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- Zhu

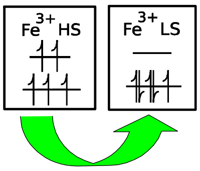
Volume and spin collapse in orthoferrite $LuFeO_3$ using LDA+U

Donat J. Adams[1,2] and Bernard Amadon[1]
[1]CEA,DAM,DIF, F 91297 Arpajon, France
[2] Centre de Physique Théorique, École Polytechnique, F91128 Palaiseau, France

INTRODUCTION

- High spin to low spin transition linked to volume collapse of ion
- Ideal material to compare calculation and experiment
- Lu: complete *f*-shell
- Simple stoichiometry and crystal structure
- Accurate experimental data up to 125 GPa [1]
- Well defined transition pressure (50 GPa)
- Perovskite structure [2,3] with strong distortion temperature effects]
- Earlier works LDA [4,5], LDA+U [6]

Volume collapse



LDA+U powerful method to predict phase transitions in transition metal oxides

METHODOLOGY

- LDA+U: Exchange correlation energy LDA and Hubbard Hamiltonian for Fe-3*d* orbitals:.
- Projector augmented waves (PAW) atomic data [7,8]
- Atomic data tested on O_2, bcc FM Fe, FeO, Lu metal
- Software: Abinit [7,9]
- Precision: *dEd* = 10meV, *dp* = 0.08 GPa, *dH* = 50 meV, p_{cr} = 0.04 GPa (36 k-points, 435 eV energy cutoff)

RESULTS

100 possible realizations of LS

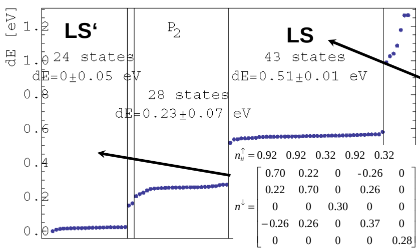


FIG. 1 : Energies of the 100 optimized LS structures. During 30 electronic steps a density matrix (10x10 possibilities) was imposed. Then the structure was fully relaxed. 3 electron configurations resulting: LS', P2 and LS. Inset: density matrix of the LS' phase.

What governs the field of stability?

$$E_U \approx \frac{U-J}{2}\underbrace{\sum_{\sigma,i} n_i^{\sigma} - (n_j^{\sigma})^2}_{=\begin{cases}0.82 & \text{HS}\\ 1.24 & \text{LS}\end{cases}}$$

(*U-J*) "punishes" LS harder

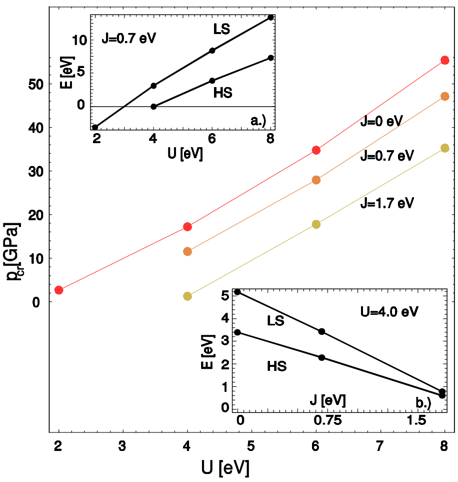


FIG. 4: Dependence of the transition pressure upon the Coulomb repulsion *U* and the exchange parameter *J*. Insets: Dependence of the ground state energy on *U* and *J* at a fixed volume.

Relaxation important for p_{cr}

Determination of *U* and *J* [10] is essential.

Non-intuitive role of *J*: *J* stabilizes LS !

$p_{cr} \propto (U-J)$

Reduced magnetic moment in HS phase

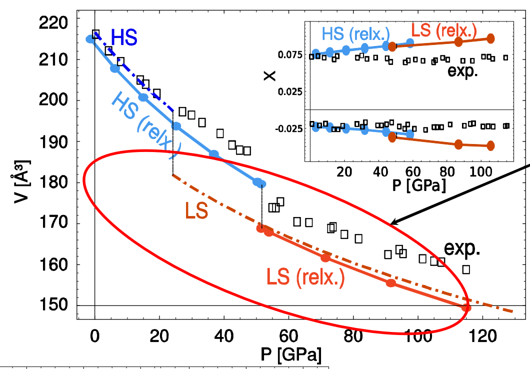
Reduction of local magnetic moment at phase trans: 3 μB
Occupation of the Fe-d orbitals. Green: Hybridized t_{2g} orbitals.
Red: main occupations.

HS:
$n_{ii}^{\uparrow}$ = 0.92 0.92 0.97 0.93 0.97
$n_{ii}^{\downarrow}$ = 0.07 0.07 0.25 0.07 0.25

Hybridized orbitals reduce magnetic moment. (4.01 μ_B, ionic value 5 μ_B)

LS:
$n_{ii}^{\uparrow}$ = 0.92 0.92 0.28 0.92 0.27
$n_{ii}^{\downarrow}$ = 0.91 0.91 0.24 0.09 0.23

Hybridized orbitals compensate each other and magnetic moment (1 μ_B) is conserved.



Volume collapse 6% (Exp. 5.5%)

Why is bulk modulus underestimated?

Overestimation of *U*? Metallization?

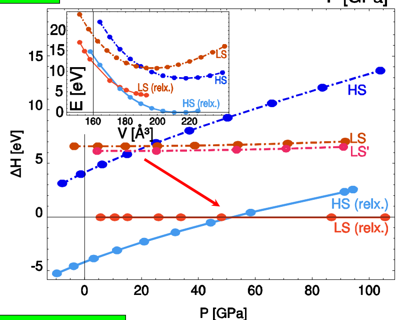


FIG. 2: EOS for *p* between 0 and 120 GPa. Calculated values (•) and experimental data (□) Ref. [1]. Dashed lines: Calculation without relaxation (transition pressure 21 GPa). Inset: Reduced atomic coordinates of Lu.

FIG. 3: Enthalpy of the HS, the LS and the LS' phase. Crossings: phase transitions. Transition HS to LS at 22 GPa (unrelaxed) and 51 GPa (relaxed). Transition to LS' lower by 4 GPa. Inset: the energy of the HS and LS phase at the corresponding volumes.

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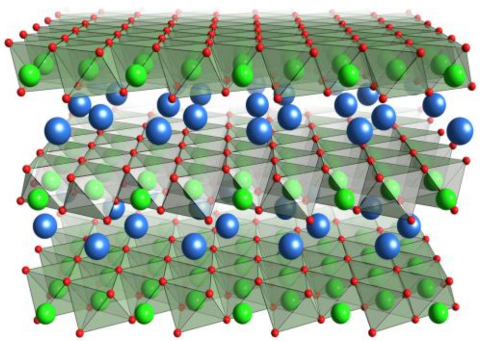
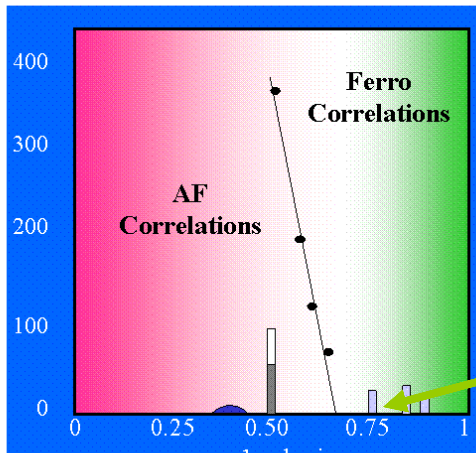
Na ORDERING, Co CHARGE ORDER AND METALLIC MAGNETISM OF THE Na COBALTATES Na_xCoO_2

H. Alloul, J. Bobroff, G. Lang , I. Mukhamedshin*, T. Platova* and G. Collin

Laboratoire de Physique des Solides, UMR CNRS 8502, Université Paris-Sud Orsay

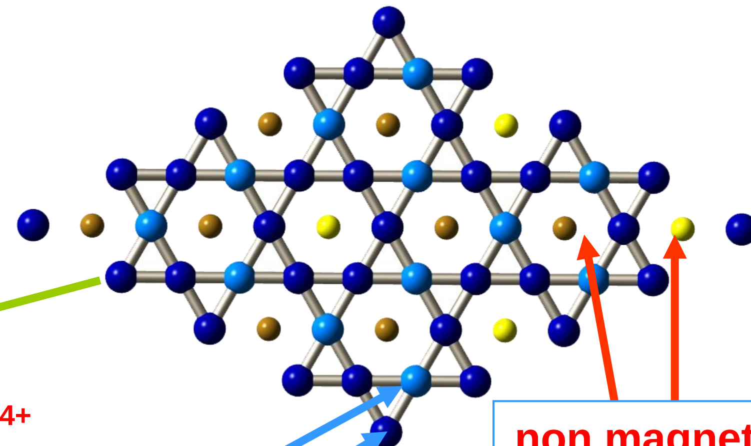
** Also Magnetic Resonance Spectroscopy Group, Kazan University (Russia)*





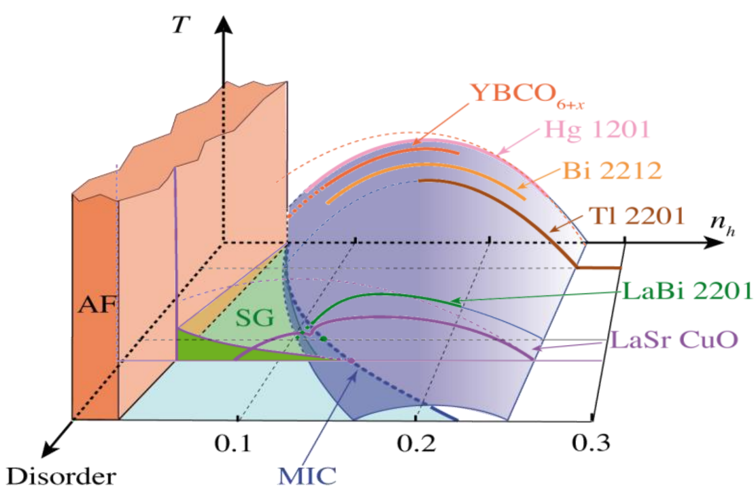
Co $^{3+}$ x Co $^{4+}$

Na order and charge order for x=2/3



delocalised holes
Co $^{3.44+}$
Kagome lattice

non magnetic
Co $^{3+}$



Different charge orders
for other values of x
Different ground state properties

LPS ORSAY

TRIANGLE DE LA PHYSIQUE

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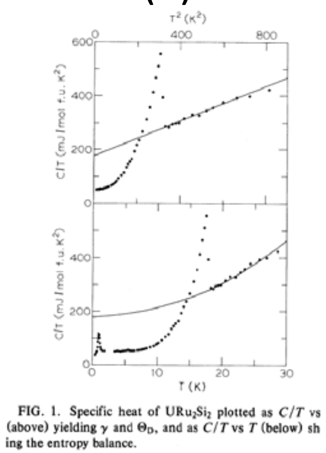
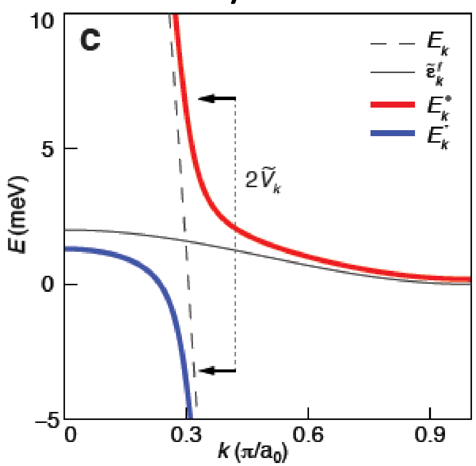
'Hidden Order' State from the 'Fano Lattice' Electronic Structure of URu_2Si_2F:

A.R. Schmidt *etal* (2009)

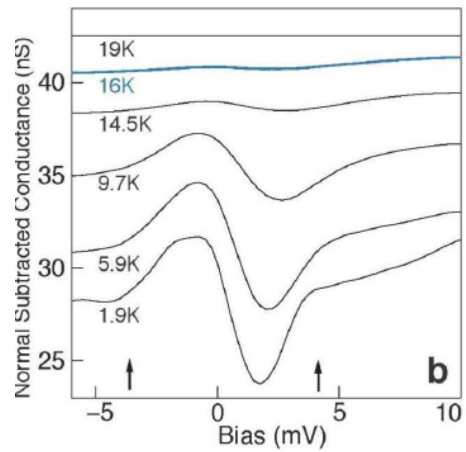
C(T)



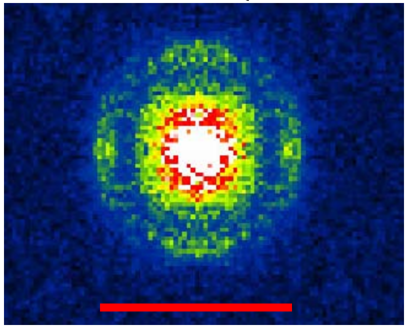
HF hybridization



STM Visualization of Fano lattice



STM QPI



(0.6,0)

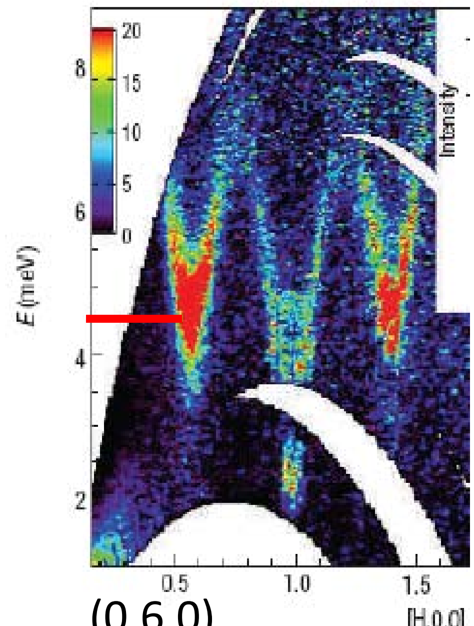
*Nature of Kondo Lattice?: Fano Lattice. Visualization of HF band onset

*Nature of HO: itinerant vs intracell? dual, both intra cell –R coherence U lattice changes (Haule, Myake…) and itinerant K (Varma,Gorkov,AVB…).

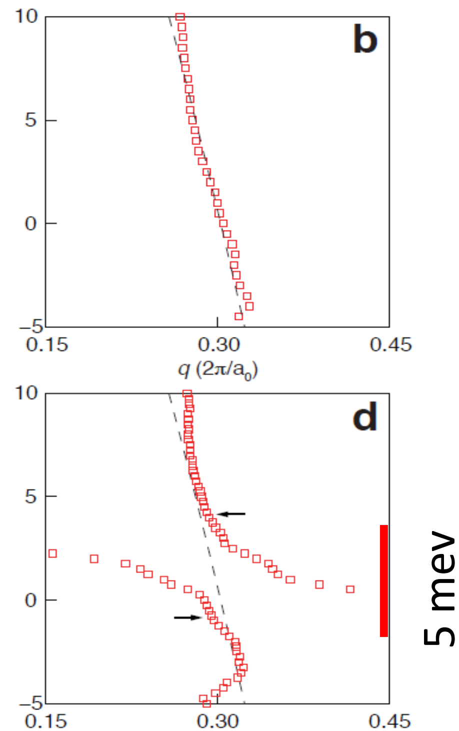
*QPI change:Sharp change in QP dispersion T_HO

attendant Q resonant features: **E = 5 meV, Q* = (0.6,0), (0,0.6)** Consistent with INS data Wiebe,Bourdarot et al

INS, Wiebe (2007)



(0.6,0)



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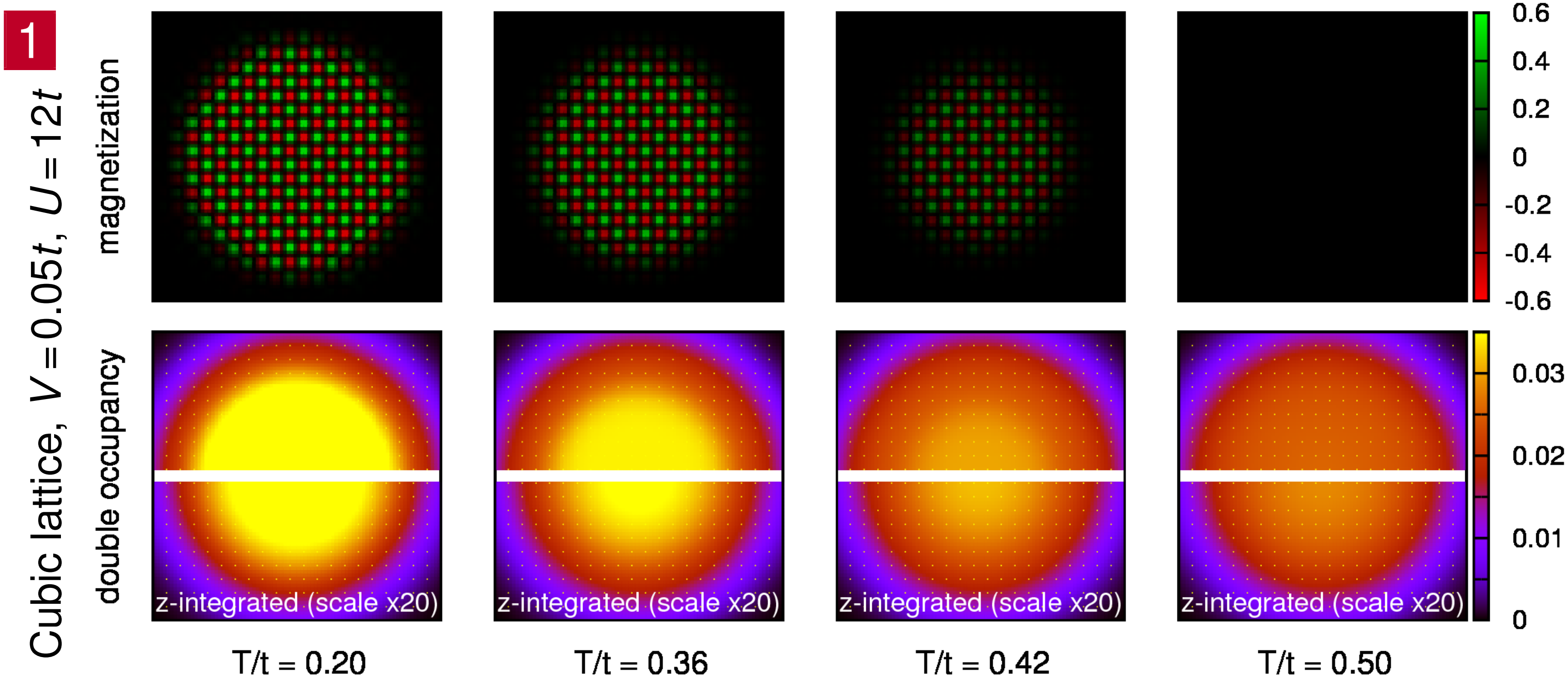
- Zhu

Néel transition of fermionic atoms in an optical trap: a real-space DMFT study

Elena Gorelik,[a] Irakli Titvinidze,[b] Walter Hofstetter,[b] and Nils Blümer[a]
[a] Institut für Physik, Johannes Gutenberg-Universität, Mainz, Germany
[b] Institut für Theoretische Physik, Johann Wolfgang Goethe-Universität, Frankfurt/Main, Germany

1



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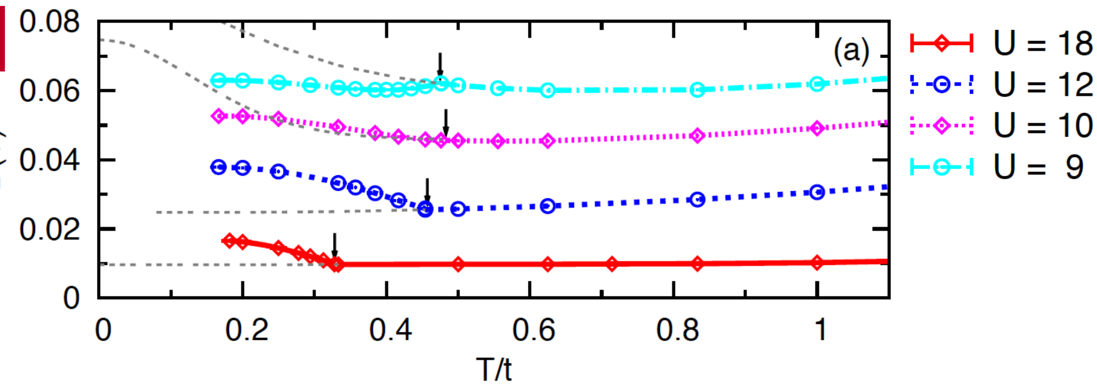

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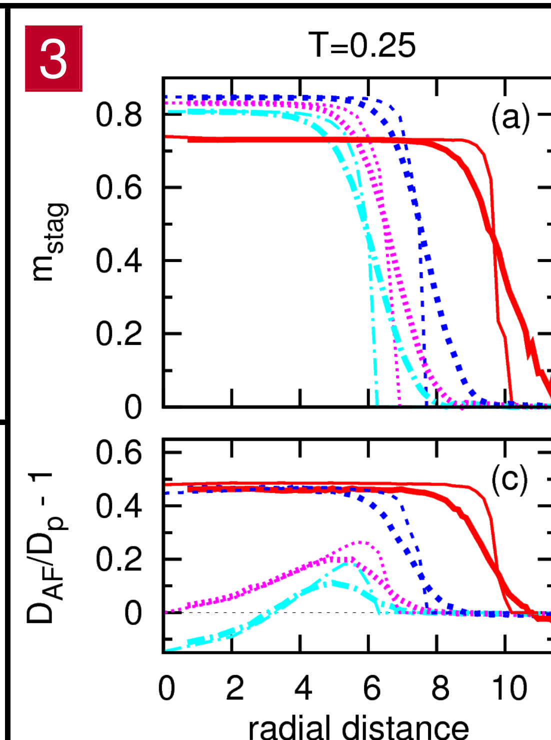

4

Summary

AF phases signaled by enhanced double occupancy

LDA fails for ordered phases: misses proximity effects

Simulations of $\mathcal{O}(100000)$ particles at full DMFT level

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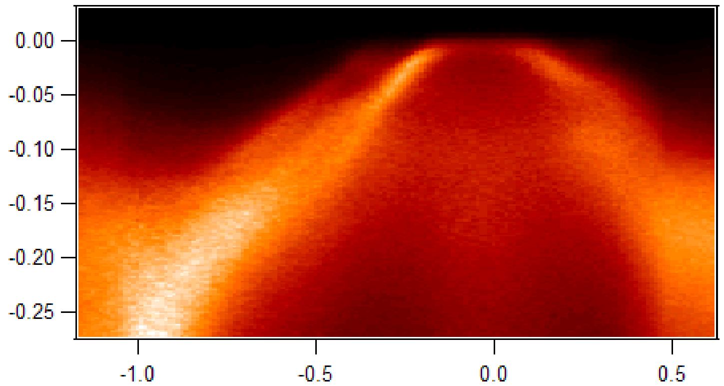
Comparaison of Fermi Surface and Band Structure measured with ARPES of $Ba(Fe_{1-x}Co_x)_2As_2$ and $Ba(Fe_{1-x}Ru_x)_2As_2$

Véronique Brouet, *LPS Orsay, France*

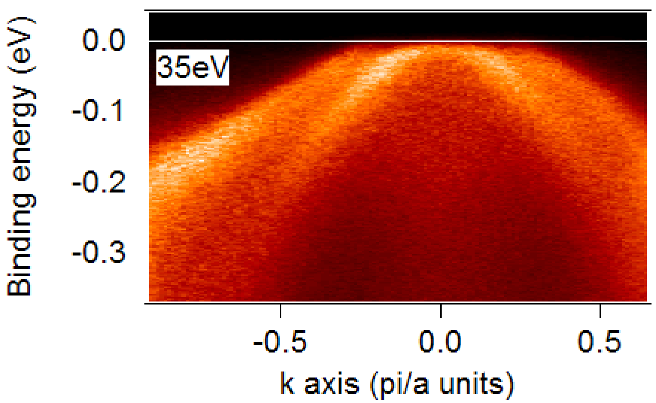
$BaFe_2As_2$



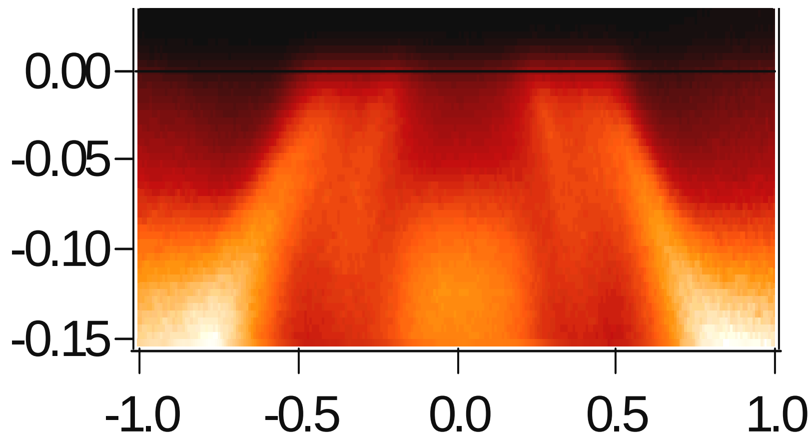
Co substitution
= electron doping

Ru substitution
= isovalent

$Ba(Fe_{0.93}Co_{0.07})_2As_2$



$Ba(Fe_{0.65}Ru_{0.35})_2As_2$



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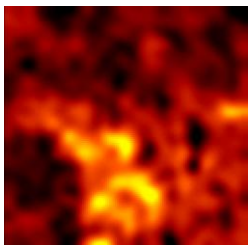
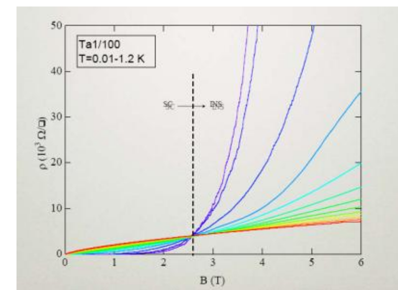
Phase Fluctuations and the Superconductor-Insulator Transition in Thin Films

Yonatan Dubi, Sasha Balasky
Los Alamos National Lab

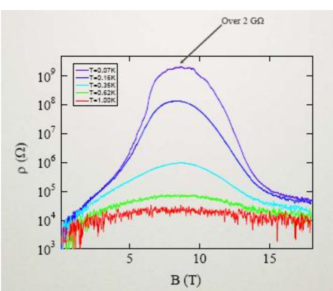
We argue that the interplay between disorder and phase fluctuations can explain many of the phenomena observed in disordered thin superconducting films:



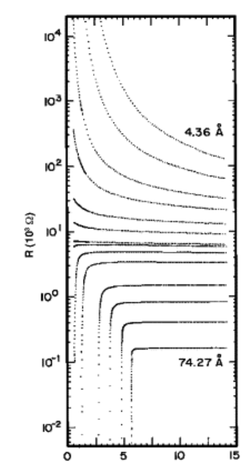
• Disorder and magnetic field give rise to the formation of “superconducting islands”.



• The magnetic-field-tuned superconductor-insulator-transition (SIT) is a percolation transition of inter-island phase-coherence.



•The huge magneto-resistance peak is due to the competition of transport through the SC islands and coulomb blockade.



•The thickness-induced transition is due to scaling of the phase stiffness with film thickness, and Tc enhancement in parallel fields is due to surface-roughness-enhanced phase fluctuations.

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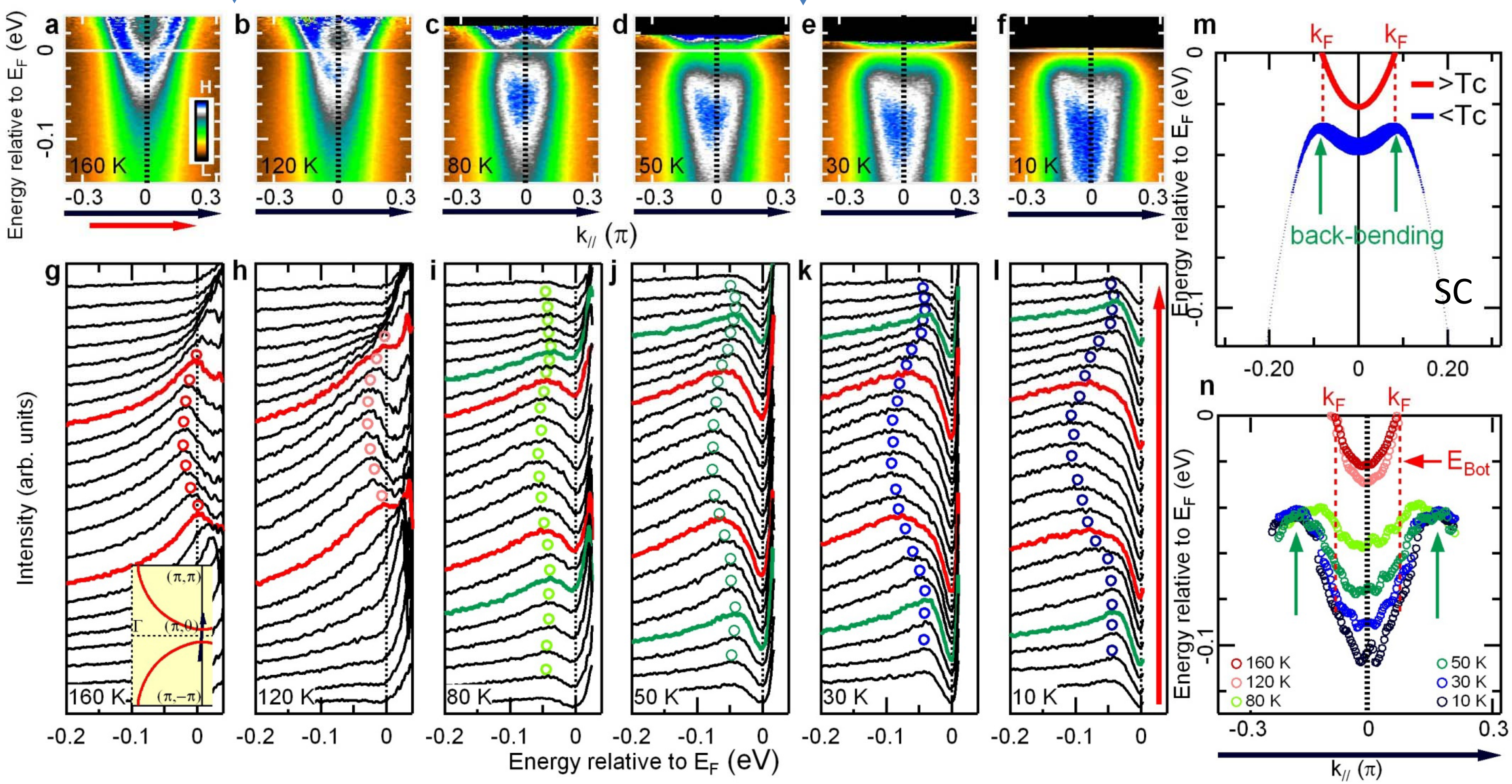
Particle-hole symmetry broken pseudogap in Bi2201

T* ~ 125 K

Tc ~ 34 K



Fermi-Dirac function divided

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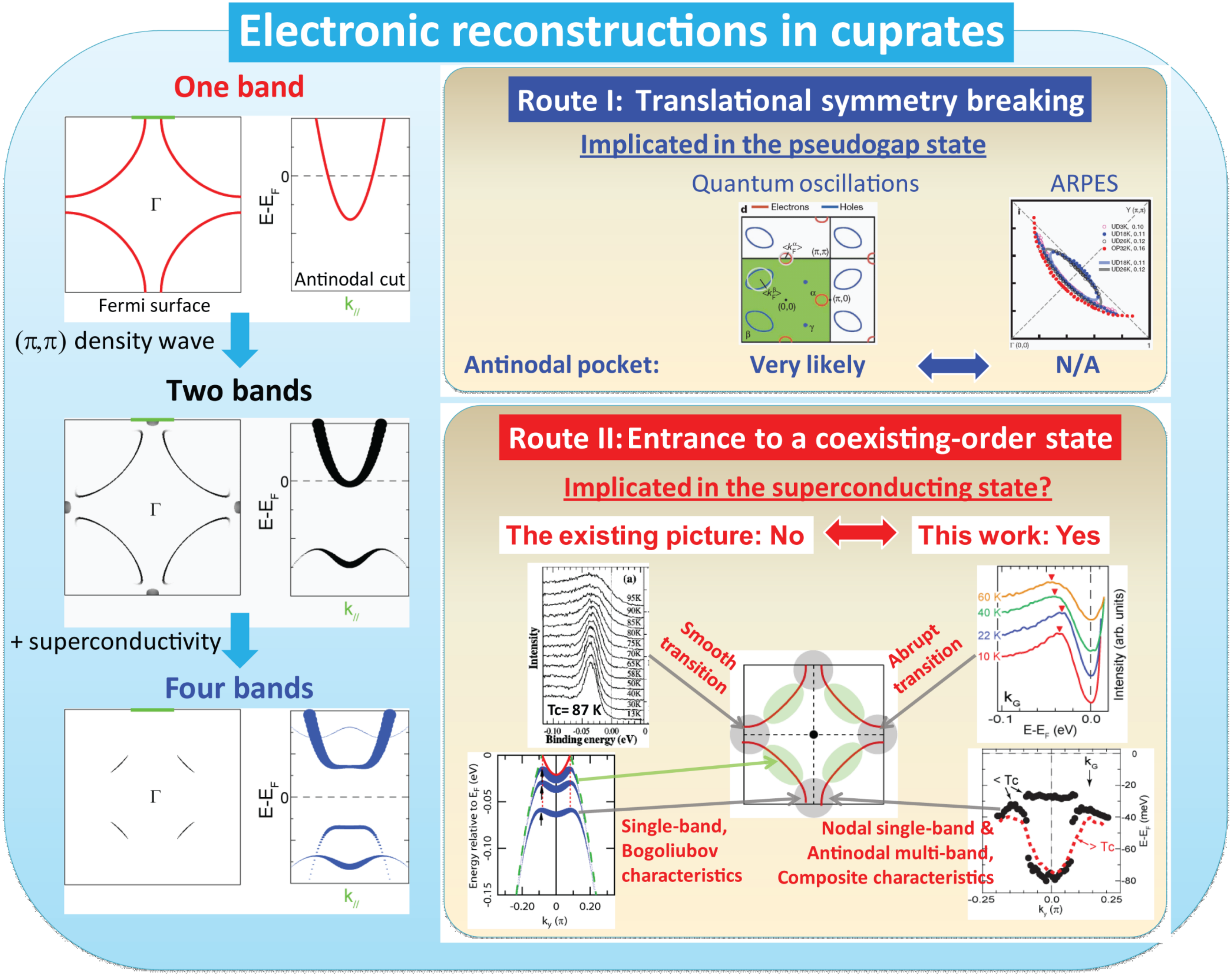

Electronic reconstructions in cuprates
One band
Γ
Fermi surface
E-E_F
0
Antinodal cut
k_//
(π,π) density wave
Two bands
Γ
E-E_F
0
k_//
+ superconductivity
Four bands
Γ
E-E_F
0
k_//
Route I: Translational symmetry breaking
Implicated in the pseudogap state
Quantum oscillations
ARPES
Electrons
Holes
(π,π)
(0,0)
(π,0)
Antinodal pocket:
Very likely
N/A
Route II: Entrance to a coexisting-order state
Implicated in the superconducting state?
The existing picture: No
This work: Yes
Binding energy (eV)
Intensity
Tc= 87 K
Smooth transition
Abrupt transition
60 K
40 K
22 K
10 K
k_G
E-E_F (eV)
Intensity (arb. units)
Energy relative to E_F (eV)
k_y (π)
Single-band, Bogoliubov characteristics
Nodal single-band & Antinodal multi-band, Composite characteristics
< Tc
> Tc
E-E_F (meV)

- Adams
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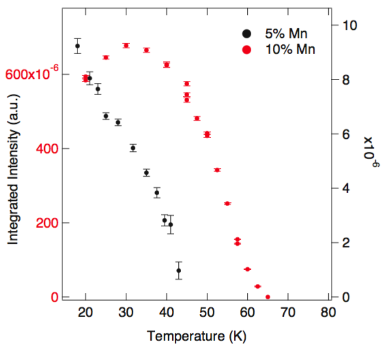
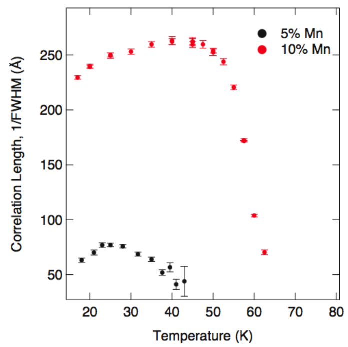
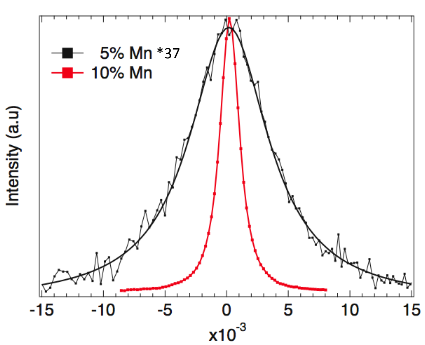
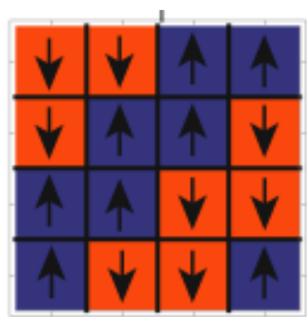
Spatially inhomogeneous metal-insulator transition in Mn-$Sr_3Ru_2O_7$

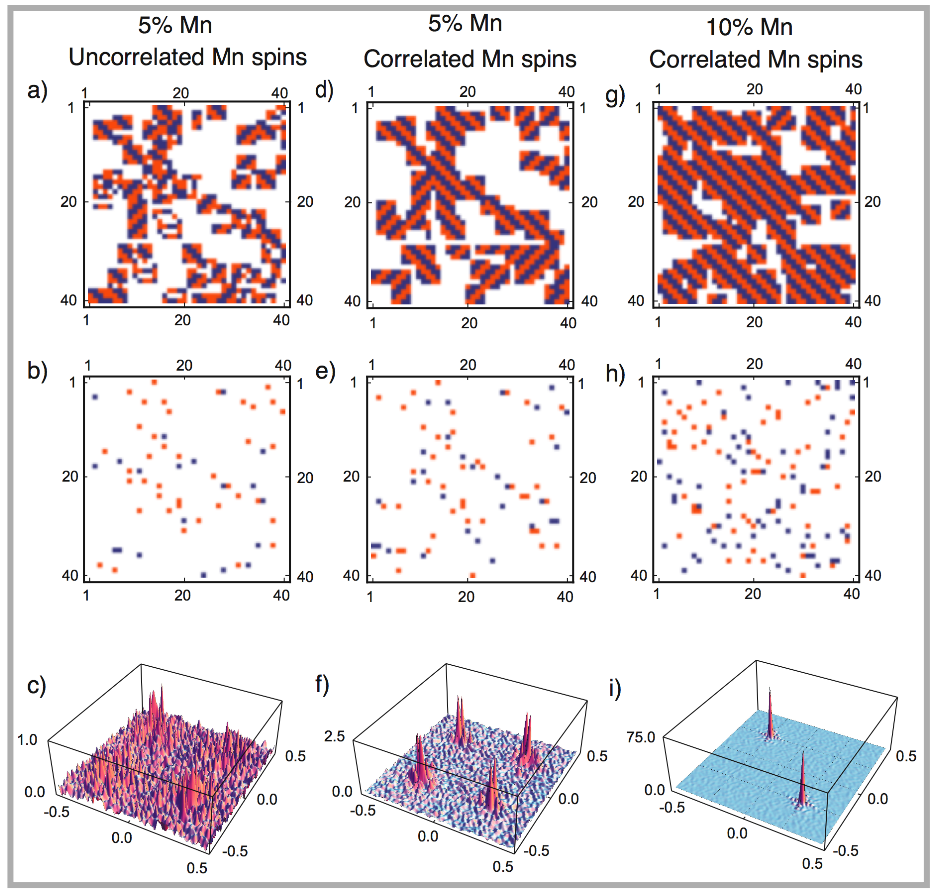
M.A. Suman Hossain et al. (UBC)
Now at SIMES, Stanford











Resonant diffraction is possible even at the impurity edge!

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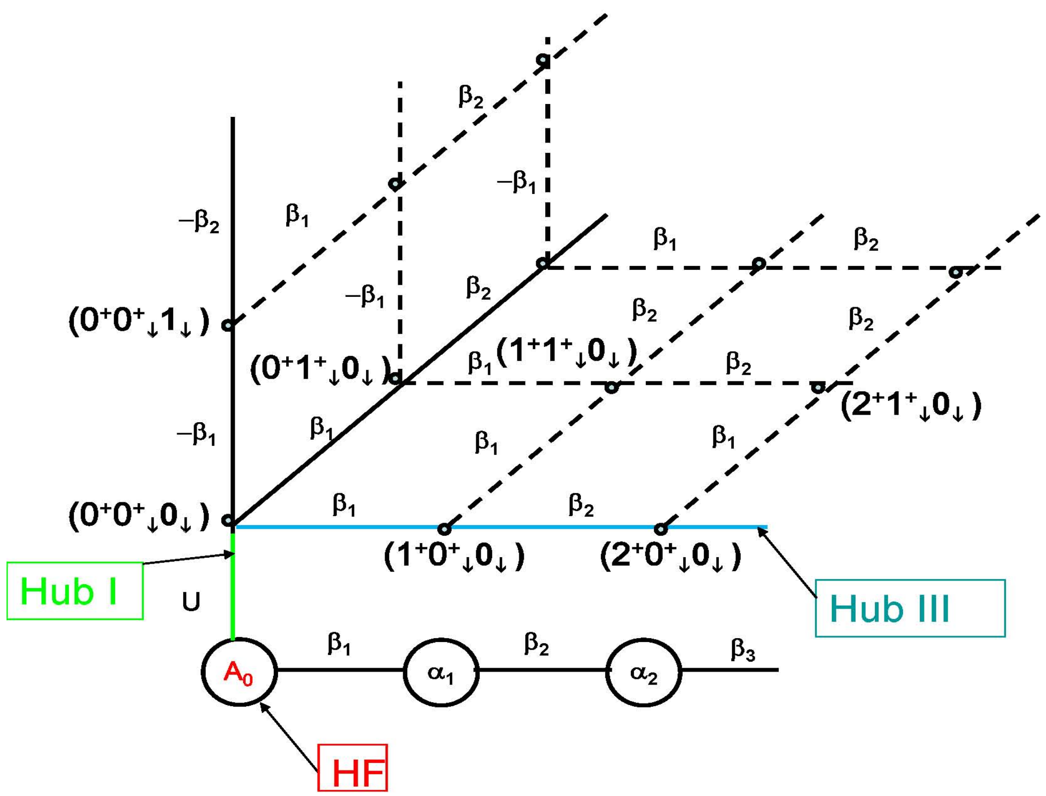
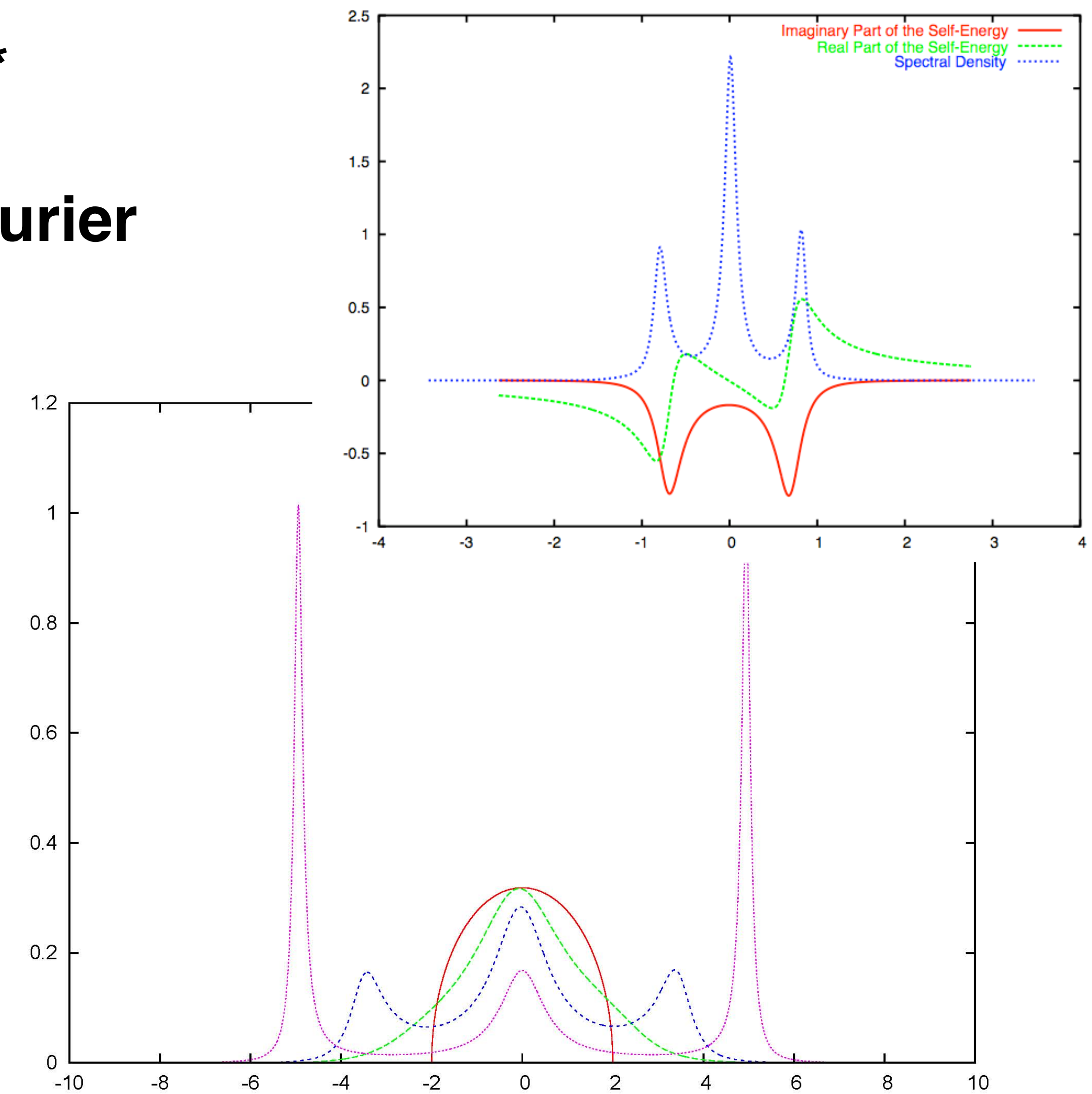
New impurity recursion based solver for Dynamical Mean Field Theory

Jean-Pierre Julien*† and R. C. Albers*

* Group T-4, LANL,

† Institute Neel CNRS and Universite J. Fourier France





$$\Sigma(z) = A_0 + \cfrac{B_1^2}{z - A_1 - \cfrac{B_2^2}{z - A_2 - \cfrac{B_3^2}{z - \cdots}}}$$

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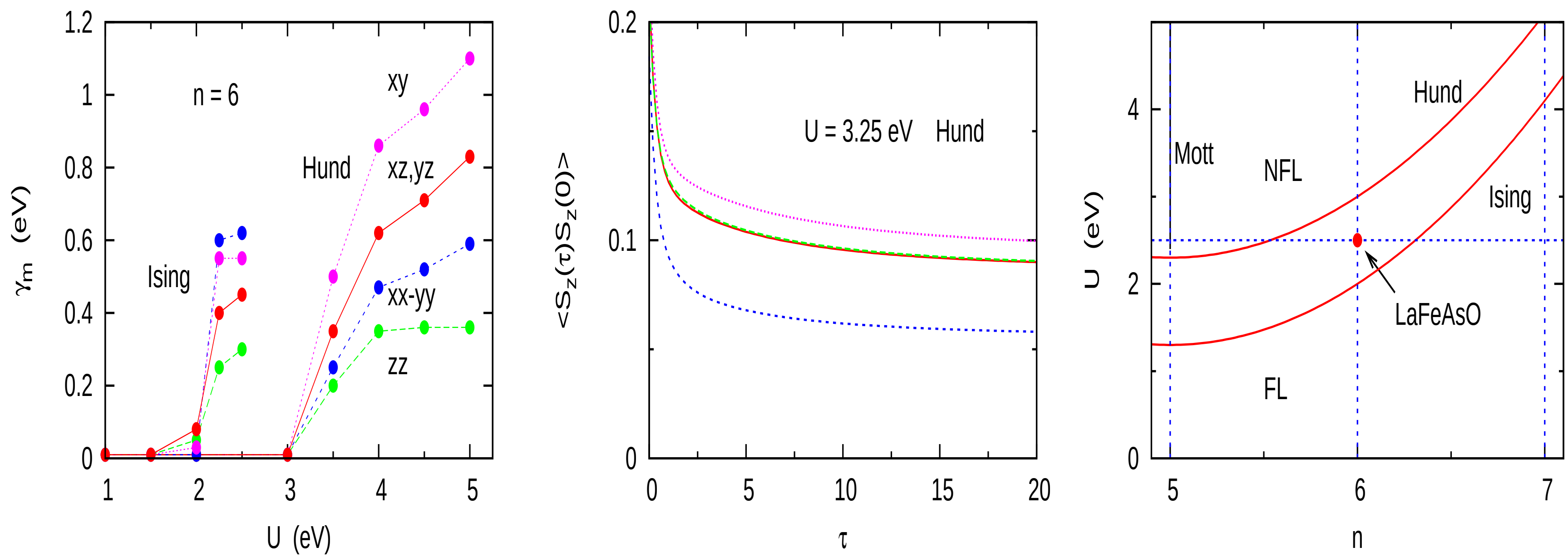
LaFeAsO: Spin Freezing Transition

H. Ishida, A. Liebsch, PRB 81 (2010)



- extension of finite-T ED / DMFT to 5 bands
- Hund exchange: $U_c \approx 3$ eV, Ising coupling: $U_c \approx 2$ eV
- $n \rightarrow 5$: 'parent' Mott insulator, $n > 6$: Fermi liquid
- phase diagram qualitatively similar to cuprates
- $U,\ J\ \rightarrow\ U_{mn},\ J_{mn}$ Miyake et al:
- FeSe vs. LaFeAsO: on opposite sides of spin freezing?

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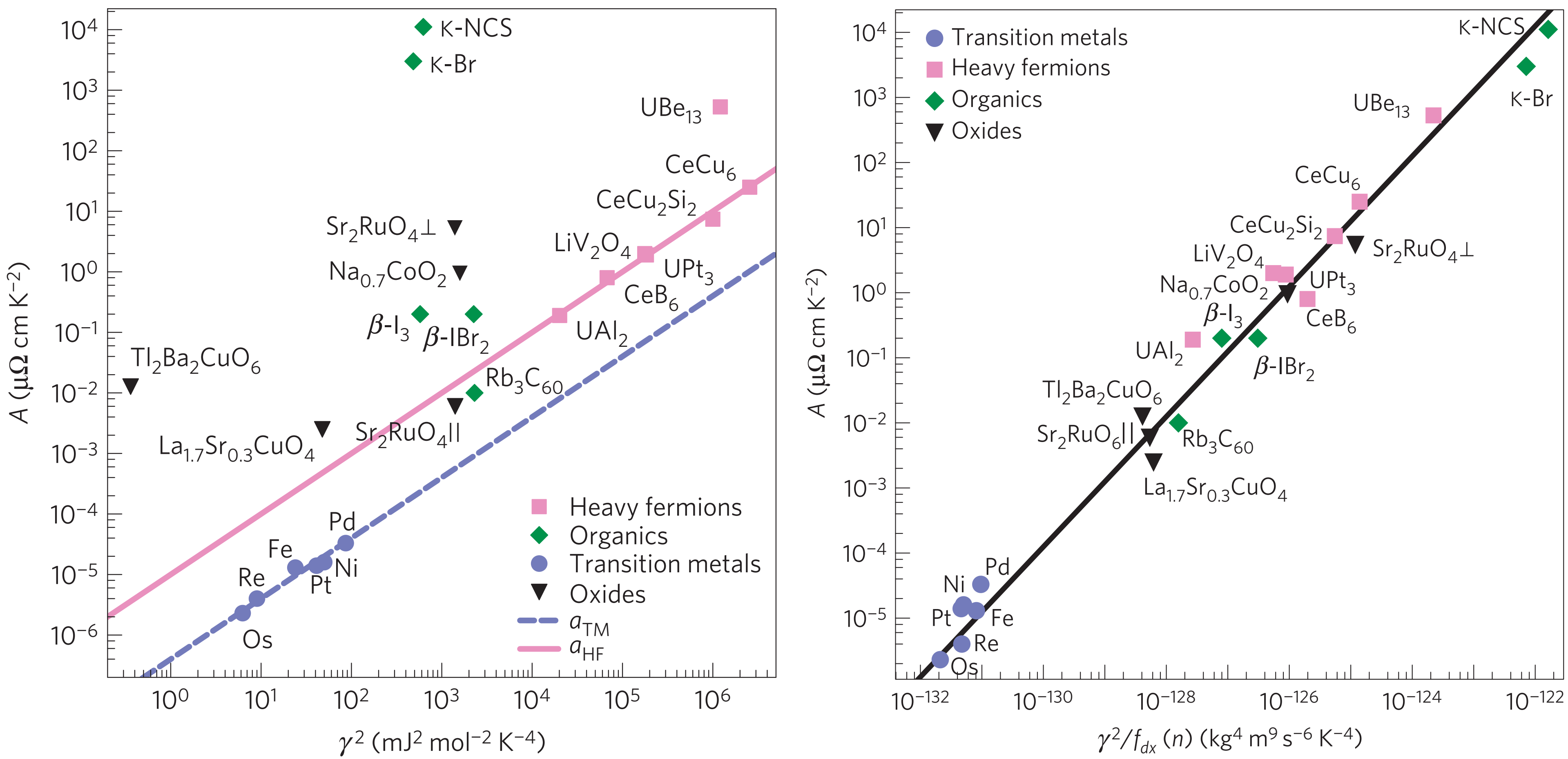
A unified explanation of the Kadowaki-Woods ratio

[Jacko, Fjærestad & Powell, Nature Phys. **5**, 422 (2009)]



We introduce a ratio, closely related to the Kadowaji-Woods ratio, that includes the effects of carrier density and spatial dimensionality and takes the same (predicted) value in a wide range of strongly correlated metals

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- Liebsch
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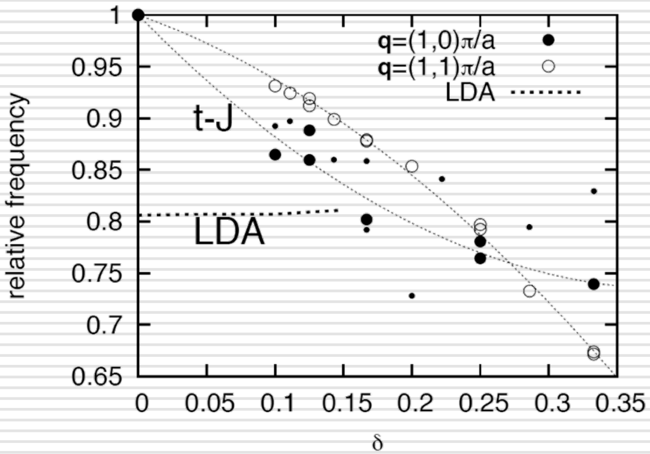
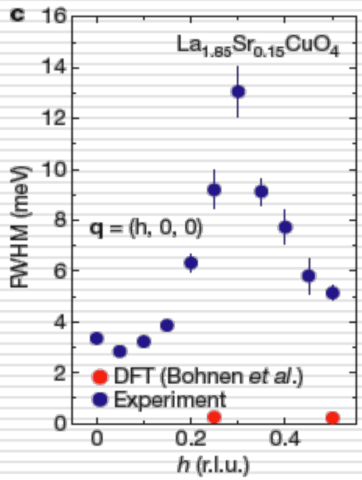
Electron-phonon interaction in strongly correlated systems

Giorgio Sangiovanni (*Vienna Tech*) and Olle Gunnarsson (*MPI Stuttgart*)

- oxygen-breathing modes in cuprates:
  <u>strong coupling</u> in experiments *but* <u>negligible coupling</u> in LDA/GGA





NATURE|Vol 455|2 October 2008 **BRIEF COMMUNICATIONS ARISING**

Photoemission kinks and phonons in cuprates

D. Reznik[1], G. Sangiovanni[2], O. Gunnarsson[3] & T. P. Devereaux[3]

- Adams
- Alloul
- Balatsky
- Bluemer
- Brouet
- Dubi
- Hashimoto
- He
- Held
- Hossain

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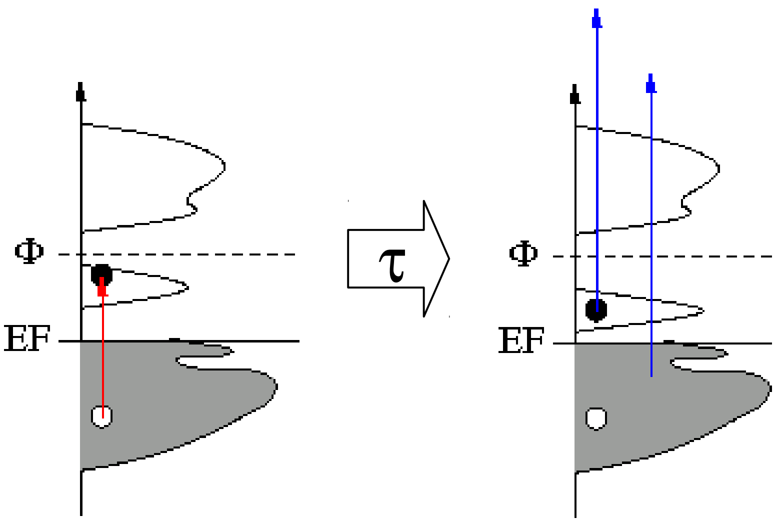
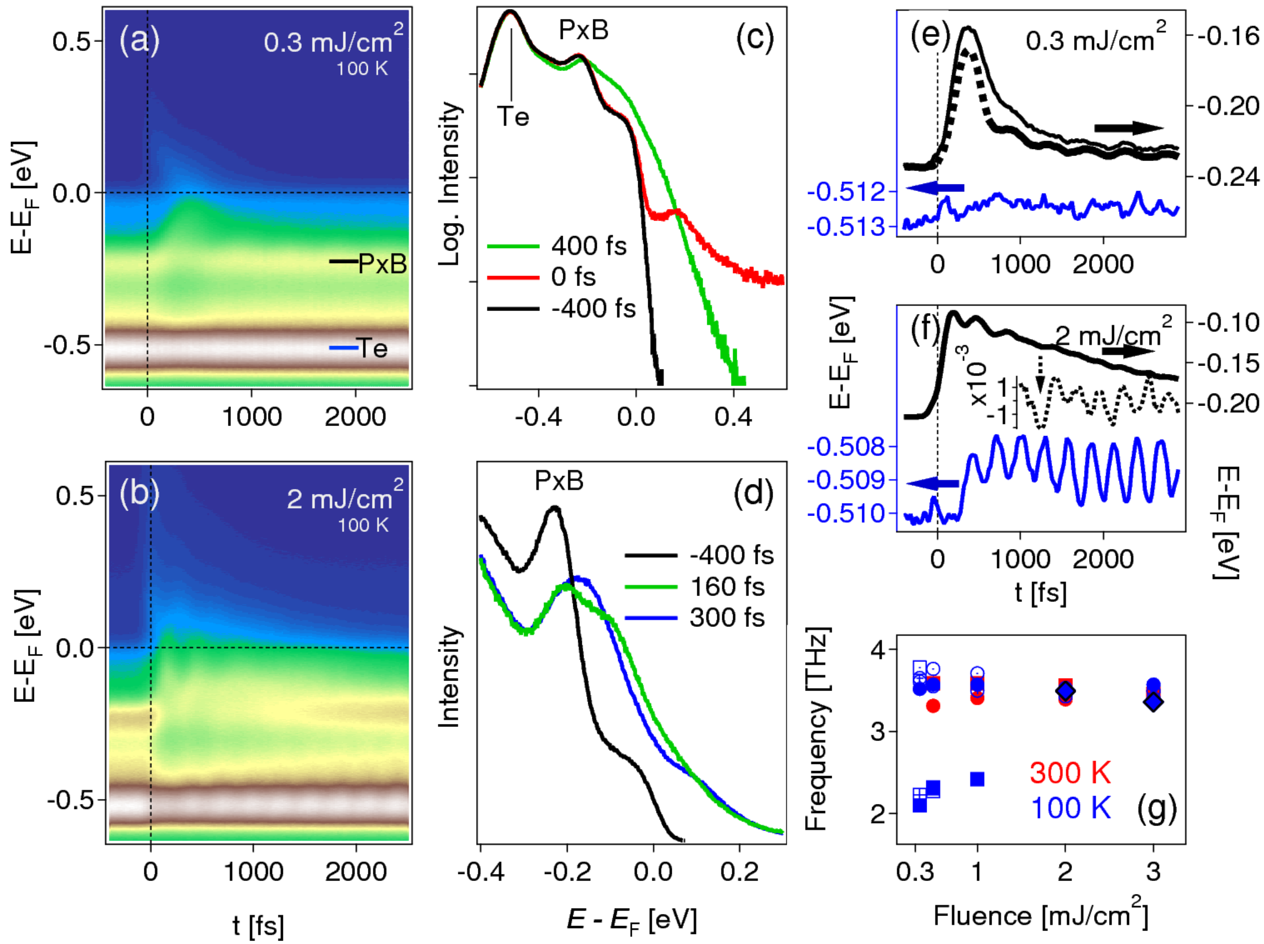
Time-resolved ARPES on the charge-density-wave material $TbTe_3$: collective modes and phase transitions

Felix Schmitt





- Novel technique, allowing access to both quasiparticles and collective modes at the same time
- Access correlations through their effect on quasiparticles

→ We believe to have observed the CDW amplitude mode

→ time-resolved closing of CDW gap

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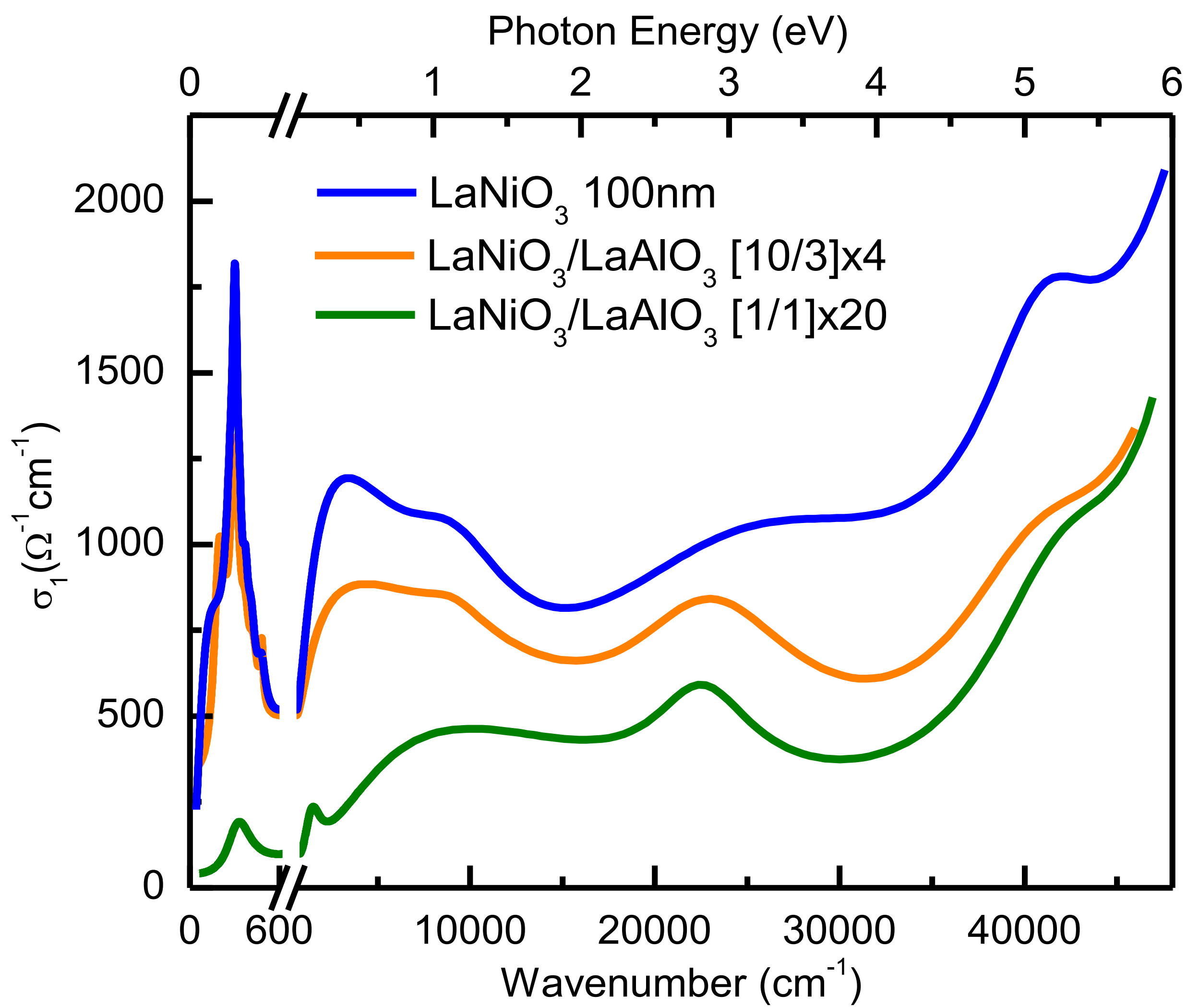
Optical Probe of Strong Correlations in $LaNiO_3$ Thin Films and Superlattices

M. K. Stewart, J. Liu, R. Smith, B. Chapler, C. Yee, K. Haule, J. Chakhalian, D. N. Basov



$$\frac{K_{\mathrm{exp}}}{K_{\mathrm{band}}} = 0.07$$

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Magnetic interaction mechanism in Europium monochalcogenide

Xiangang Wan[1], Sergej Y. Savrasov[2]

[1]Nanjing University, China

[2]University of California, Davis

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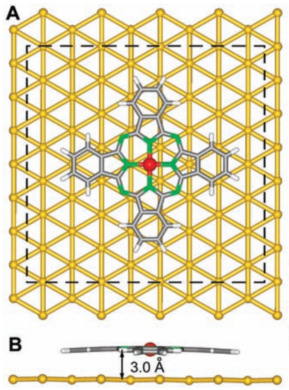
Towards DMFT in Quantum Chemistry

Dominika Zgid and Garnet Chan

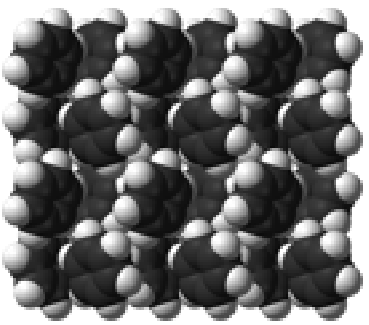
Department of Chemistry and Chemical Biology
Cornell University, Ithaca, NY, USA

Surface chemistry



- metallic surface with coverage
- theoretical surface spectroscopy, excited states of a molecule and conductance

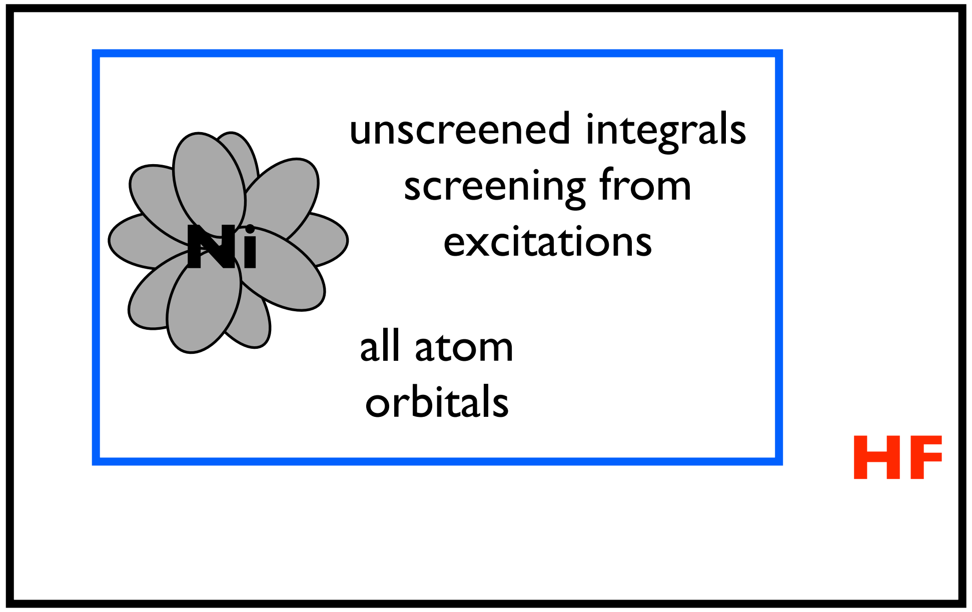
Problem of solids



- molecular crystals with large unit cell in which the overlap between molecular orbitals is moderate

Quantum Chemistry DMFT

- explicit extended basis in the cluster treated with quantum chemistry solver based on variational wave function
- local screening of integrals progressively achieved through increasing the basis
- long range interaction via HF
- no double counting



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Band Narrowing and Mott Localization in Iron Oxychalcogenides $La_2O_2Fe_2O(Se,S)_2$

Jian-Xin Zhu (Los Alamos National Laboratory) and co-workers