d- only vs. dp- basis sets for DMFT et al.

2p or not 2p...

N. Parragh et al. arXiv:1303.2099

P. Hansmann PhD thesis

Philipp Hansmann

ÉCOLE POLYTECHNIQUE ParisTech

cnrs dépasser les frontières

ERC Kick Off

Baumschlagerberg, September 2013

People

Würzburg

- N. Parragh
- G. Sangiovanni

Wien

- S. Hummel
- A. Toschi
- K. Held

MPI Stuttgart

- O.K. Andersen

MPI Stuttgart

- B. Keimer

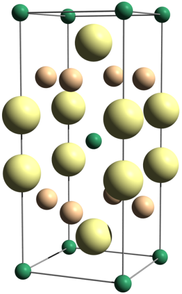
Tokyo / Riken

- Y. Tokura

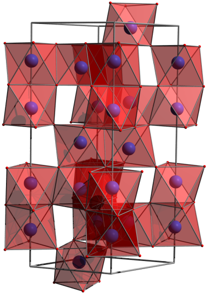
Outline

The usual suspects

$CeSi_2Cu_2$: 4f



V_2O_3: 3d(t_{2g})



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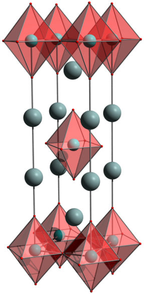

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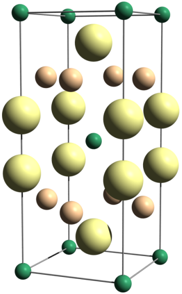

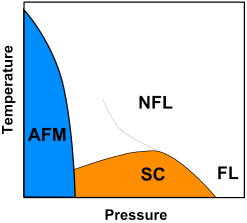

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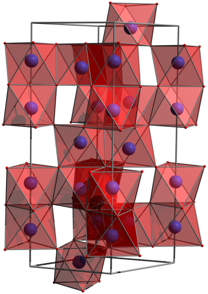

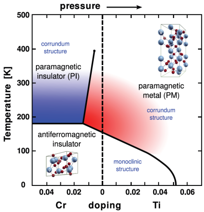

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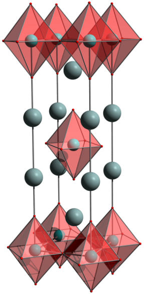
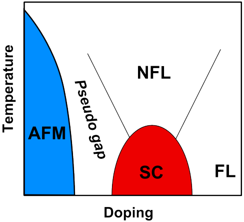




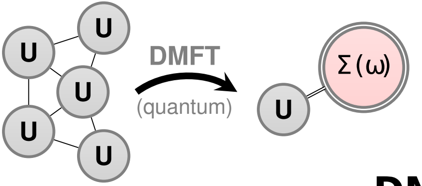
DMFT and beyond

DΓA

cluster DMFT

Dual Fermions

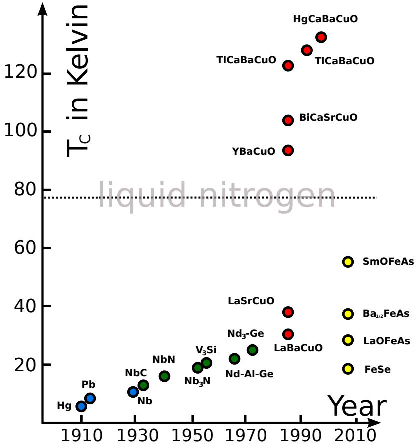
DCA



DMF²RG

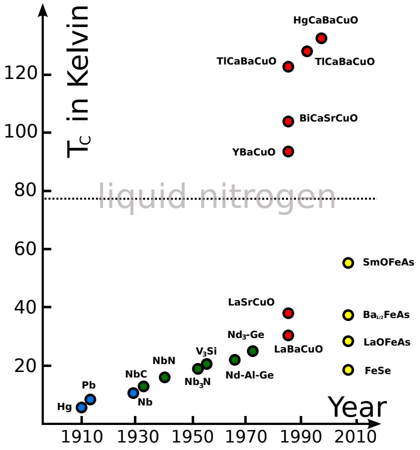
GW+DMFT

The last crusade



Where is the holy grail?

The last crusade



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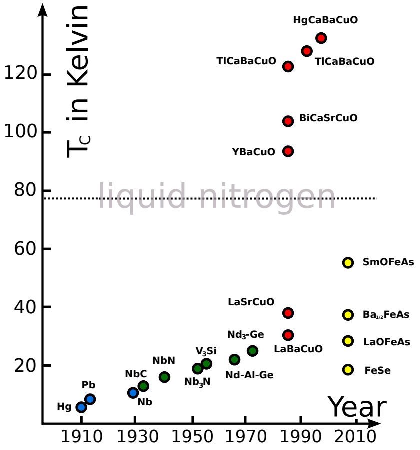

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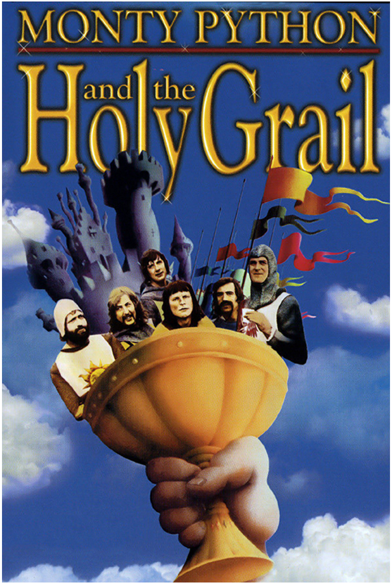

First things first: Bands

Pergamon

J. Phys. Chem. Solids Vol. 56, No. 12, pp. 1573–1591, 1995

0022–3697/95 $9.50 + 0.00

0022–3697(95)00269-3

LDA ENERGY BANDS, LOW-ENERGY HAMILTONIANS, t', t'', $t_\perp(\mathbf{k})$, and $J_\perp$.

O. K. ANDERSEN, A. I. LIECHTENSTEIN, O. JEPSEN and F. PAULSEN
Max-Planck Institut für Festkörperforschung, D-70569 Stuttgart, Germany

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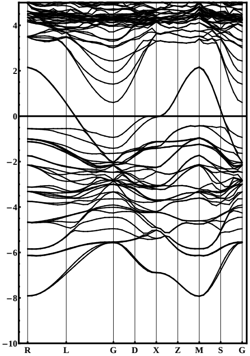

e.g. La_2CuO_4

- -10eV to 2eV: Cu 3d and O 2p
- Due to overlap symmetry a 4band block of σ bonding orbitals can be decoupled

First things first: Bands

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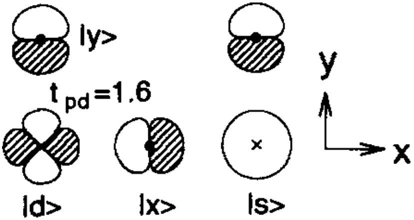

$\langle\sigma\|H\|\sigma\rangle$	$\|\mathrm{Cu}\,d\rangle$	$\|\mathrm{Cu}\,s\rangle$	$\|\mathrm{O2}\,x\rangle$	$\|\mathrm{O3}\,y\rangle$
$\langle\mathrm{Cu}\,d\|$	ϵ_d	0	$2t_{pd}\sin\frac{a}{2}k_x$	$-2t_{pd}\sin\frac{a}{2}k_y$
$\langle\mathrm{Cu}\,s\|$	0	ϵ_s	$2t_{sp}\sin\frac{a}{2}k_x$	$2t_{sp}\sin\frac{a}{2}k_y$
$\langle\mathrm{O2}\,x\|$	$2t_{pd}\sin\frac{a}{2}k_x$	$2t_{sp}\sin\frac{a}{2}k_x$	ϵ_p	0
$\langle\mathrm{O3}\,y\|$	$-2t_{pd}\sin\frac{a}{2}k_y$	$2t_{sp}\sin\frac{a}{2}k_y$	0	ϵ_p

First things first: Bands

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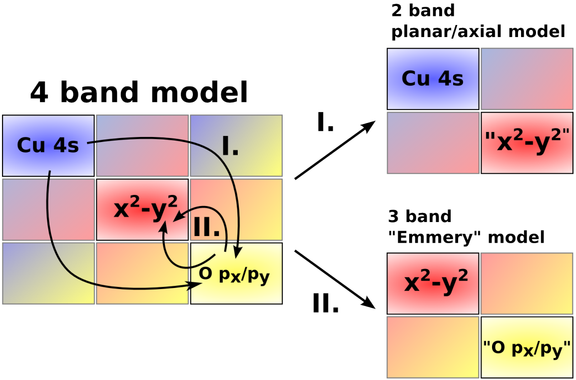
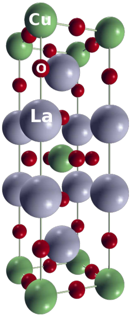
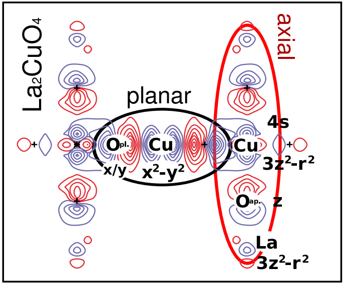
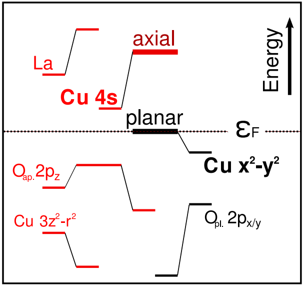


high-T_c cuprates

Pavarini et al., PRL **87**, 047003 (2001)







Two hybridized bands:

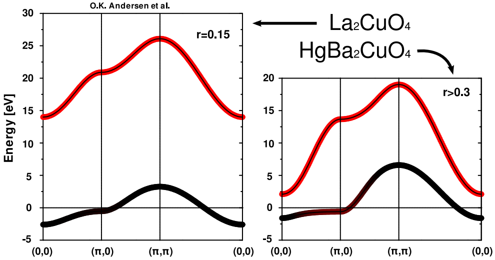
1. Cu-3d x^2-y^2
   dressed with O $p_{x/y}$
2. Cu-4s axial orbital
   dressed with Cu $3z^2$-r^2, $O_{ap.}$ p_z, La $3z^2$-r^2, etc.

high-T_c cuprates

The parameter "r"

ϵ_{axial}-ϵ_F small $\rightarrow$ r large

Material dependent parameter



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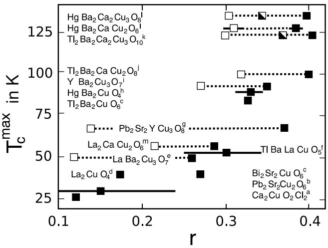
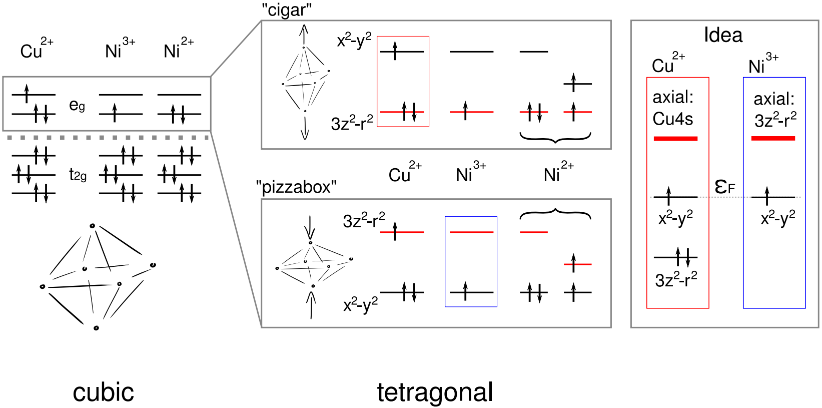


high-T_c nickelates?!?

The crackpot approach to high T_c superconductivity...

high-T_c nickelates?!?

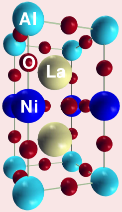
The crackpot approach to high T_c superconductivity...

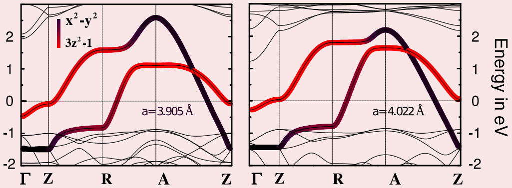


J. Chaloupka & G. Khaliullin, Phys. Rev. Lett. **100**, 016404 (2008)

Fermisurface of $LaNiO_3/LaAlO_3$

Correlation effects on the Fermi Surface





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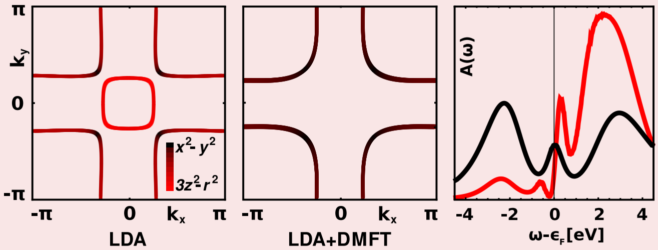
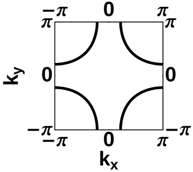


- LDA+DMFT (V=5.0eV)
- $\Re[\Sigma(\omega \to 0)]$ enhances Δ_{CF}
- $\mu' = \mu - \Re[\Sigma(\omega \to 0)]$
- t,t' one band–model for cuprates



$(t' = 0.4t)$

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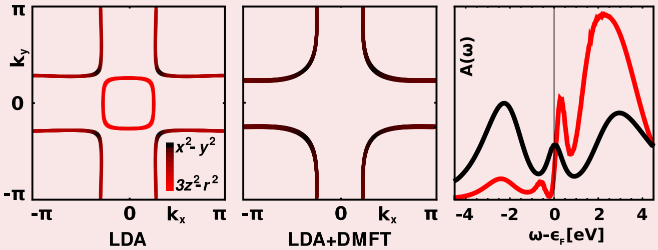
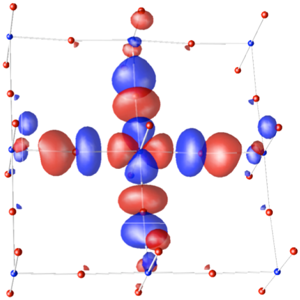


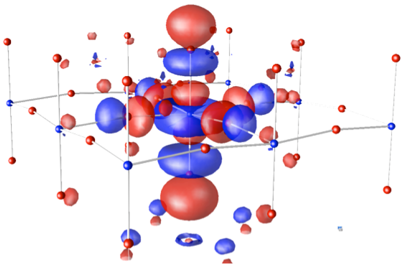
- metalic **single – sheet surface** situation
- but Fermisurface remains **mixed**!
- "sheet selective" transition
  - PH *et al.*, Phys. Rev. Lett. **103**, 016401 (2009)
  - PH *et al.*, Phys. Rev. B **82**, 235123 (2010)

Wannierfunctions from NMTO

x^2-y^2



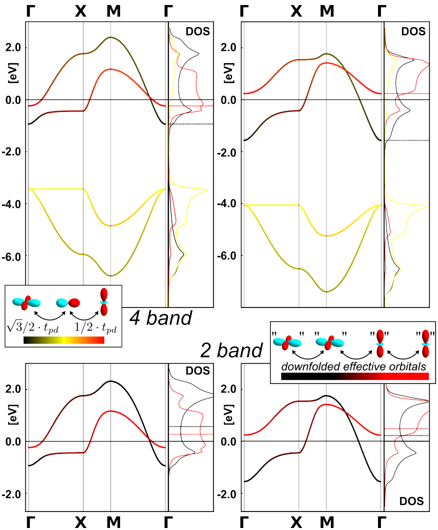
$3z^2$-r^2



Is this an appropriate basis?

$$\hat{H} = \hat{H}_{\text{kin.}} + U \cdot \sum_{i,m,\sigma} \hat{n}_{im\uparrow}\hat{n}_{im\downarrow} + \sum_{i,\sigma<\sigma'} (V - \delta_{\sigma\sigma'} J)\hat{n}_{i1\sigma}\hat{n}_{i2\sigma'}$$

Disclaimer: MODEL



(dp-Ham.): $N = 4\ p\ e^{-} + 1\ d\ e^{-} = 5\ e^{-}$

(d-Ham.): $N = 1\ d\ e^{-} = 1\ e^{-}$

Disclaimer: MODEL

Four to two bands...

With “Loẅdin” downfolding and Taylorexpansion of:

$$\begin{pmatrix} \varepsilon_{\text{planar}} & 0 & i\sqrt{3}t_{pd}\sin\left(\frac{k_x}{2}\right) & -i\sqrt{3}t_{pd}\sin\left(\frac{k_y}{2}\right) \\ 0 & \varepsilon_{\text{axial}} & it_{pd}\sin\left(\frac{k_x}{2}\right) & it_{pd}\sin\left(\frac{k_y}{2}\right) \\ -i\sqrt{3}t_{pd}\sin\left(\frac{k_x}{2}\right) & -it_{pd}\sin\left(\frac{k_x}{2}\right) & \epsilon_p & 0 \\ i\sqrt{3}t_{pd}\sin\left(\frac{k_y}{2}\right) & -it_{pd}\sin\left(\frac{k_y}{2}\right) & 0 & \epsilon_p \end{pmatrix}$$

(dp-Ham.): $N = 4\ p\ e^- + 1\ d\ e^- = 5\ e^-$

(d-Ham.): $N = 1\ d\ e^- = 1\ e^-$

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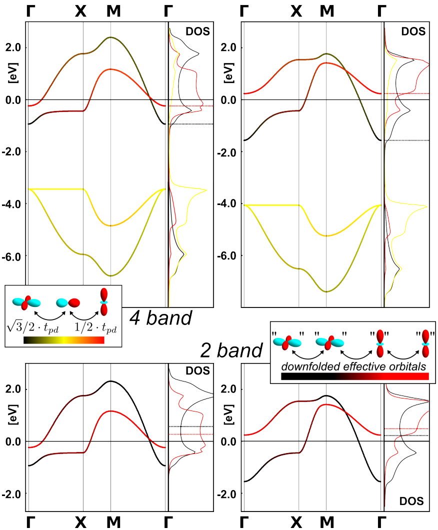

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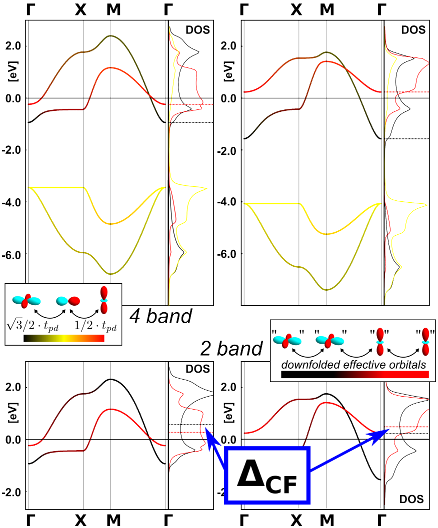

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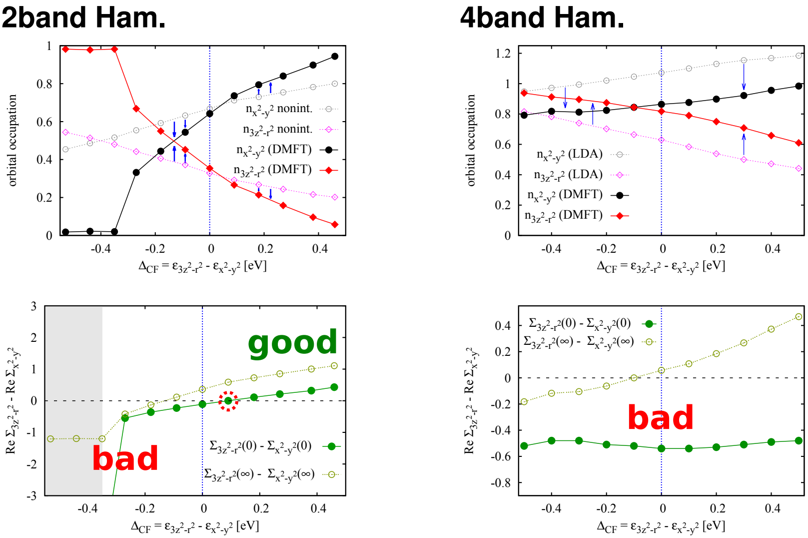
d vs. dp Hamiltonian

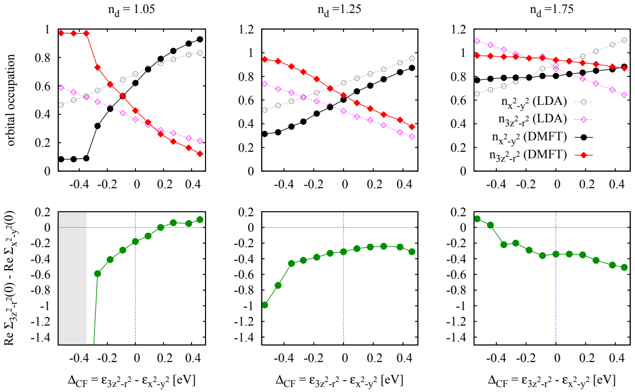


U=5eV; J=0.5eV; U'=U-2J

U=10eV; J=1.0eV; U'=U-2J

d vs. dp Hamiltonian

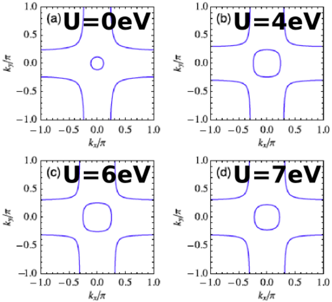
It's actually about d- **density** and **Hund's coupling**!



U=5eV; J=0.5eV; U'=U-2J

It seems clear... Or not?

M.J. Han *et al.*, PRL 2012



decreasing polarization for larger U!

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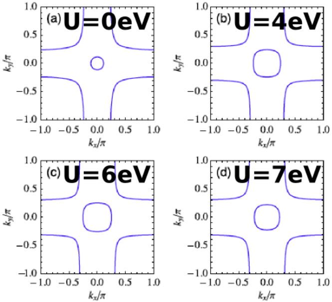
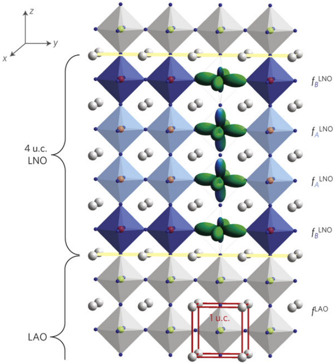


decreasing polarization for larger U!

In summary, we have shown that in a realistic many-body model of nickelate heterostructures, it is essentially not possible to achieve a significant degree of orbital polarization, so that the idea[14] of obtaining a single-band electronic structure must be discarded. Further,

It seems clear... Or not?



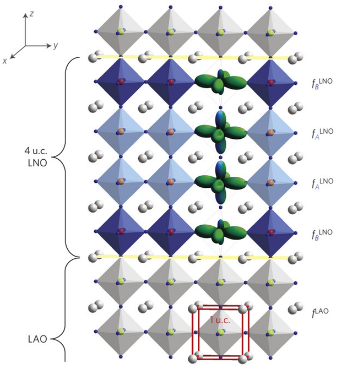
$$P = \frac{n_{x^2-y^2} - n_{\mathrm{axial}}}{n_{x^2-y^2} + n_{\mathrm{axial}}}$$

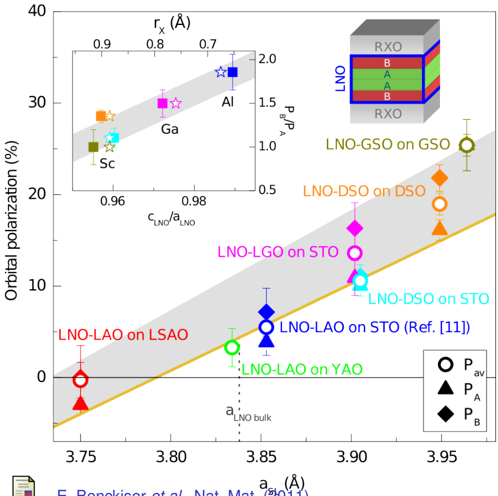
$P_{\mathrm{d}} > 40\%$ $P_{\mathrm{dp}} \approx 10\%$

E. Benckiser *et al.*, Nat. Mat. (2011)

E. Benckiser *et al.*, arXiv 1308.6389 (2013)

It seems clear... Or not?





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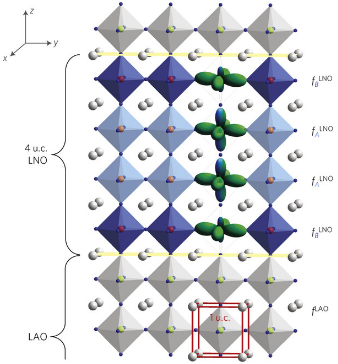

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IV. CONCLUSION

In summary, we have shown that tensile epitaxial strain can enhance the occupation of the x^2-y^2 orbital to 25% in nickelate superlattices. The combined analysis of XAS and resonant reflectivity at the Ni L edge revealed that strain induced by the lattice mismatch with the substrate has the largest effect on the orbital polarization. Especially when combined with other control parameters such as the conduction electron density in the LNO layers, the prospects for orbital engineering of the electronic properties of the nickelates and other oxide superlattices are therefore brighter than suggested by recent experimental and theoretical work.

E. Benckiser *et al.*, Nat. Mat. (2011)

E. Benckiser *et al.*, arXiv 1308.6389 (2013)

More questions than answers...

Summing up...

- d and dp basis sets give qualitatively different result
- **d Ham.** at quarter filling: large orb. polarization
- **dp Ham.** with $N_d>1$: polarization spoiled by Hund's coupling

However...

- Experimentally there seems to be hope
- Control of effective N_d with strain, ...

Emery model revisited

Pergamon

J. Phys. Chem. Solids Vol. 56, No. 12, pp. 1573–1591, 1995

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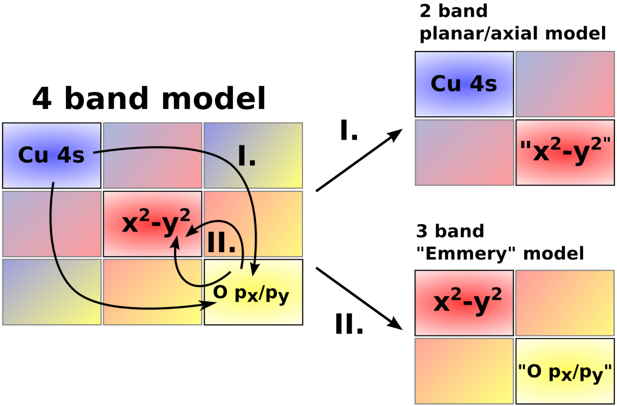
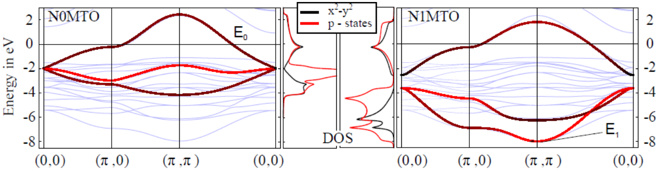


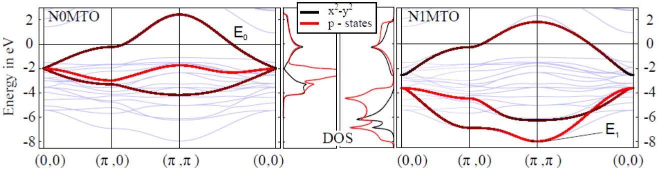
Cuprates in the Emery NMTO basis



Emery

- axial band → WF tails on the oxygens...
- ... and so is the materials dependence.

Cuprates in the Emery NMTO basis

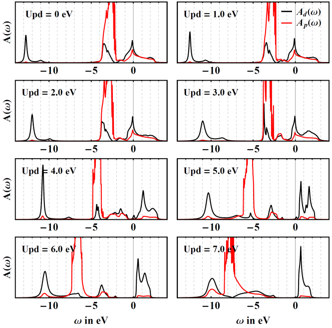


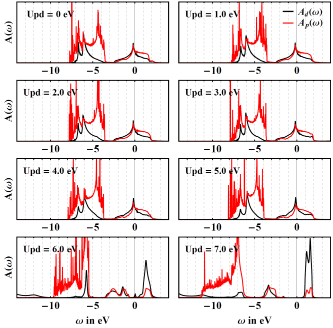
Emery

- axial band → WF tails on the oxygens...
- ... and so is the materials dependence.

proceed with DMFT for both cases:

Cuprates in the Emery NMTO basis

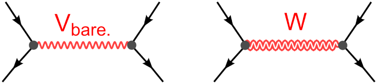




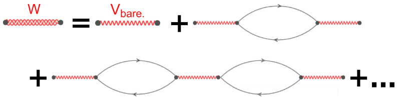
Results

- N1MTO & N0MTO “never” insulating
- Inclusion of U_{pd} (here with Hartree) might be important...
  ... likely, however, there is even something beyond.

How to obtain the interaction parameter?



In RPA (random phase approximation)

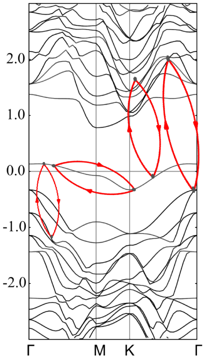


$$W = v + vP^{RPA}v + vP^{RPA}vP^{RPA}v + \ldots$$

$$W = v + vP^{RPA}(1 + vP^{RPA}v + \ldots)$$

$$W = v + vP^{RPA}W$$

$$W = \frac{v}{1 - vP^{RPA}}$$



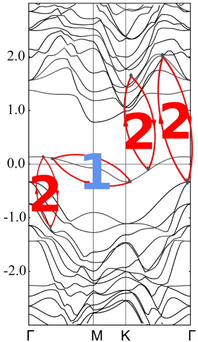
How to obtain the interaction parameter?

$$W = \frac{v}{1 - vP^{RPA}} = \frac{v}{1 - vP_1^{RPA} - vP_2^{RPA}}$$

$$W^{const.} \equiv \frac{v}{1 - vP_2^{RPA}}$$

$$U(\omega) = \langle \text{"}\Psi_{Wannier}\text{"} | W^{const.} | \text{"}\Psi_{Wannier}\text{"} \rangle$$

Also **intersite interactions** can be calculated that way



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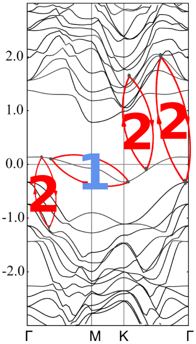

P. Seth, PH, et al., *in preparation* (TM, 4f, 5f)

PH, L. Vaugier, and S. Biermann, *in preparation* (cuprates)

More is not always better...

Conclusion

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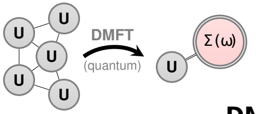
DΓA

cluster DMFT

Dual Fermions

DCA



DMF²RG

GW+DMFT