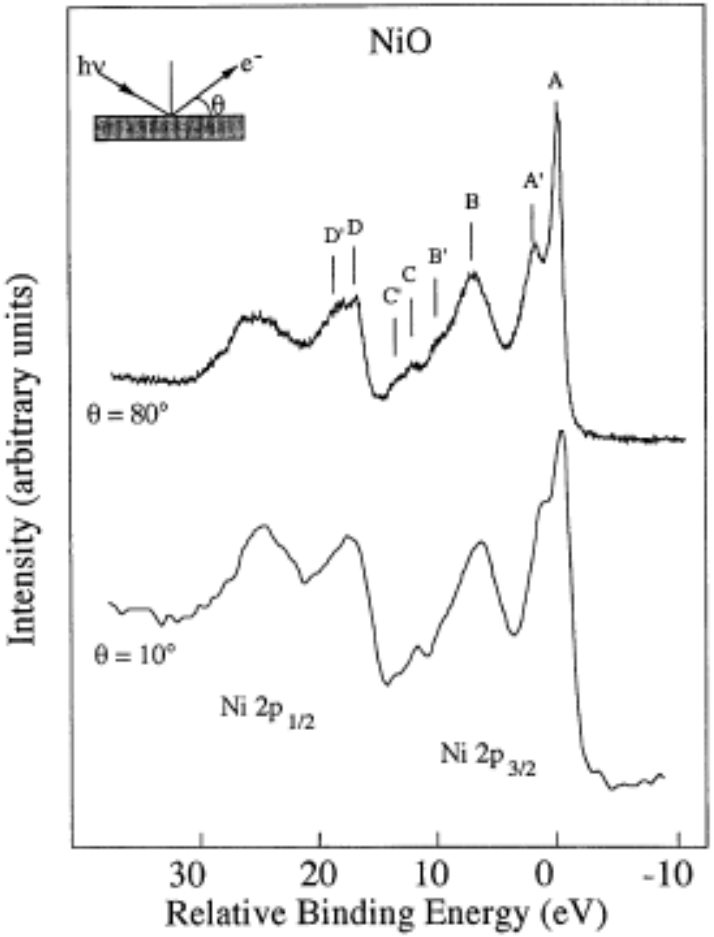
LDA+DMFT: Ren *et al.,* PRB **74** 195114 (2006)
Kunes *et al*., PRB **75** 165115 (2007)**:** PRL **99** 156404 (2007)

Zhan-Rice doublet bound states



Ni 2p HX-PES

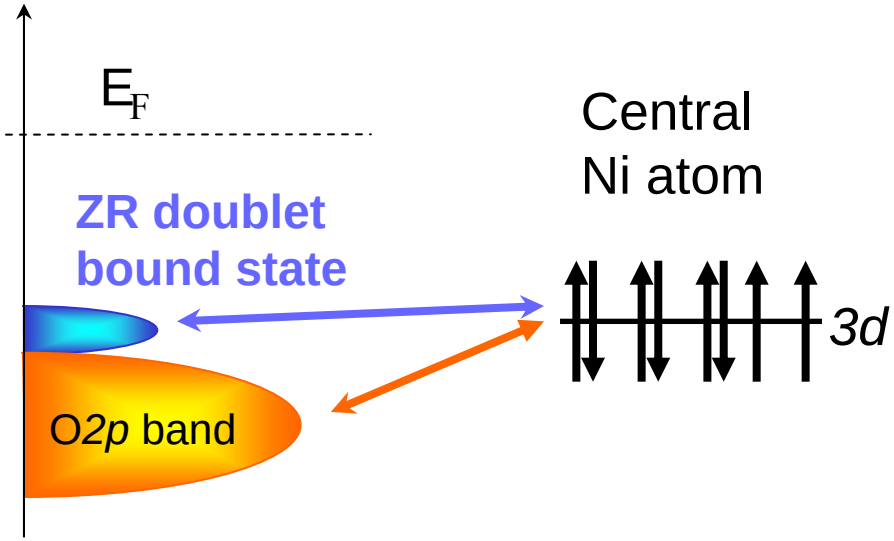


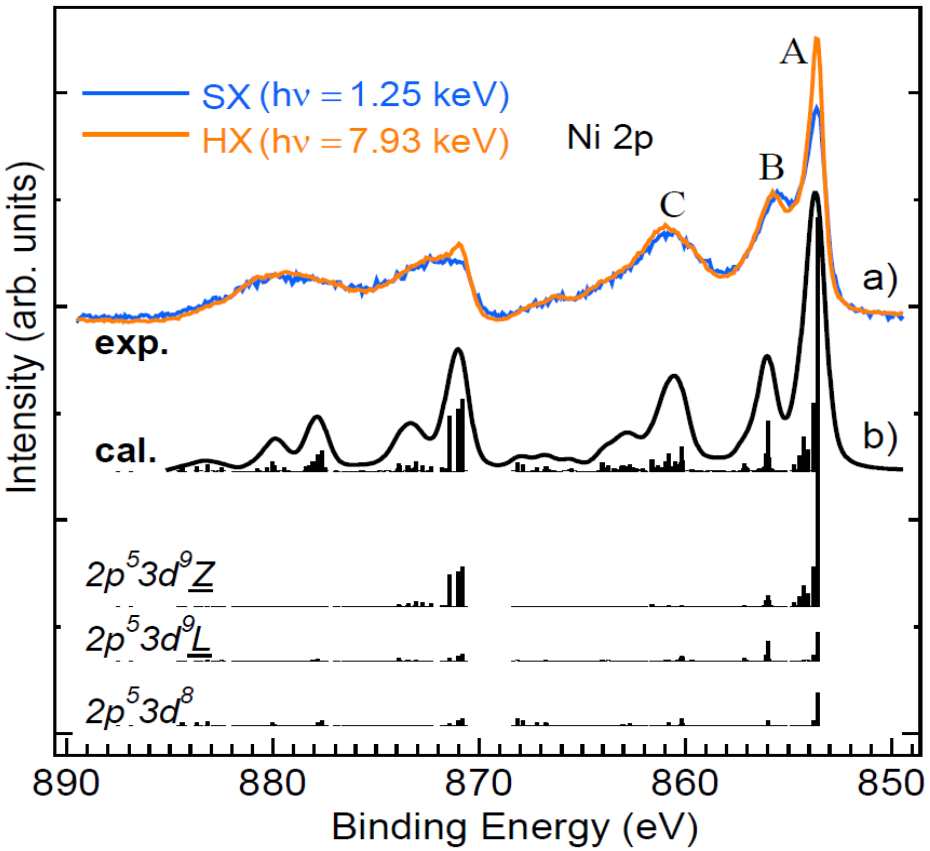


Parmigiani *et al.*,
J. Electr. Spectr. Rel. Phen. **98-99** 287(1999)

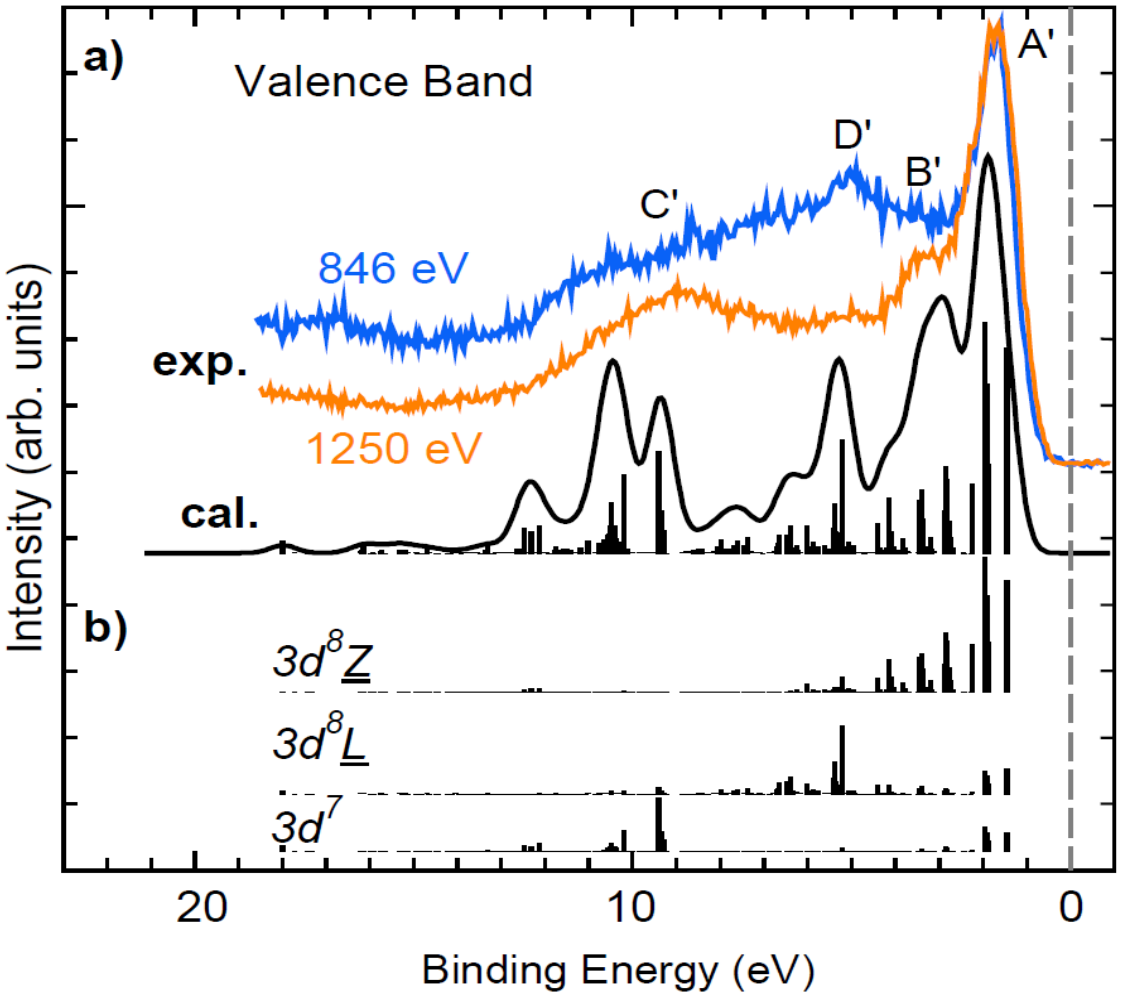
Taguchi *et al.*, PRL **100** 206401 (2008)

2p core-level HX-PES





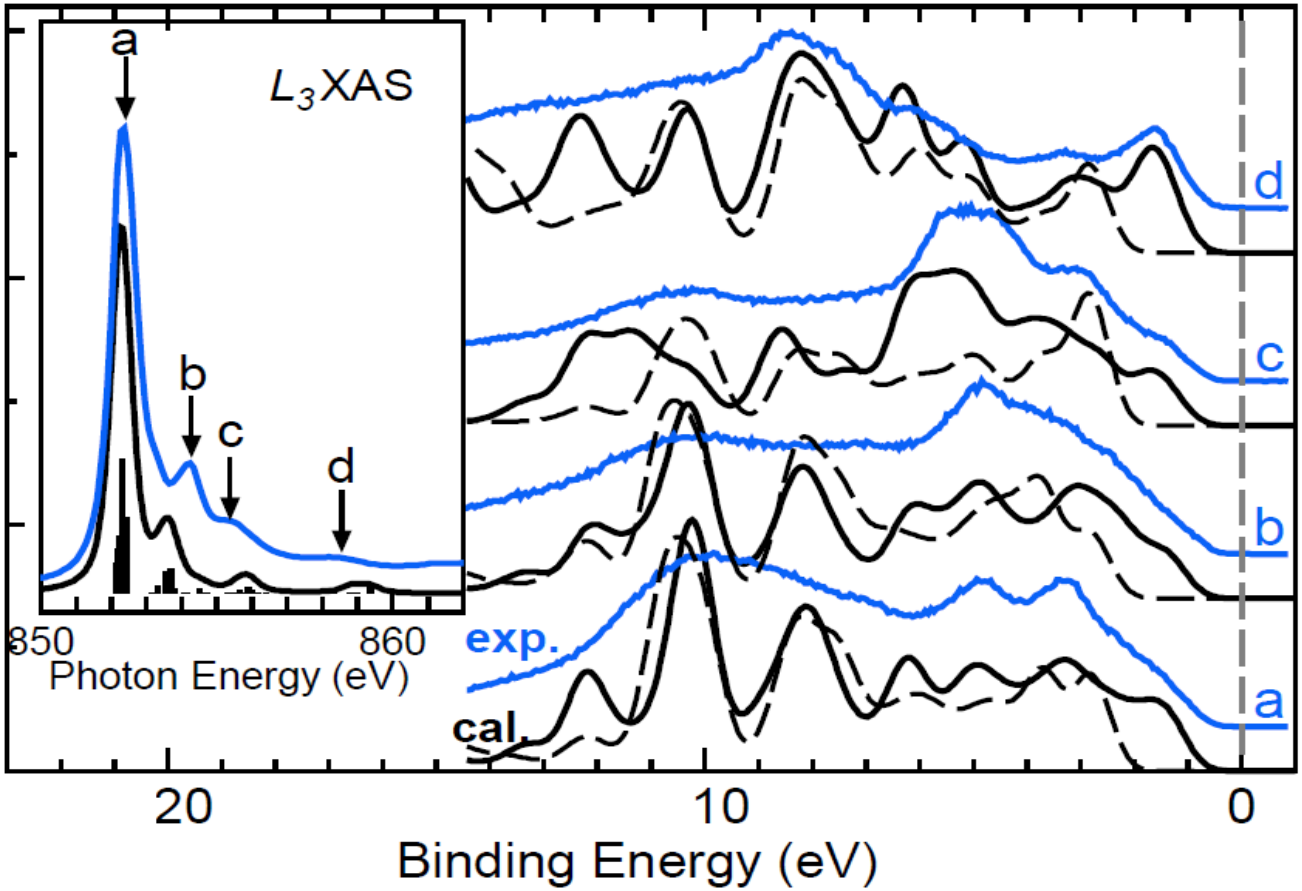
Valence band PES



Resonant PES at L_3 edge

without $3d^9\underline{Z}$

with $3d^9\underline{Z}$



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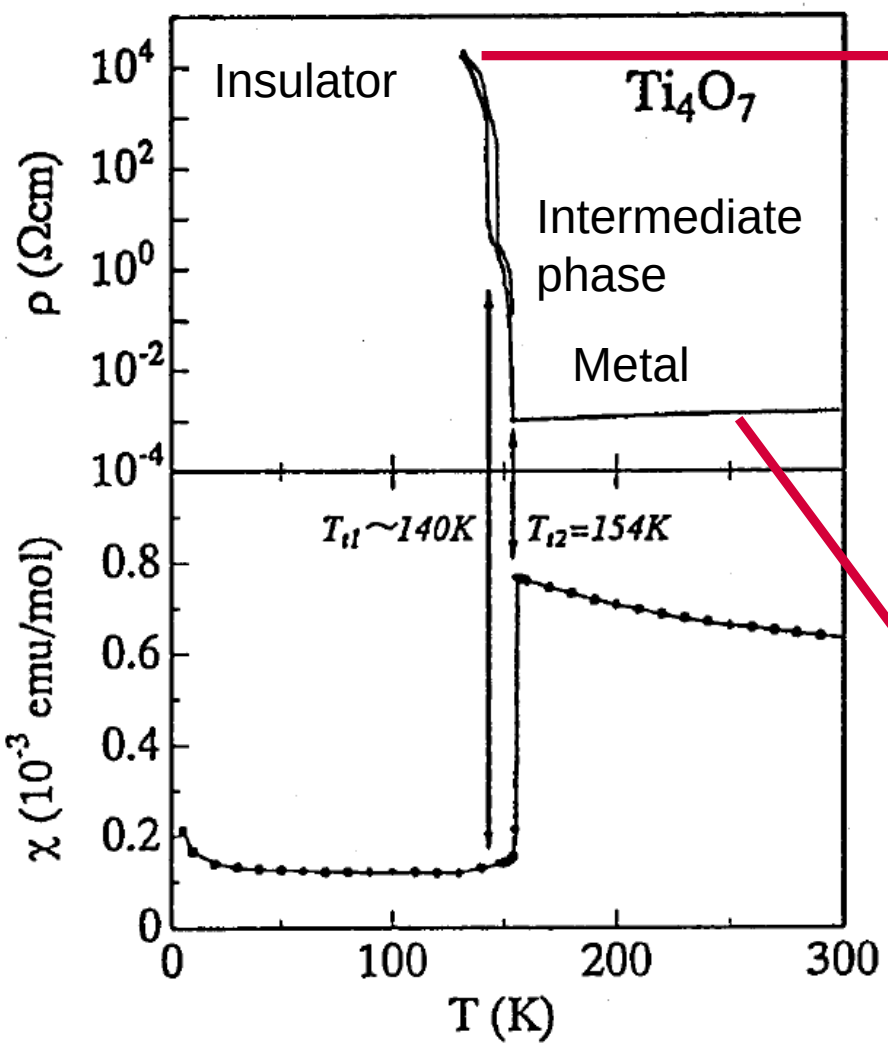
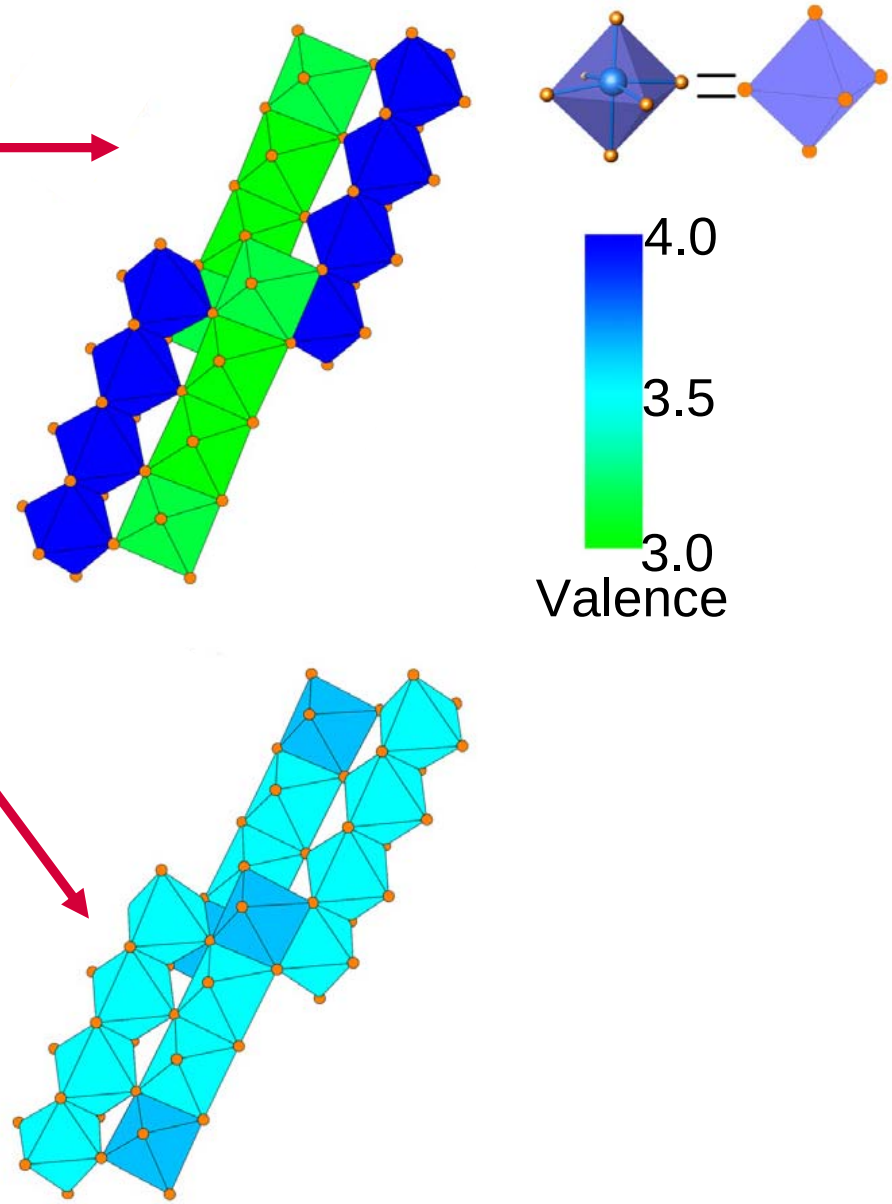
Magnéli phase: Ti_4O_7

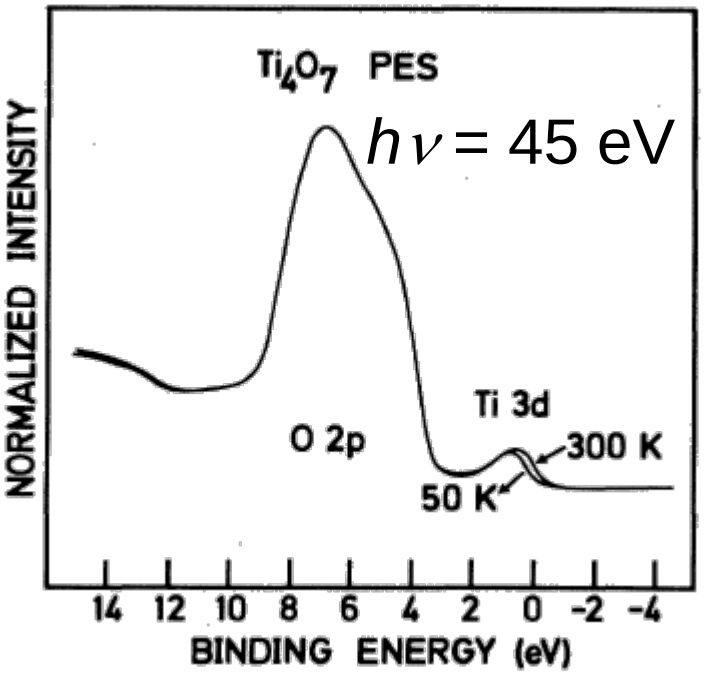




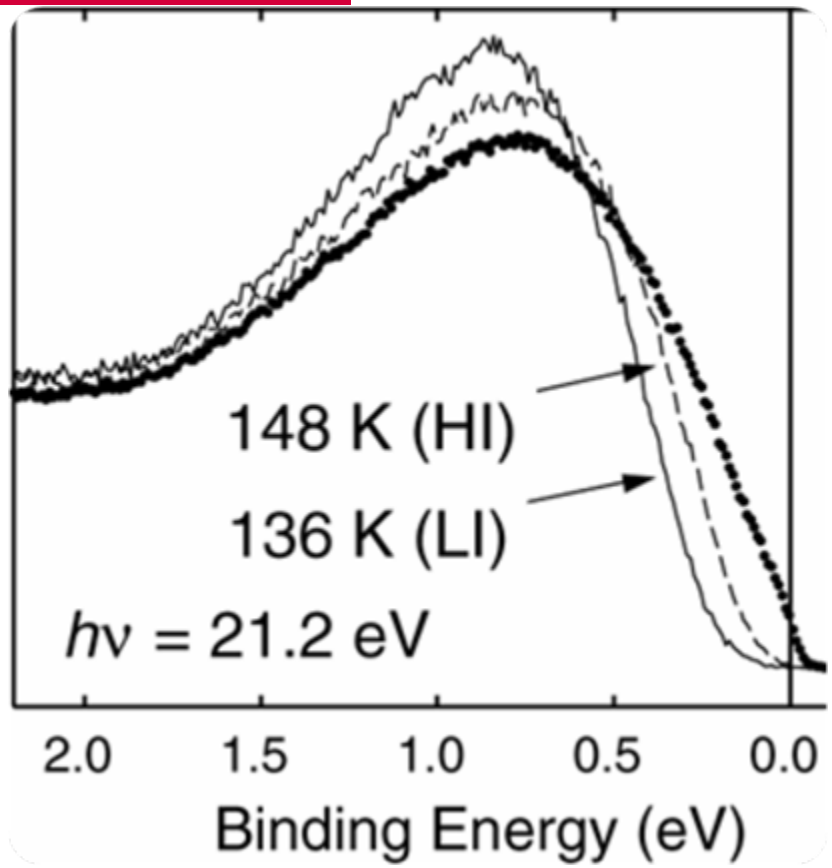
T. Tonogai (PhD thesis)

Previous results

extremely broad features

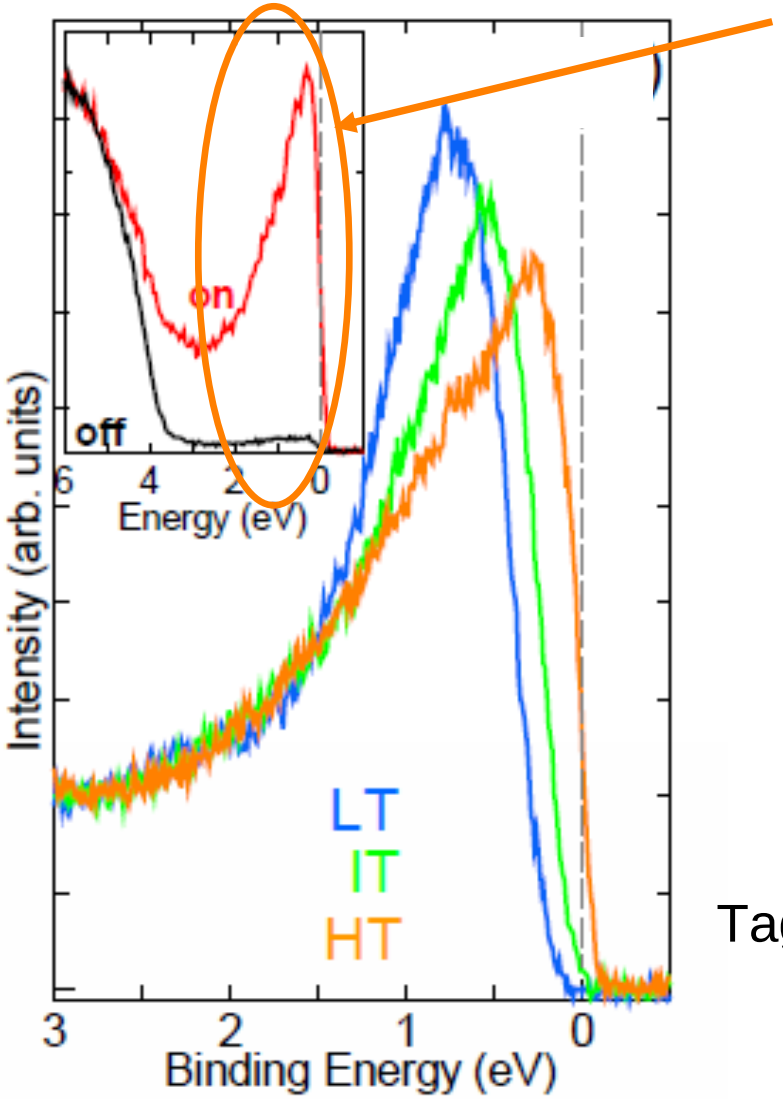


Abbate *et al*.,
PRB**51**, 10150 (1995).



Kobayashi *et al*.,
Europhys. Lett. **59**, 868 (2002).

Ti 2p resonant PES

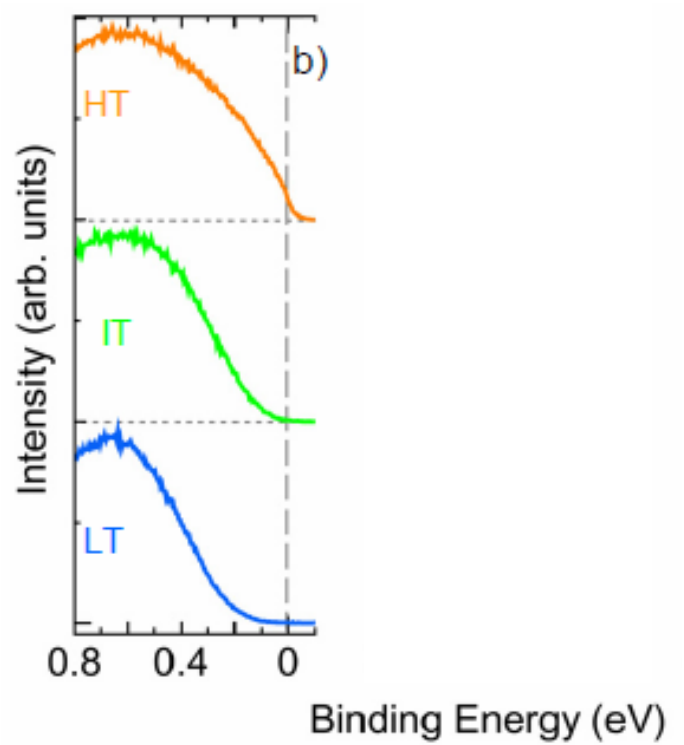


Clear Fermi-edge

Metal Phase: Fermi-Liquid state

Taguchi *et al.*, cond-mat/0902.3701

Laser PES

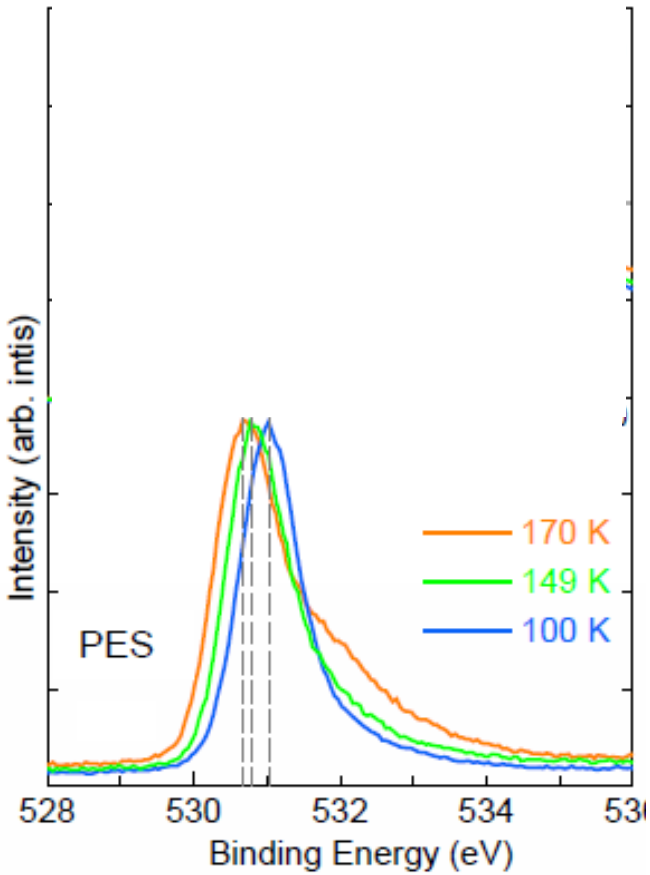


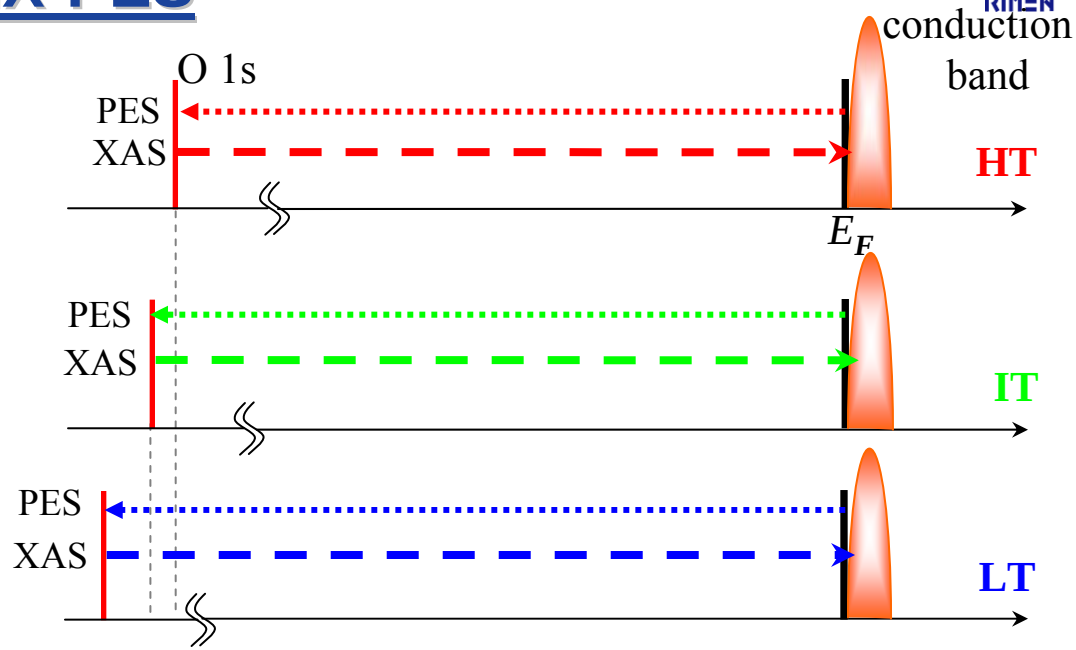
$$I(\omega) = \int d\epsilon A(\omega - \epsilon) f(\omega - \epsilon) g(\epsilon)$$

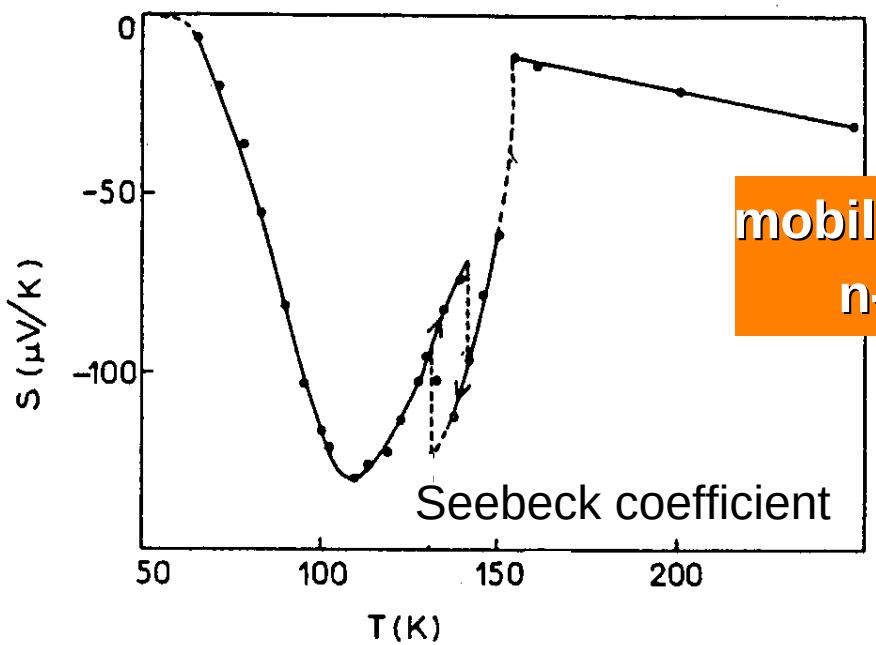
$g(\epsilon)$ Gaussian
$f(\omega)$ Fermi-Dirac
$A(\omega)$ Spectral function

Taguchi *et al.*, cond-mat/0902.3701

O 1s XAS & O 1s HX-PES

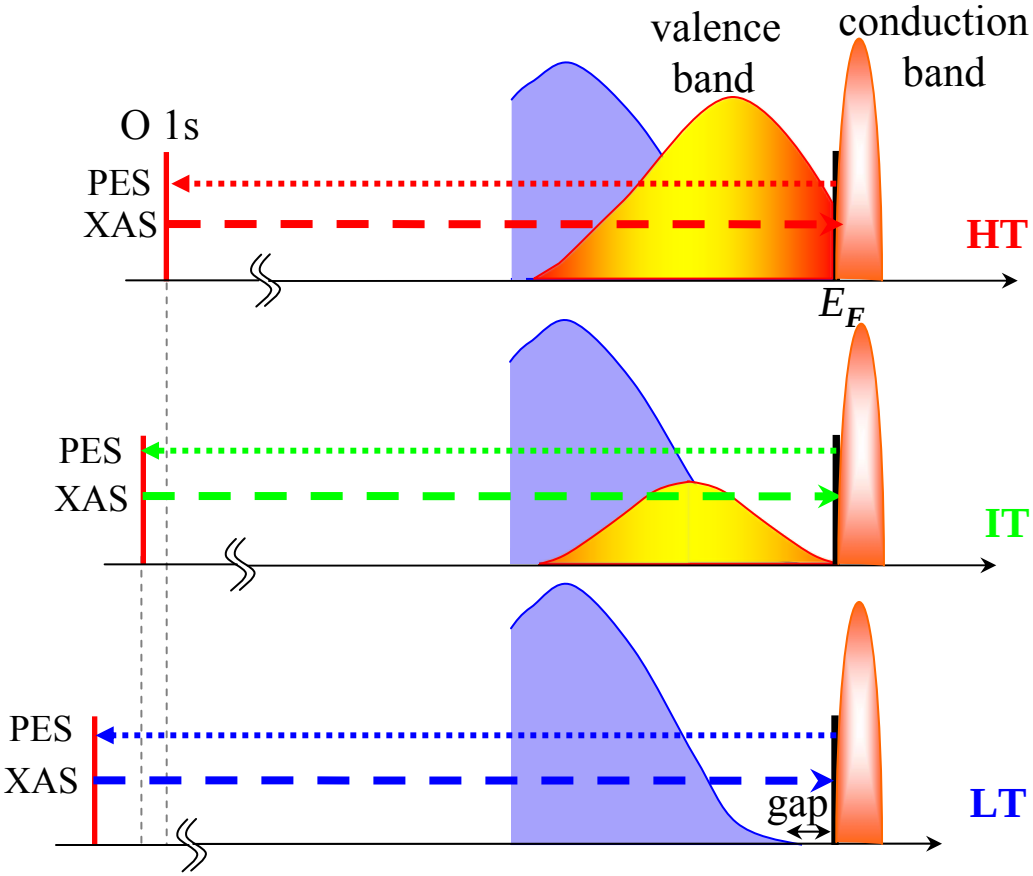




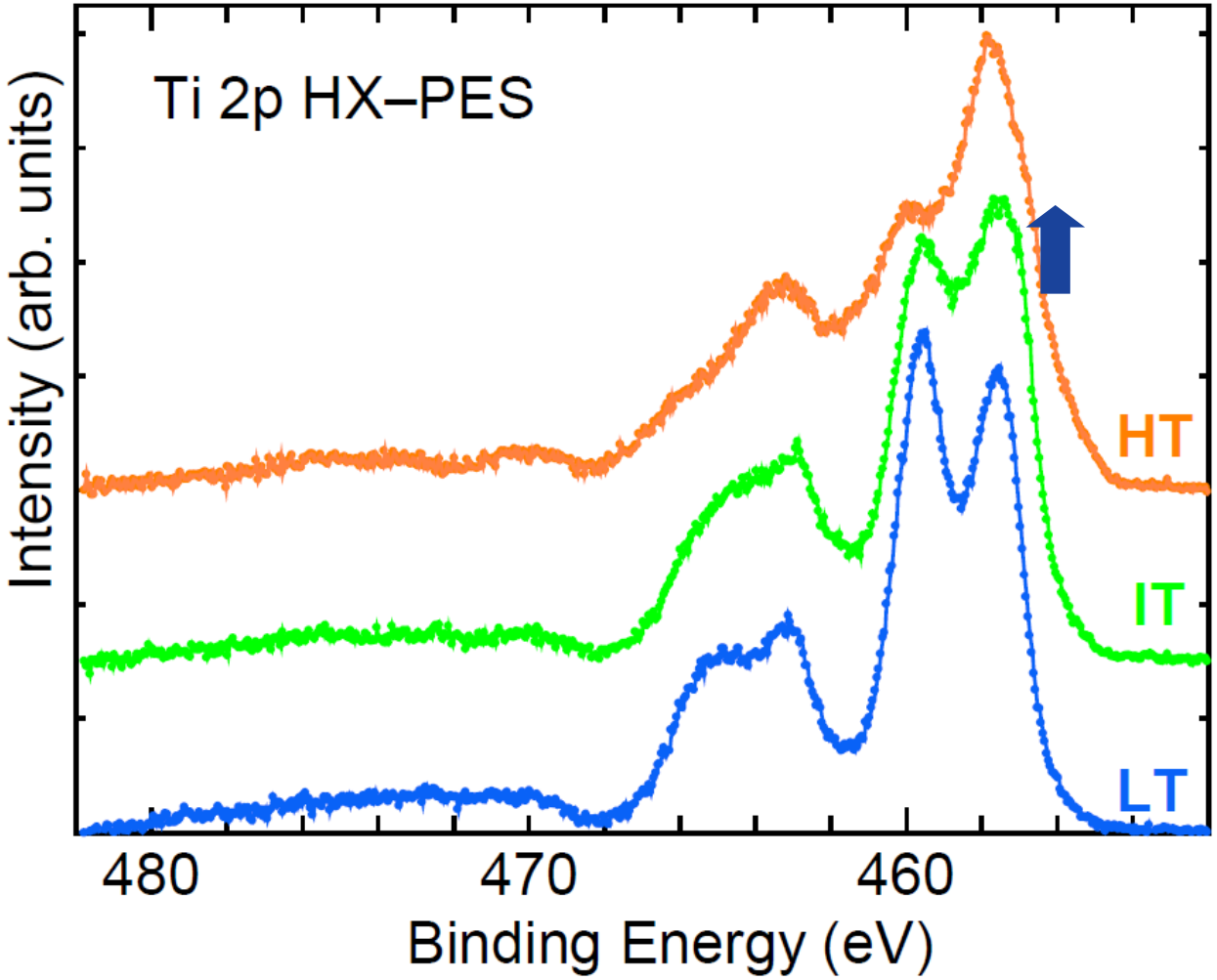


mobile carrier : n-type

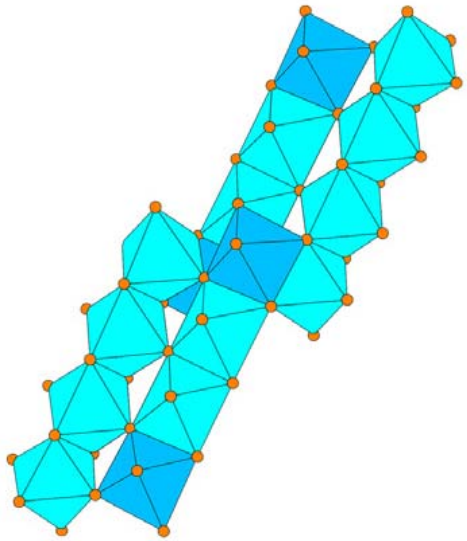
Schematic picture

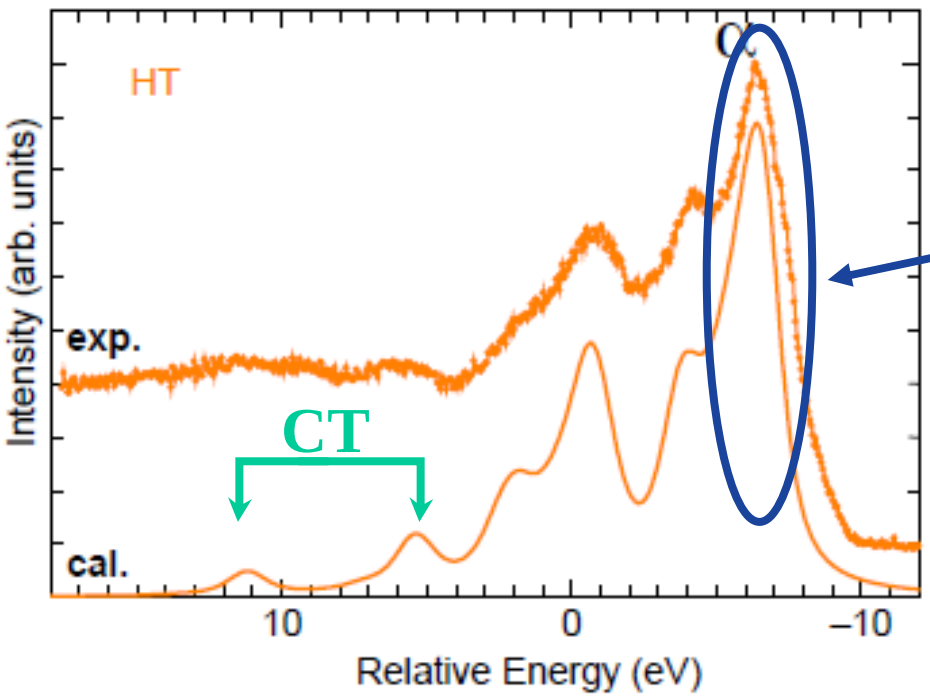


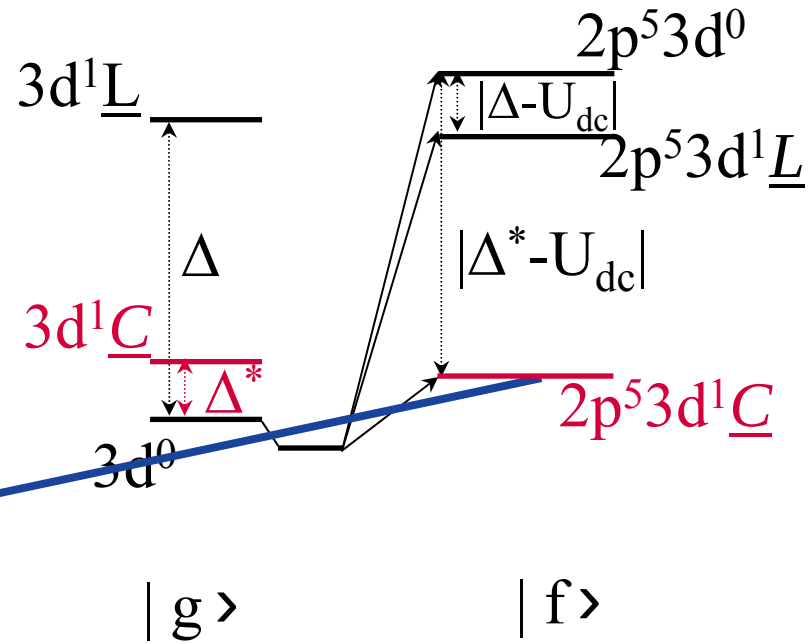
Ti 2p HX-PES

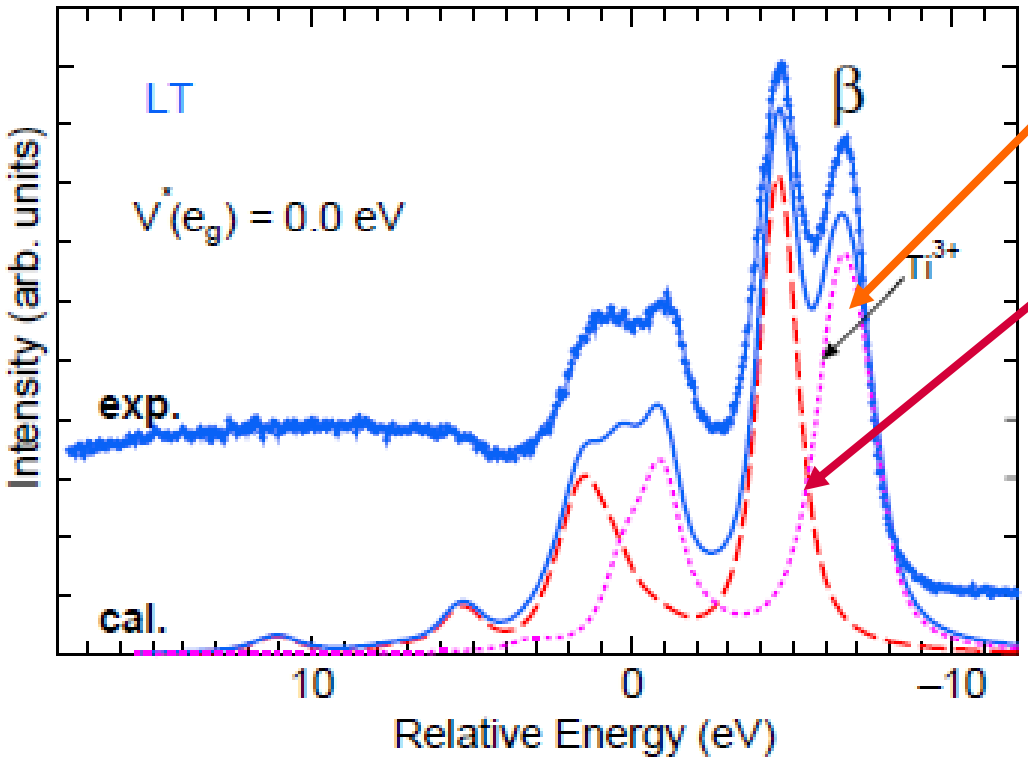


Taguchi *et al.*, cond-mat/0902.3701



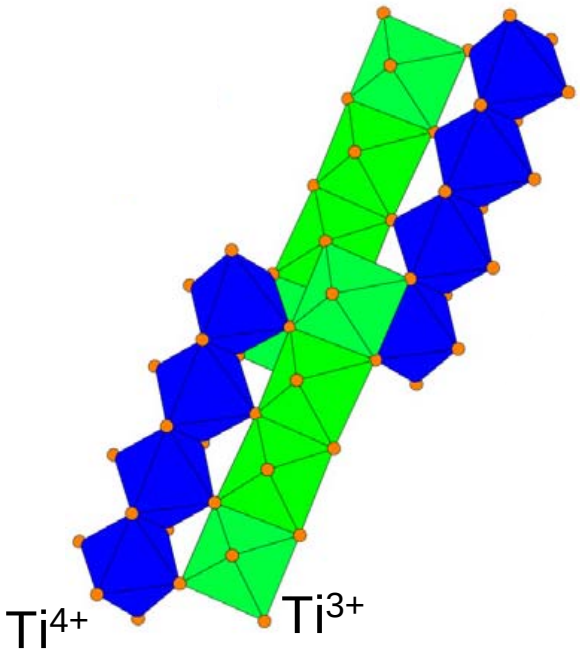

HT
CC
CT
exp.
cal.
Intensity (arb. units)
10
0
−10
Relative Energy (eV)

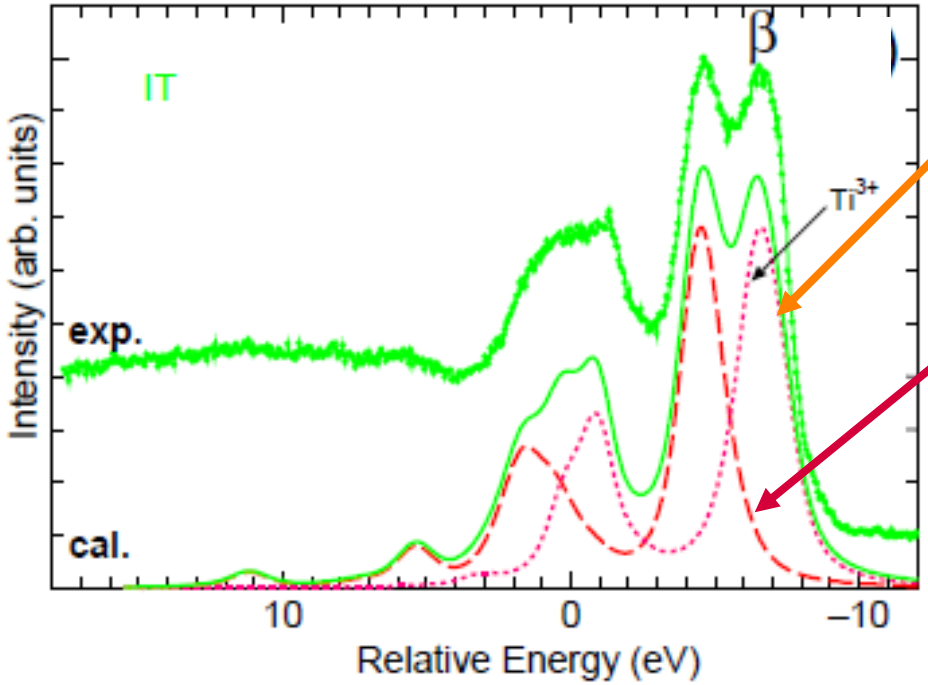

$3d^1\underline{L}$
$2p^53d^0$
$|\Delta-U_{dc}|$
$2p^53d^1\underline{L}$
Δ
$|\Delta^*-U_{dc}|$
$3d^1\underline{C}$
Δ^*
$2p^53d^1\underline{C}$
$3d^0$
$|g\rangle$
$|f\rangle$



Ti $^{3+}$

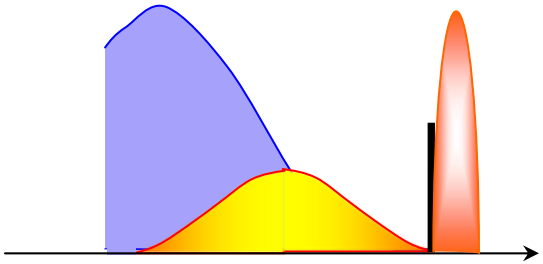
Ti^{4+} cluster
(V* =0)





Ti^{3+}

Ti^{4+} cluster



Parameters

$\Delta^* = 0.3$ eV

$V^* = 0.26$ eV

coherent nature

Summary

Further information on the nature of electronic state near E_F can be obtained from the combination of HX-PES and other techniques.

- ✓ NiO:
  All features in the VB and the core-level PES were reproduced well by extended CI model including ZR bound state screening effects.

- ✓ Ti_4O_7:
  Resonant PES …. Fermi liquid state in HT phase
  Laser PES …. Pseudo-gap feature in IT
  Ti 2p HX-PES …. This pseudo-gap feature is associated with the coherent screening states.

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