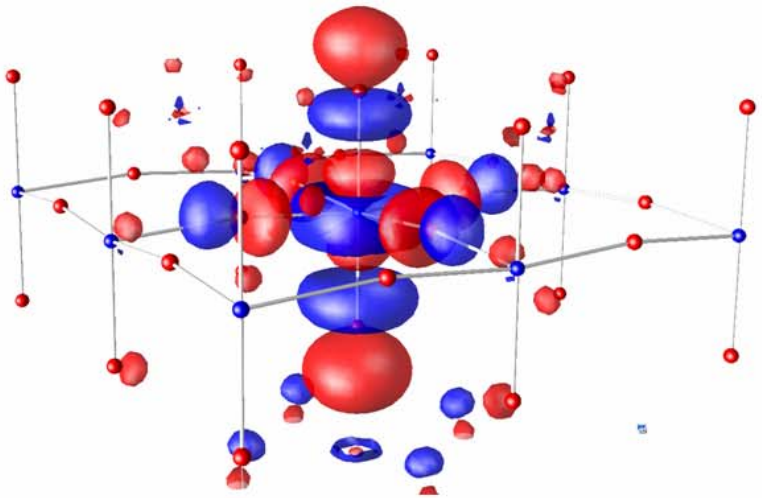
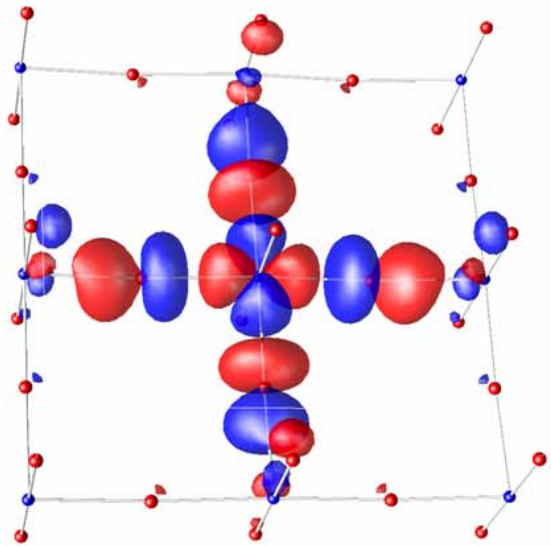
Designing nickelates that look like cuprates



$3d^7(e_g^1)$

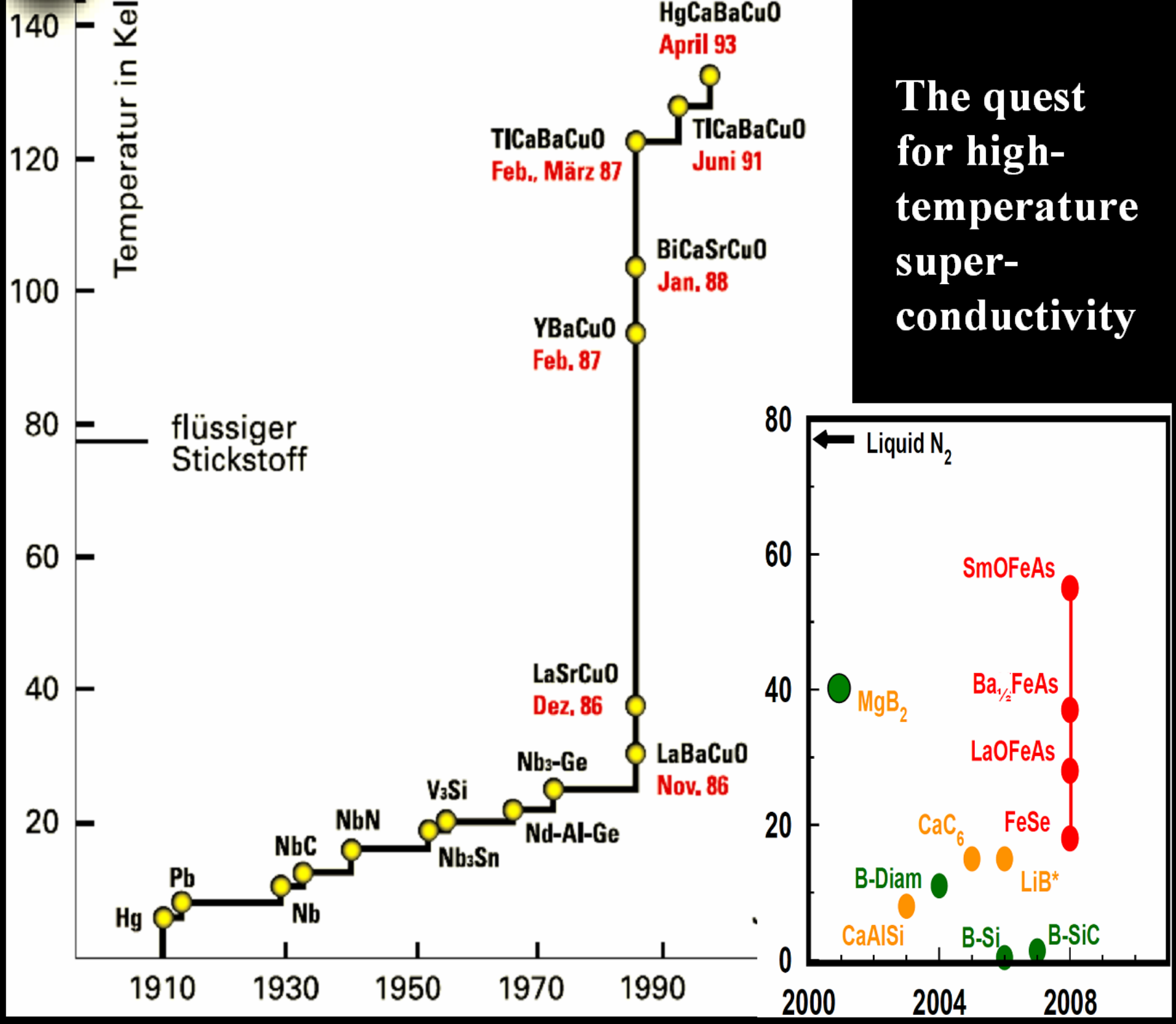


$3z^2$-1 x^2-y^2

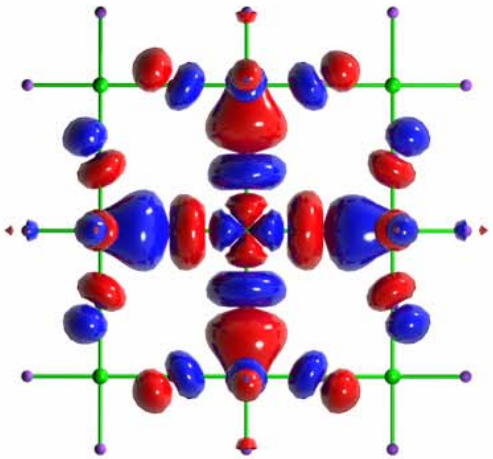
Xiaoping Yang[1], P. Hansmann[2], A. Toschi[2], K. Held[2], G. Khaliullin[1], O. K. Andersen[1]

[1] Max-Planck-Institut für Festkörperforschung, Stuttgart
[2] Institute for Solid State Physics, Vienna University of Technology

The quest for high-temperature super-conductivity



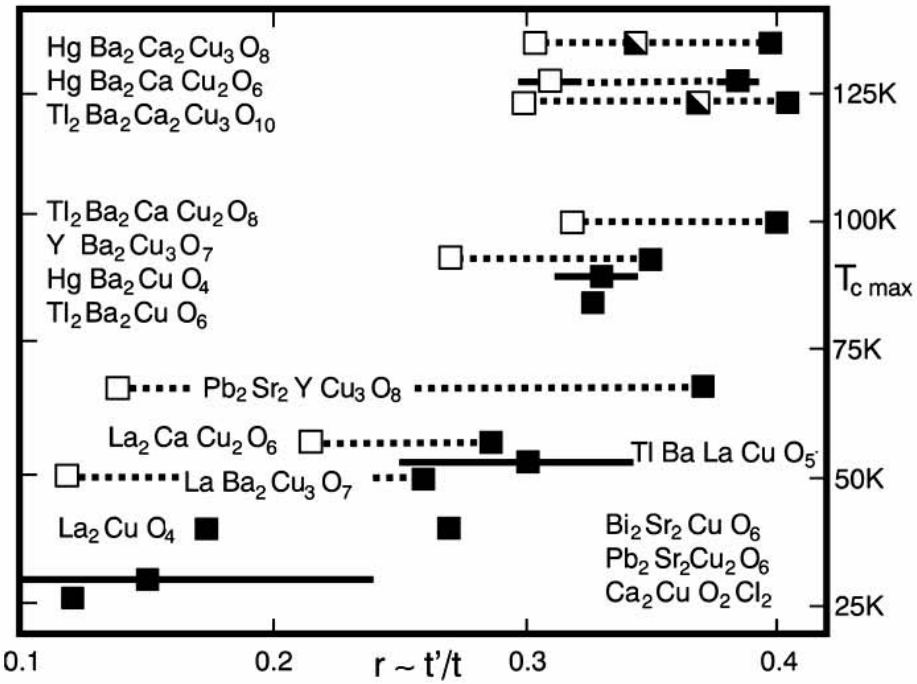
Cuprates $3d^{9-h} = 3d_{x^2-y^2}{}^{1-h}$

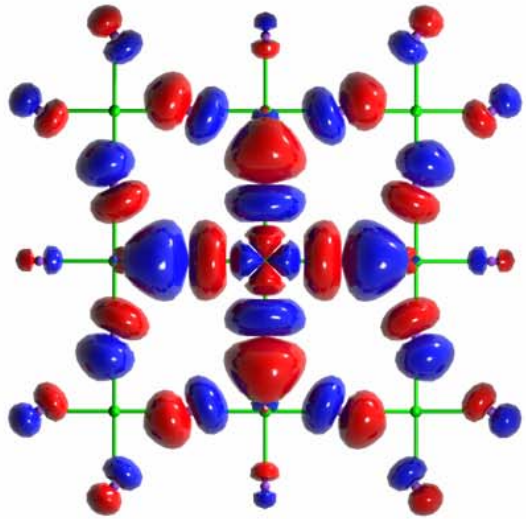


La_2CuO_4

r = 0.17, $T_{c\,max}$ = 40 K

The Materials Trend, PRL **87**, 047003 (2001)

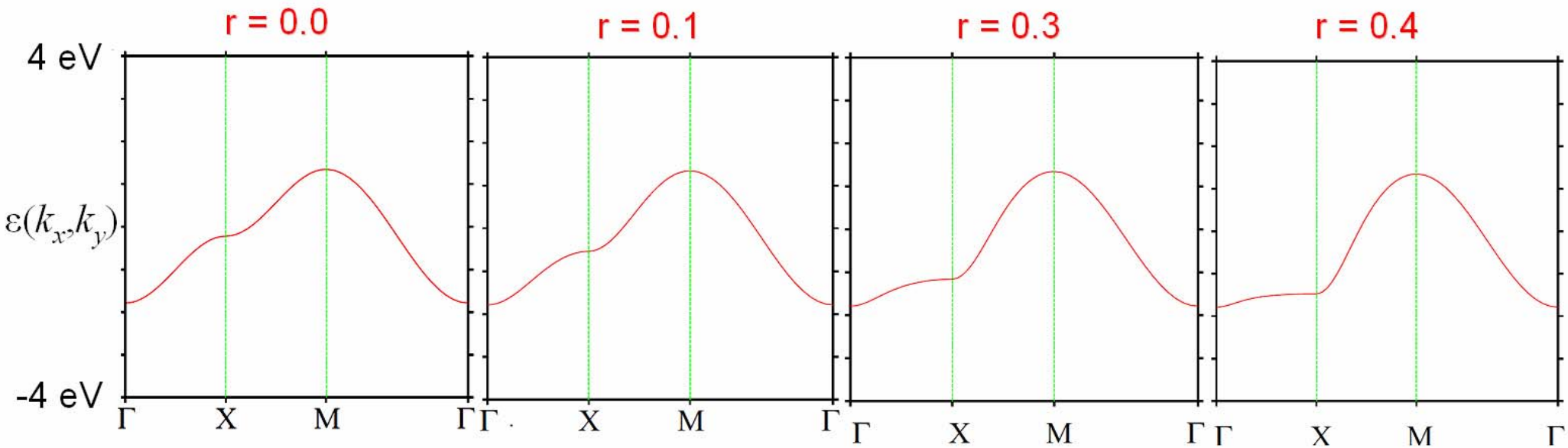




$HgBa_2CuO_4$

r = 0.33, $T_{c\,max}$ = 90 K

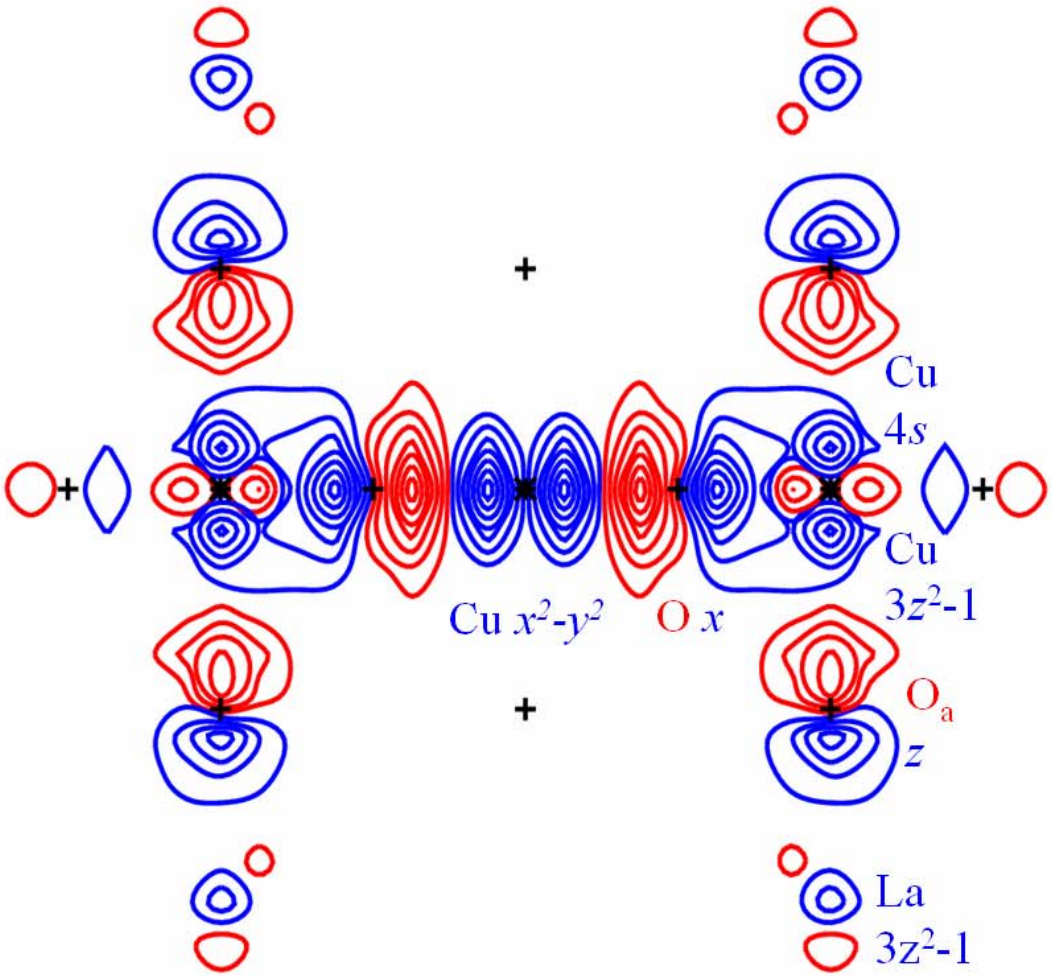
LDA conduction-band (x^2-y^2) shapes and exp Fermi surfaces for overdoped HTSCs



Which structural elements determine

$r \sim t'/t$

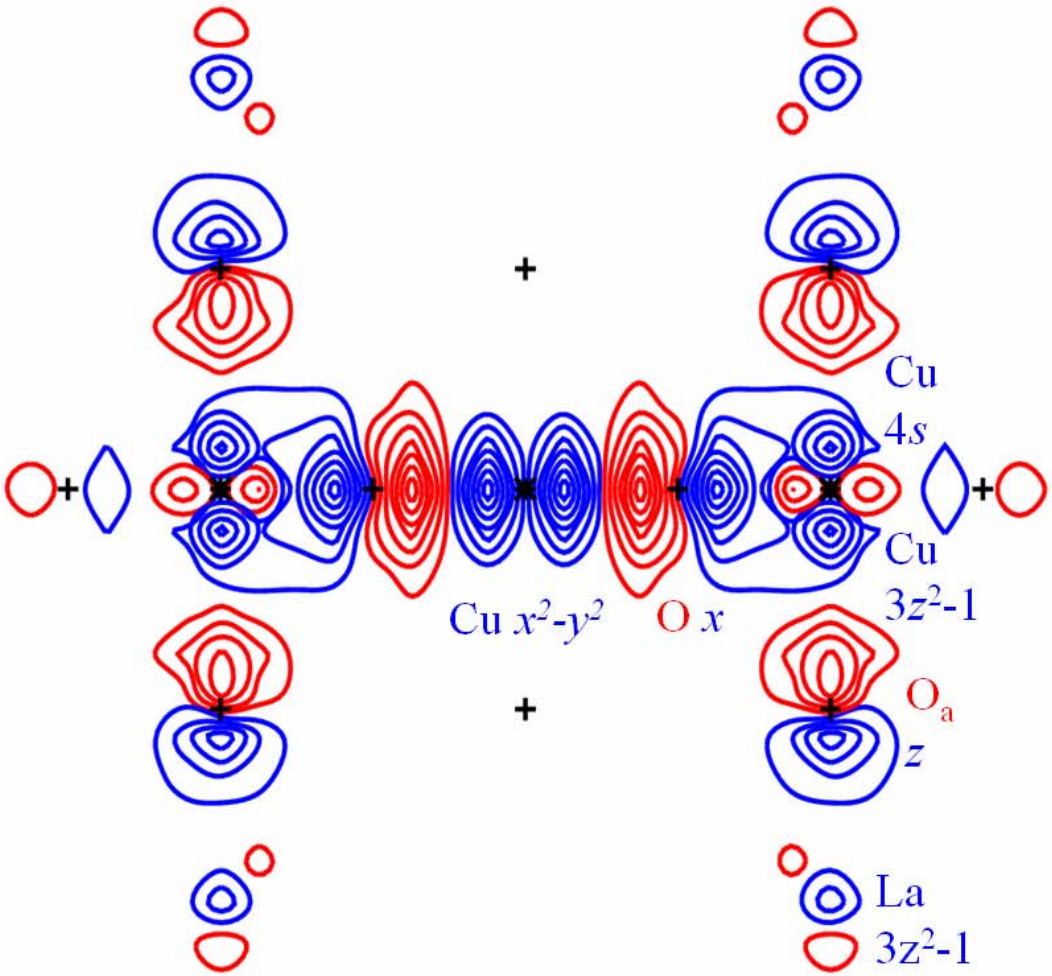
Wannier function for the cuprate conduction band



La_2CuO_4

Wannier function for the cuprate conduction band

The materials trend is best understood in terms of a tight-binding model with two orbitals:



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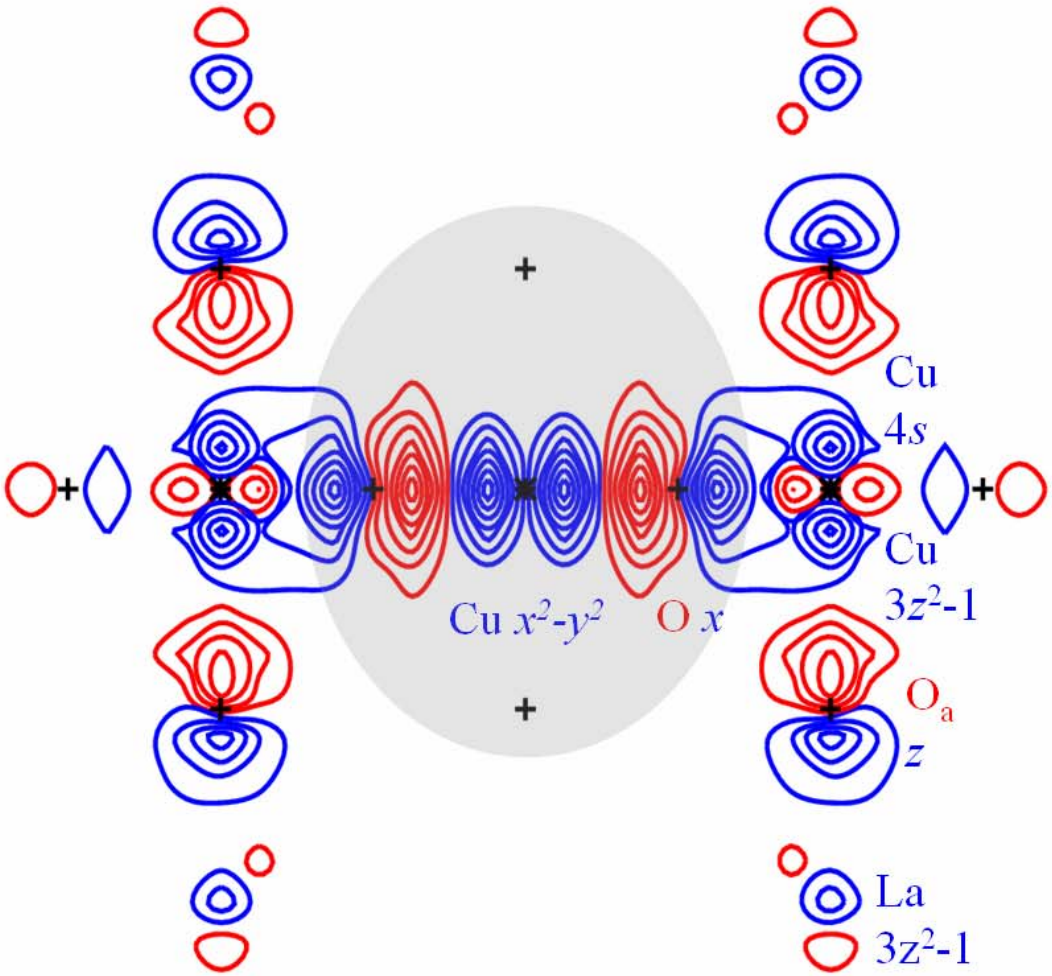

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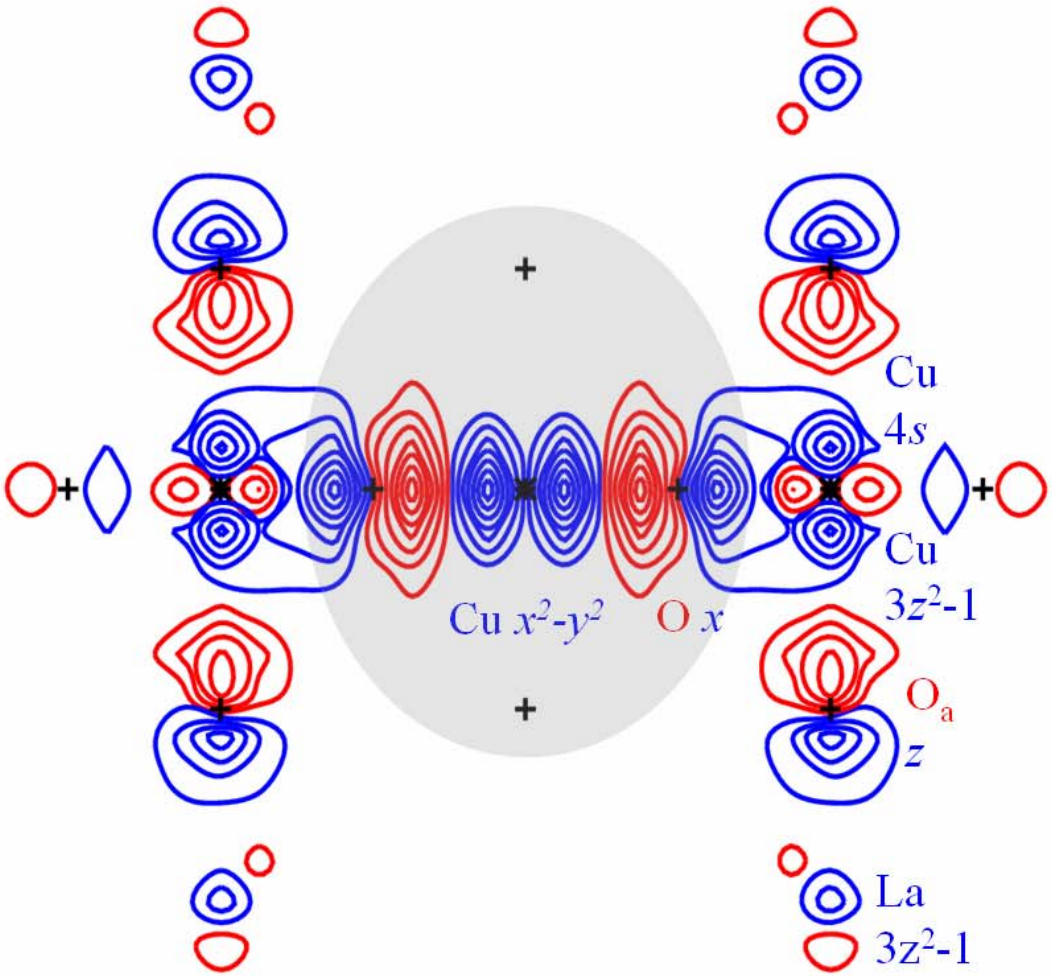

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***d* = Cu x^2-y^2**

dressed with

O *p*

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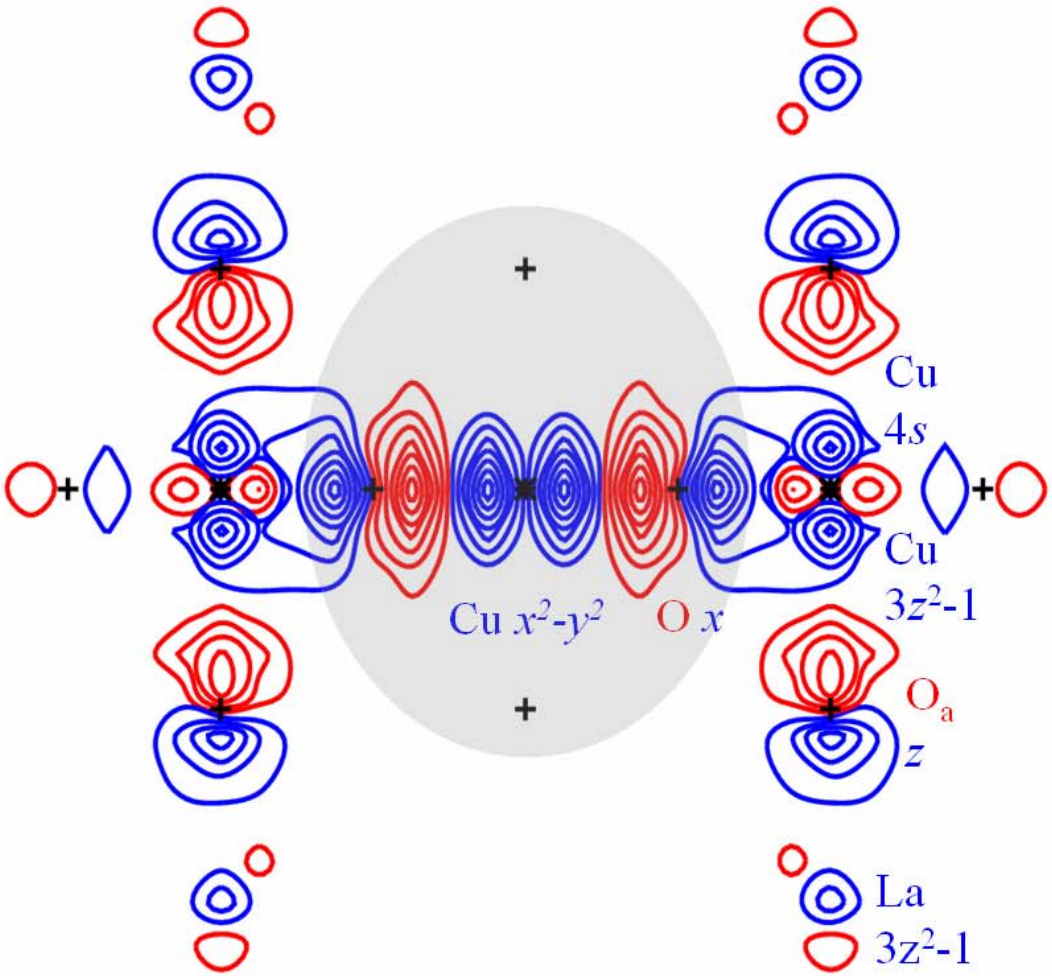

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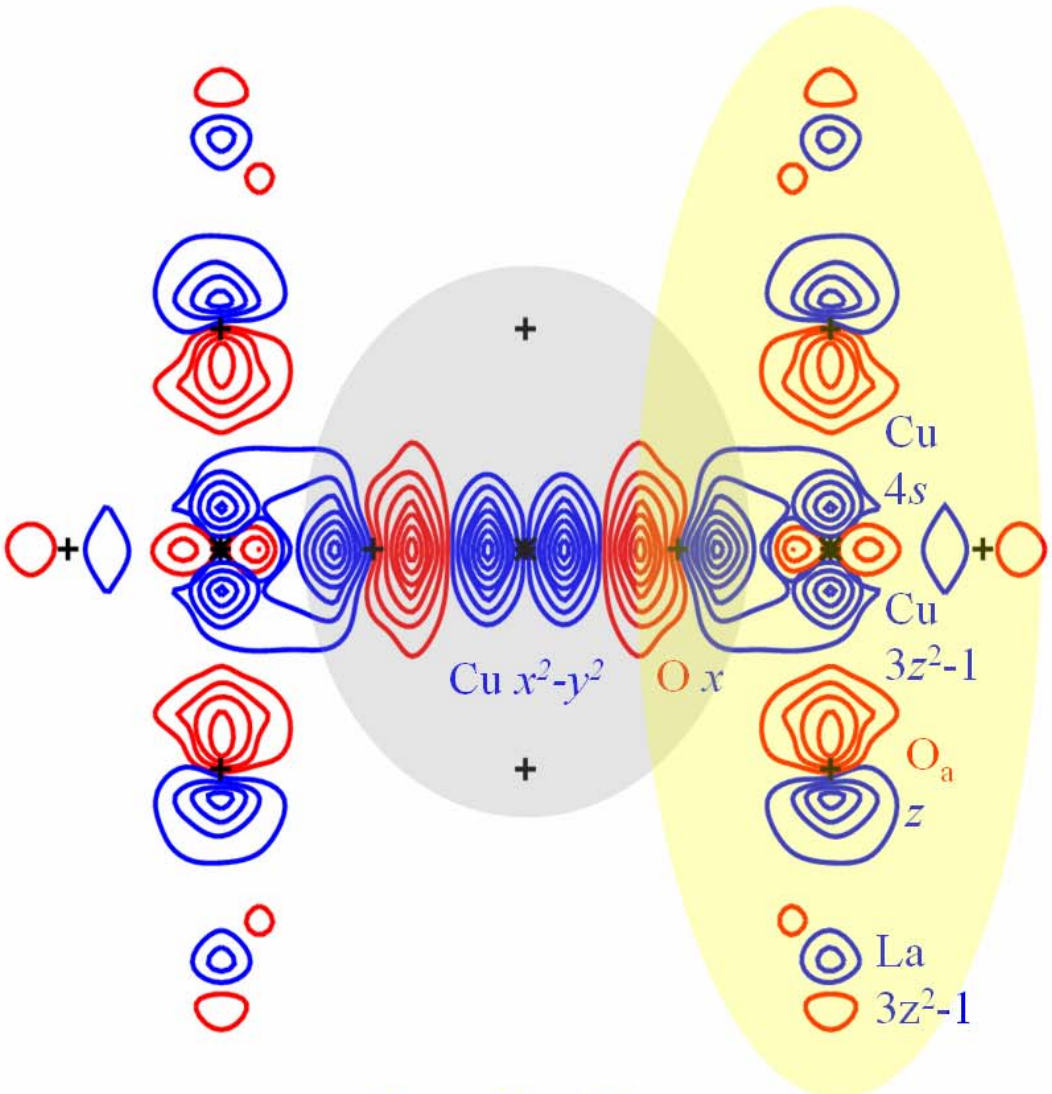

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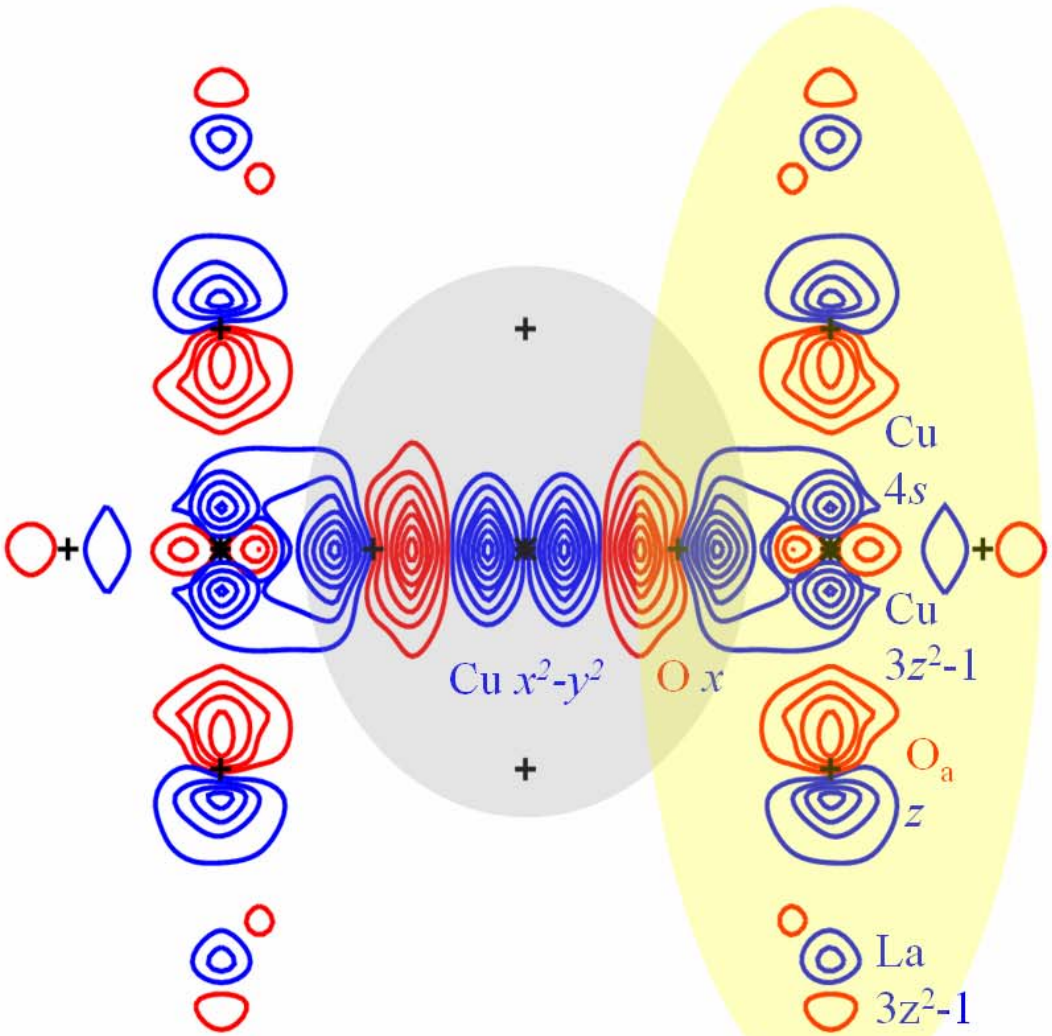

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d = Cu x^2-y^2

dressed with

O p

and

s = axial orbital = Cu 4s

dressed with

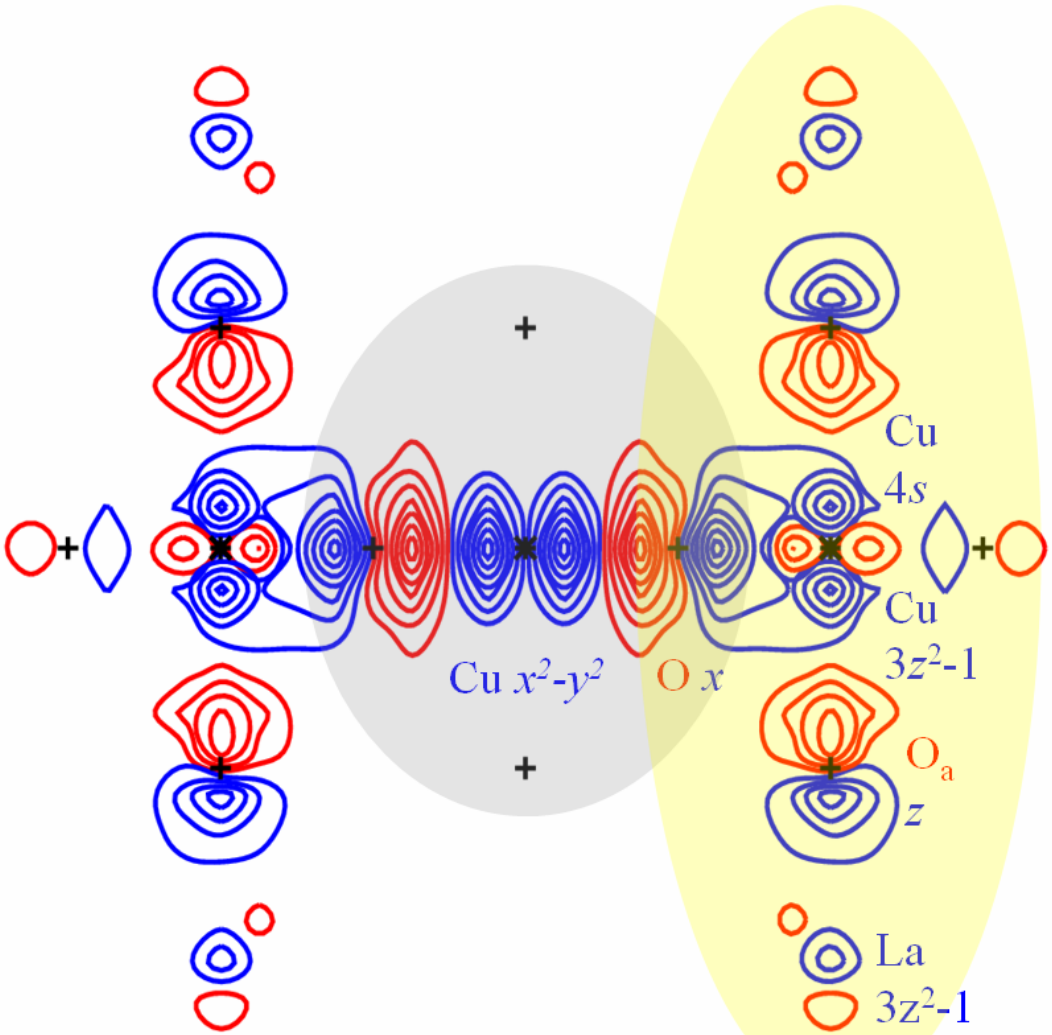
Cu $3z^2$-1,

O_a z,

La $3z^2$-1, a.s.o.

The material-dependent parameter is $\varepsilon_s - \varepsilon_F$ (> 0) . The smaller it is, the larger is $r \sim t'/t$.

Wannier function for the cuprate conduction band



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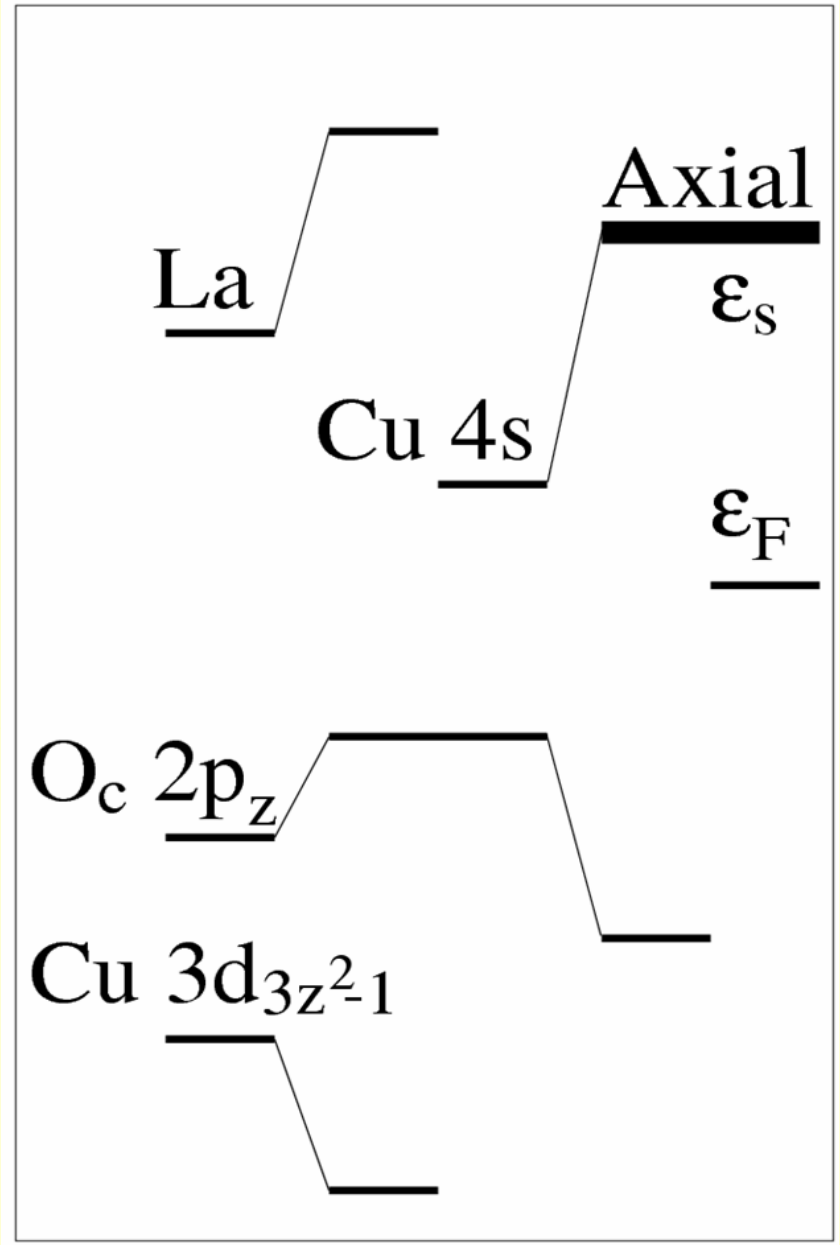

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La_2CuO_4

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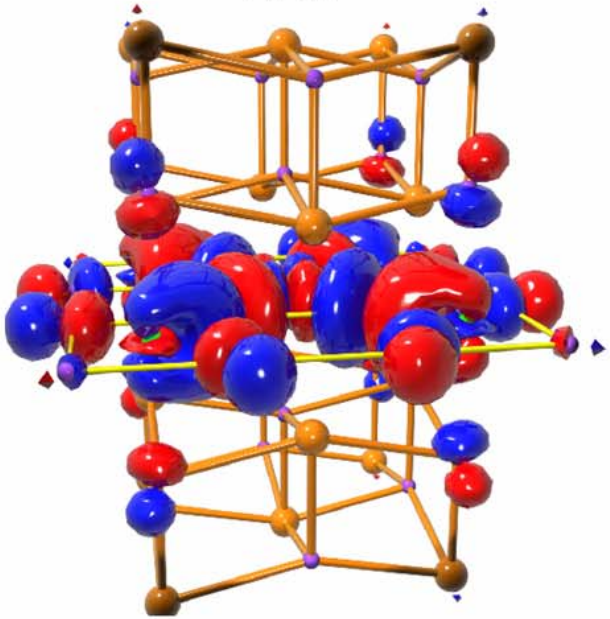
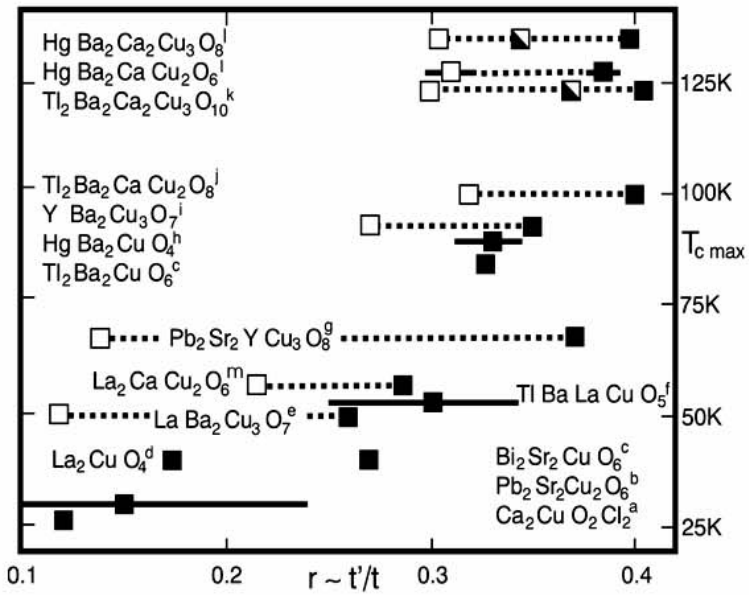
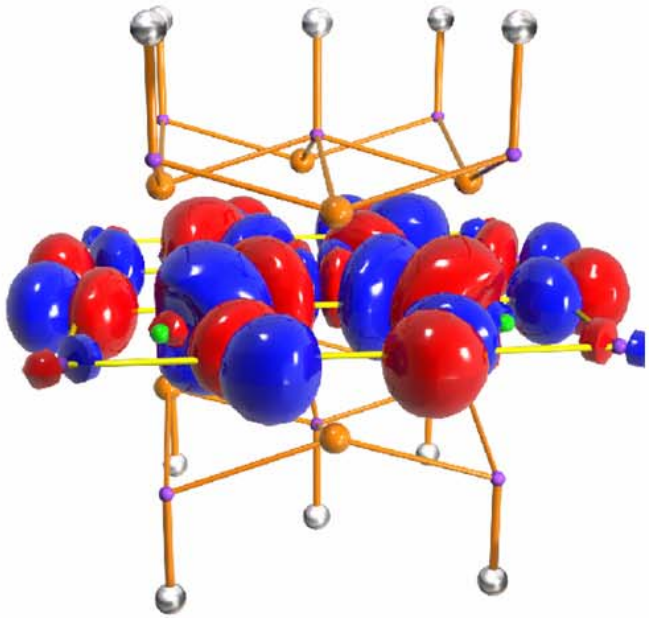
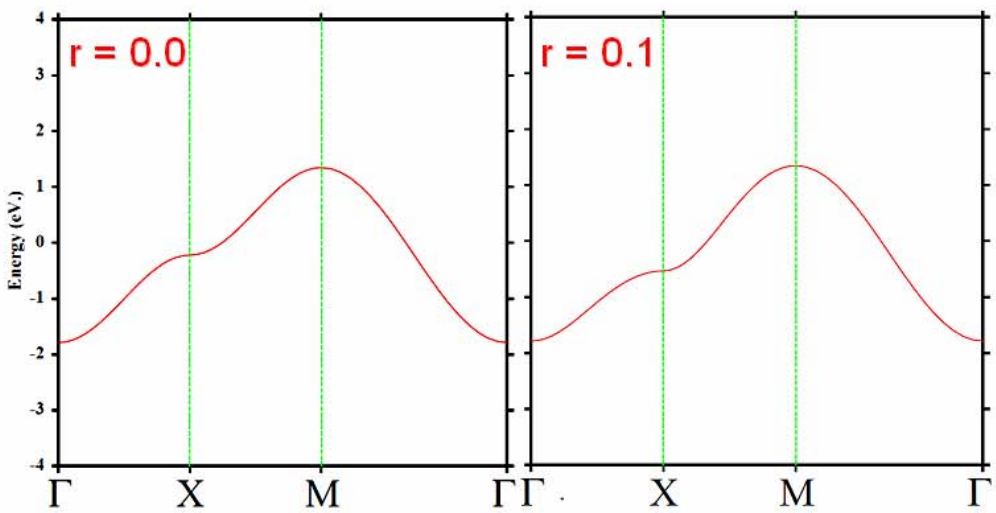


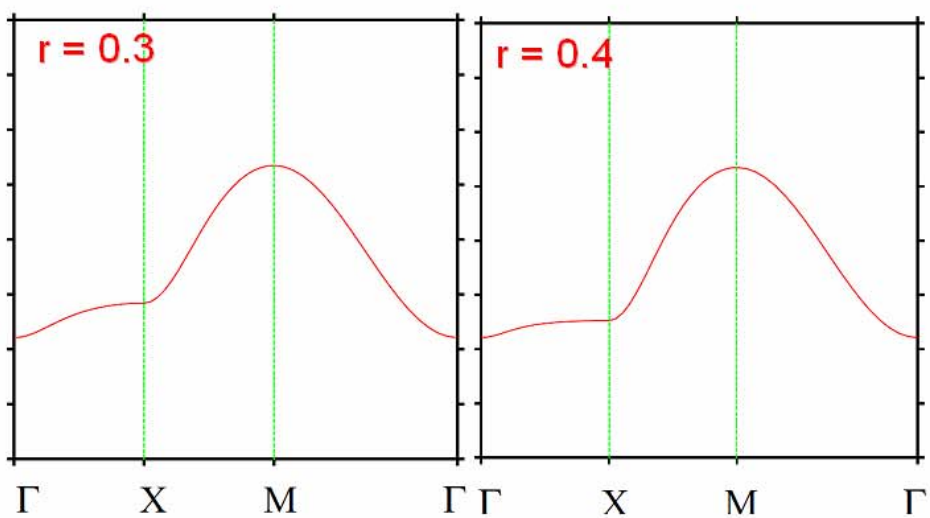


$HgBa_2CuO_4$

90 K



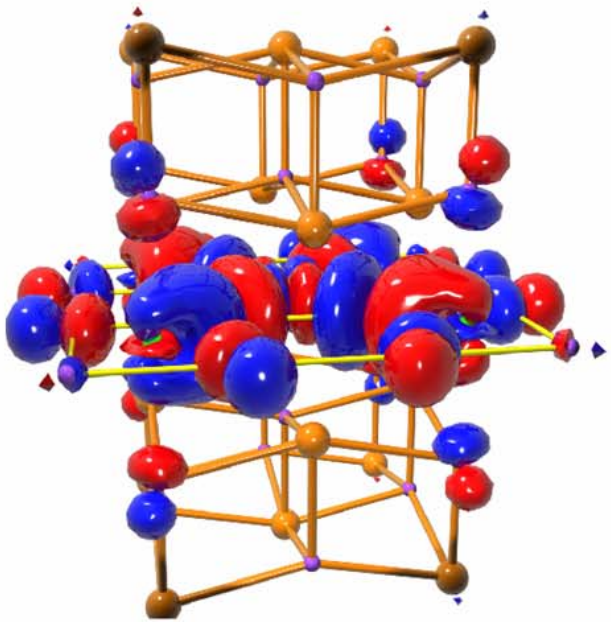


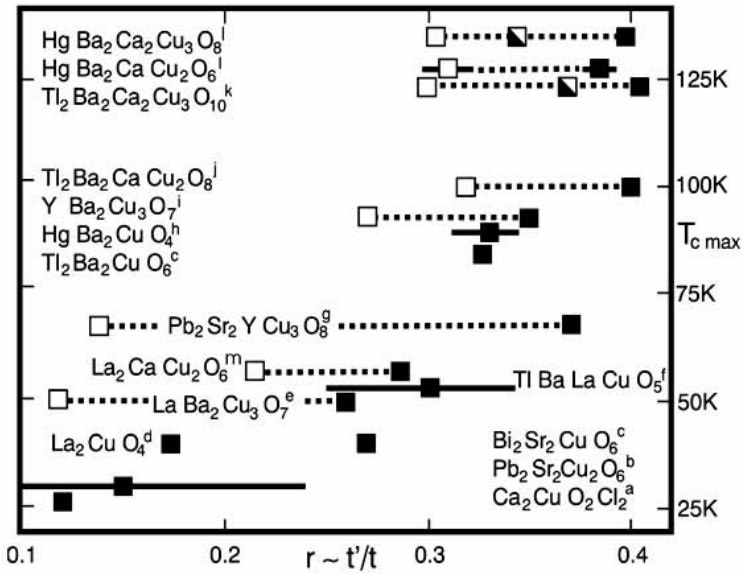


No
hybridization

Maximal
hybridization

La_2CuO_4





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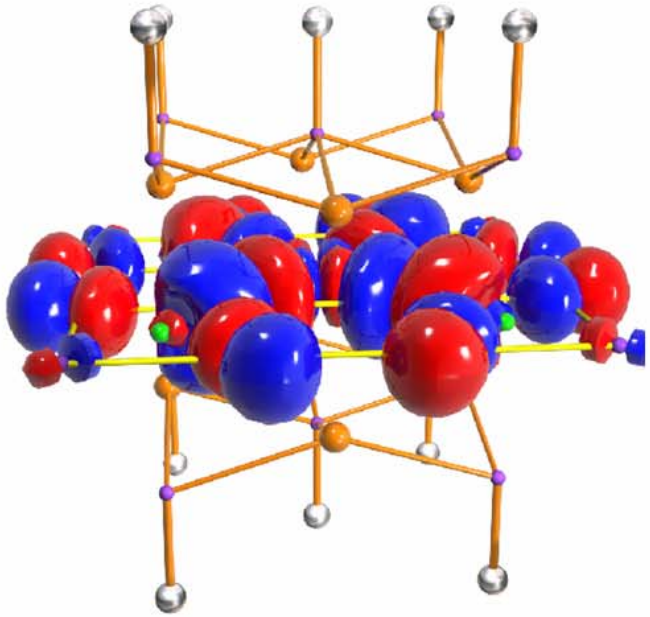
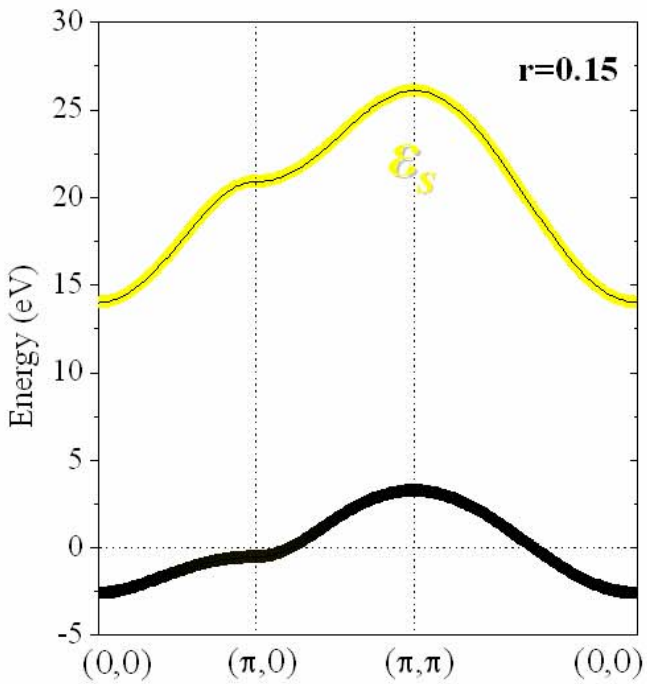
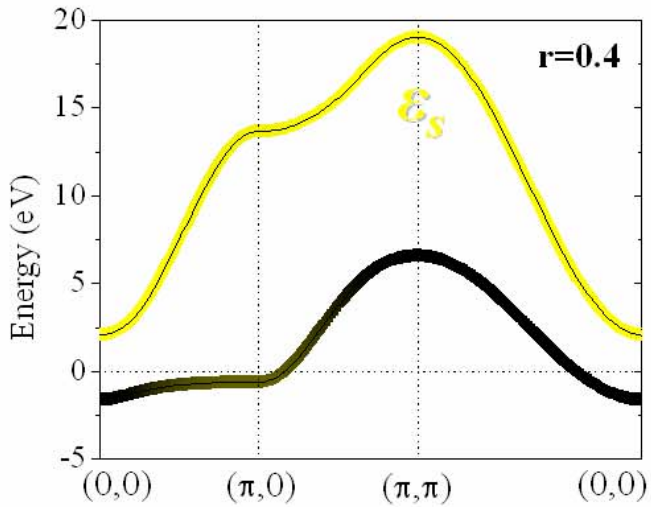




Axial 4*s*-like orbital

and x^2-y^2



These were the band structures of known families of HTSC cuprates.

Can we engineer them to get further ?

Khaliullin's idea:

J. Chaloupka and G. Khaliullin, PRL 100, 016404 (2008)

Make $Ni^{3+}(d^7)$-based HTSCs by sandwiching hole doped $LaO\text{-}NiO_2$ layers between insulating layers through heterostructuring (orbital engineering)

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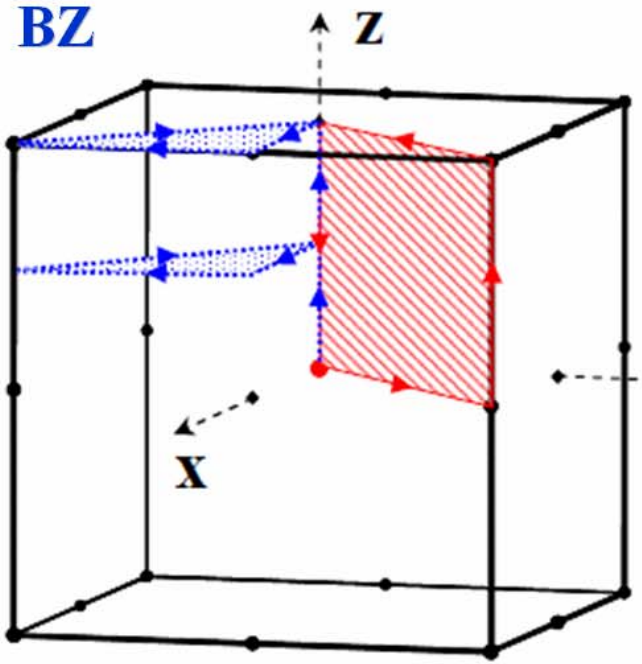
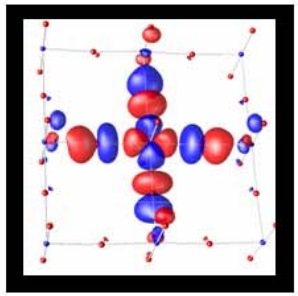
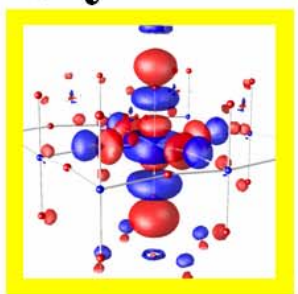
P. Hansmann, Xiaoping Yang, A. Toschi, G. Khaliullin, O.K. Andersen, K. Held, PRL 103, 016401 (2009); Xiaoping Yang et al to be published

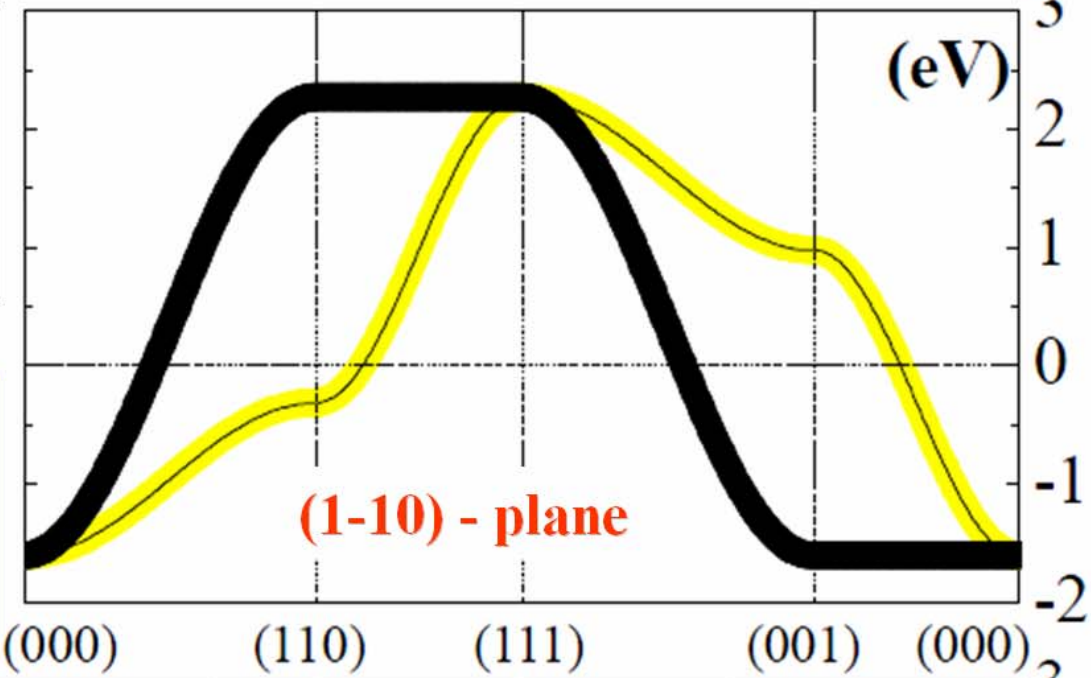
Confinement

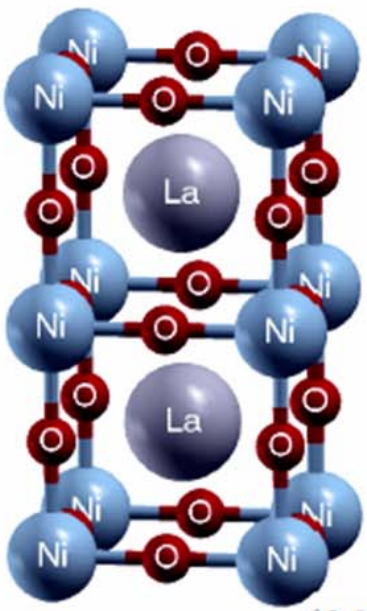
e_g bands of cubic bulk $LaNiO_3$

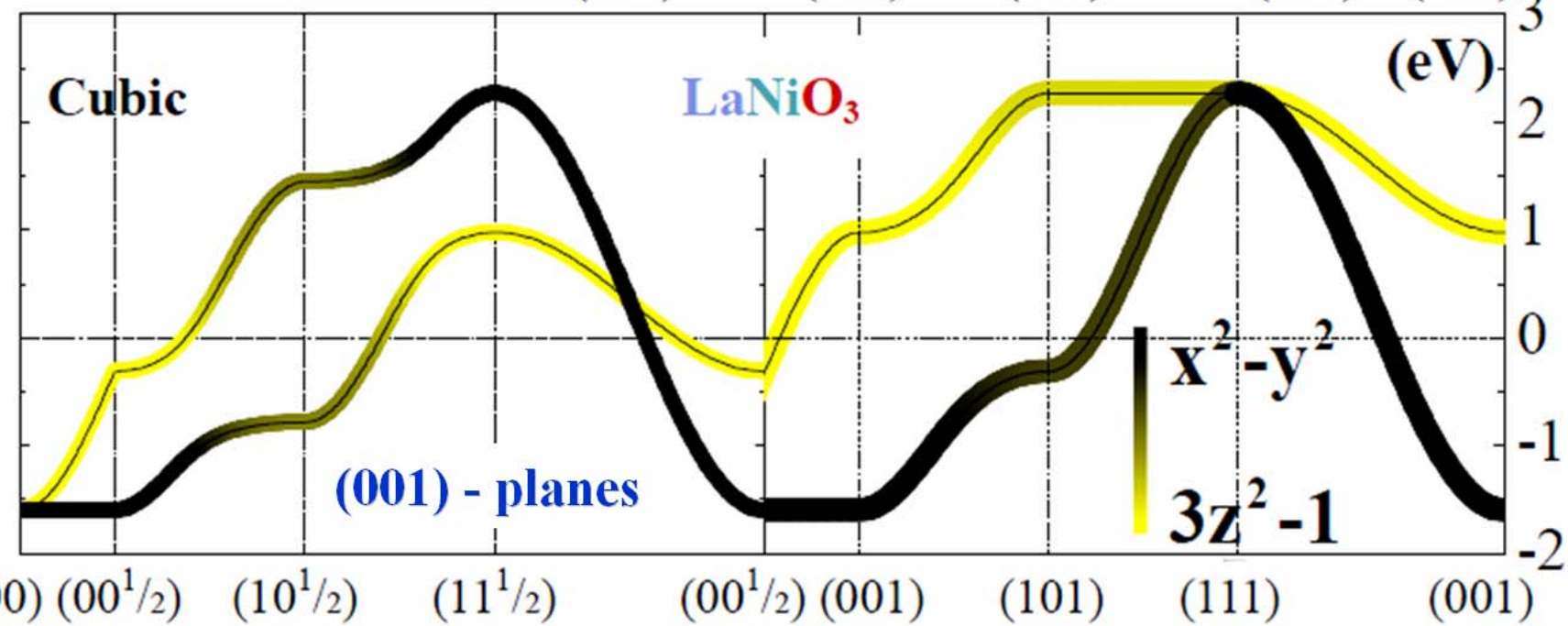




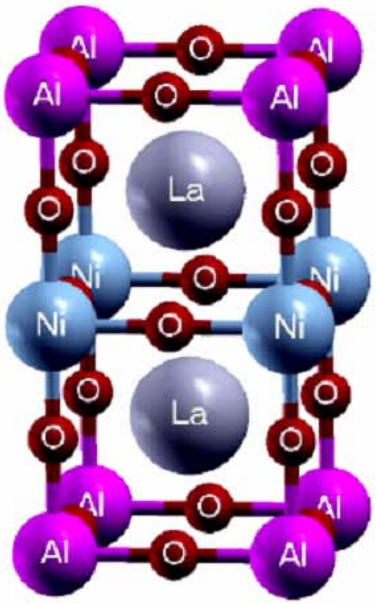






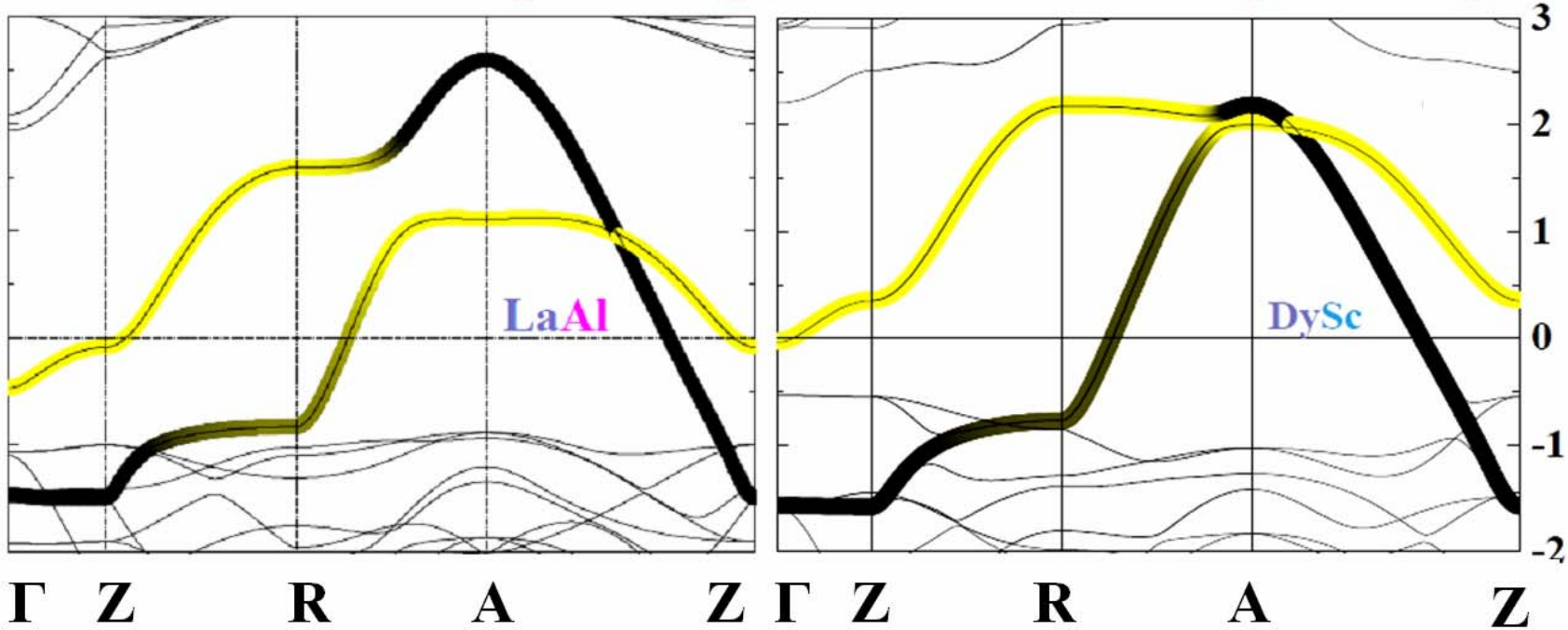


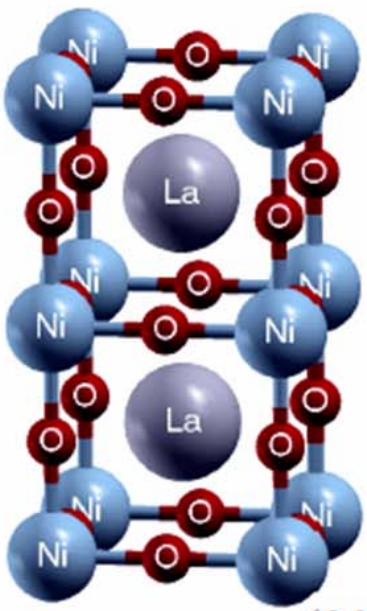
1/1 Heterostructures

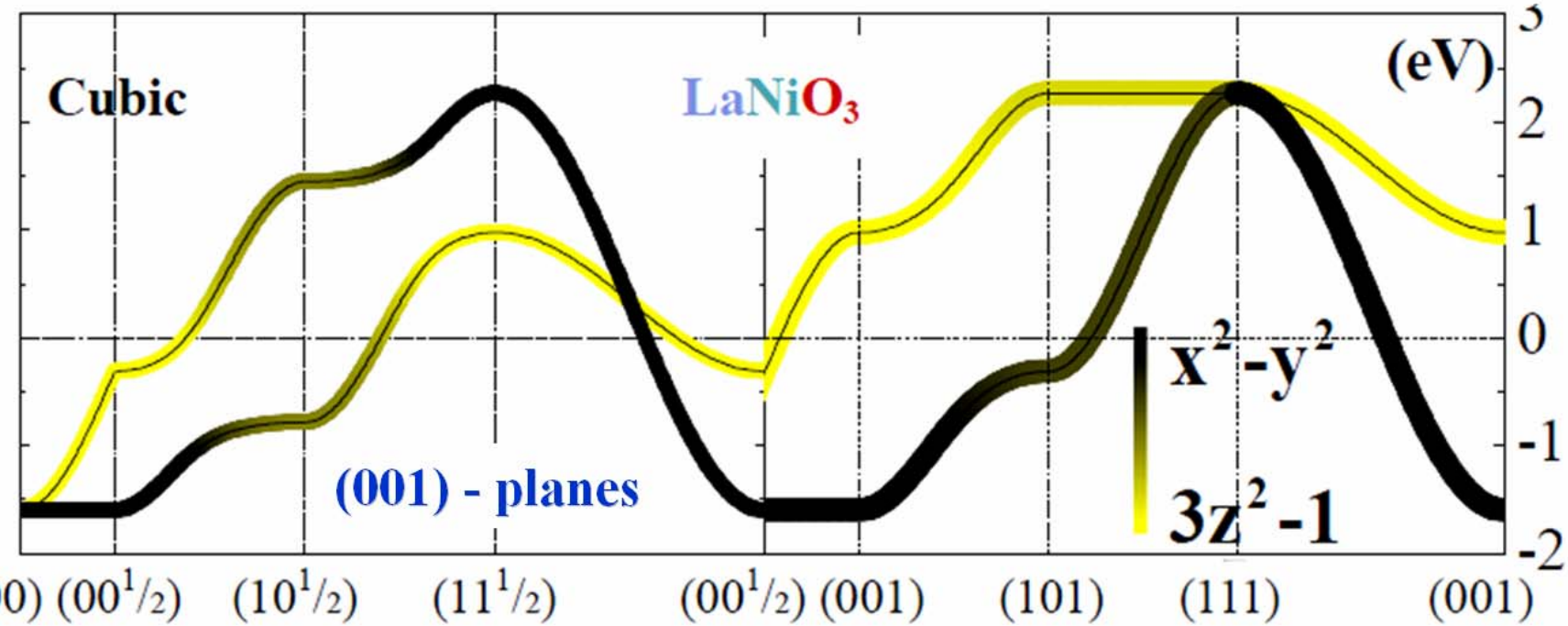


$LaNiO_3/LaAlO_3$

$LaNiO_3/DyScO_3$







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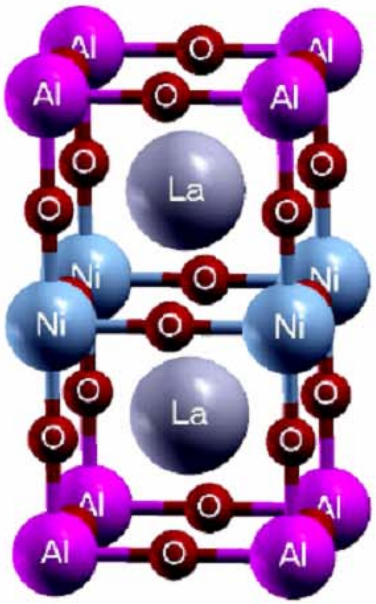

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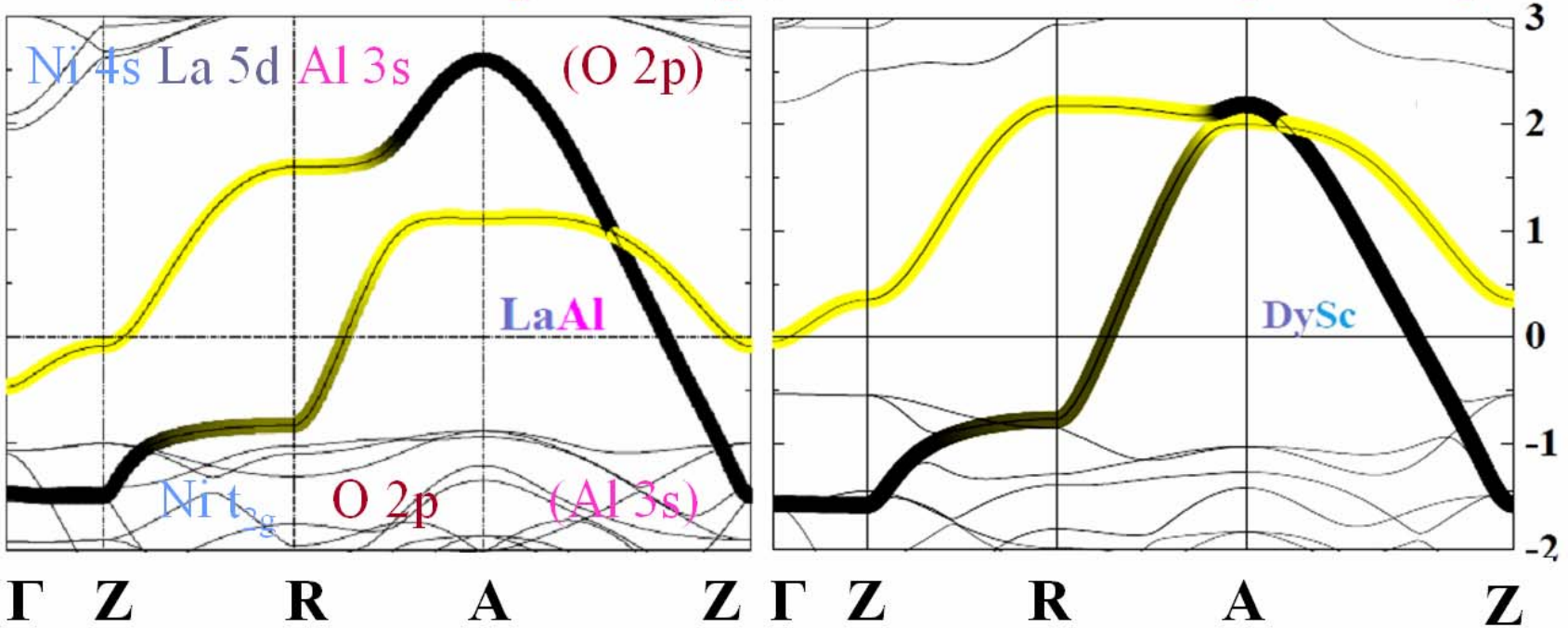

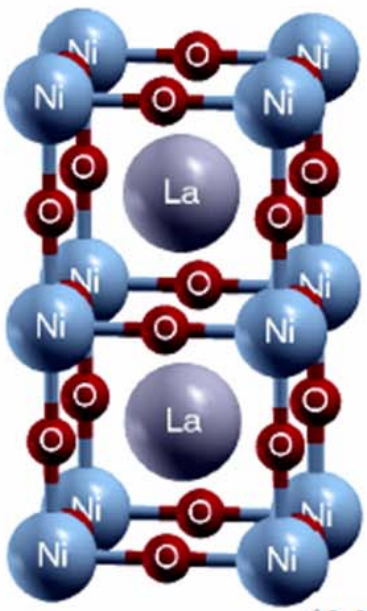

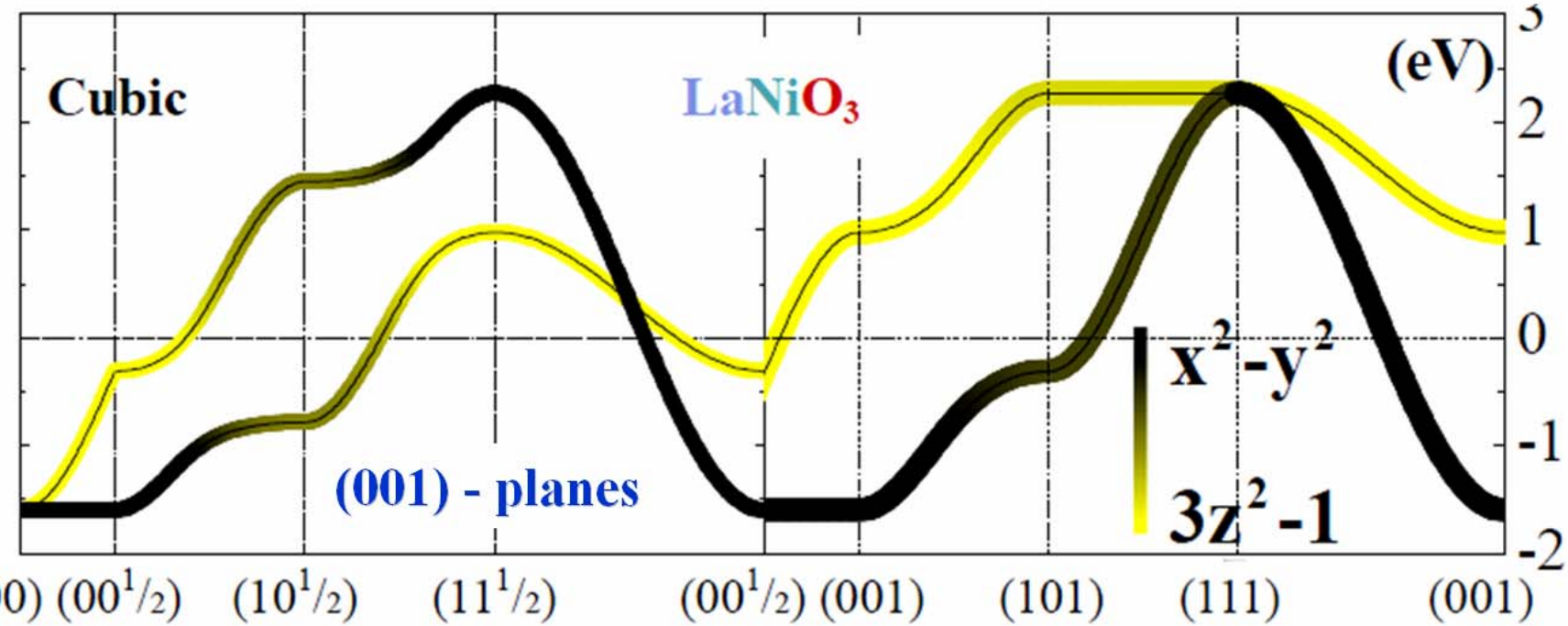

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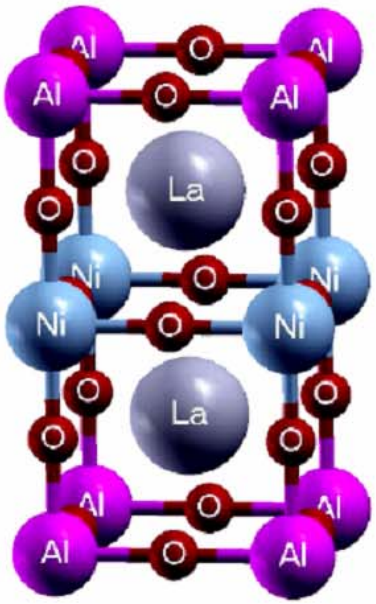

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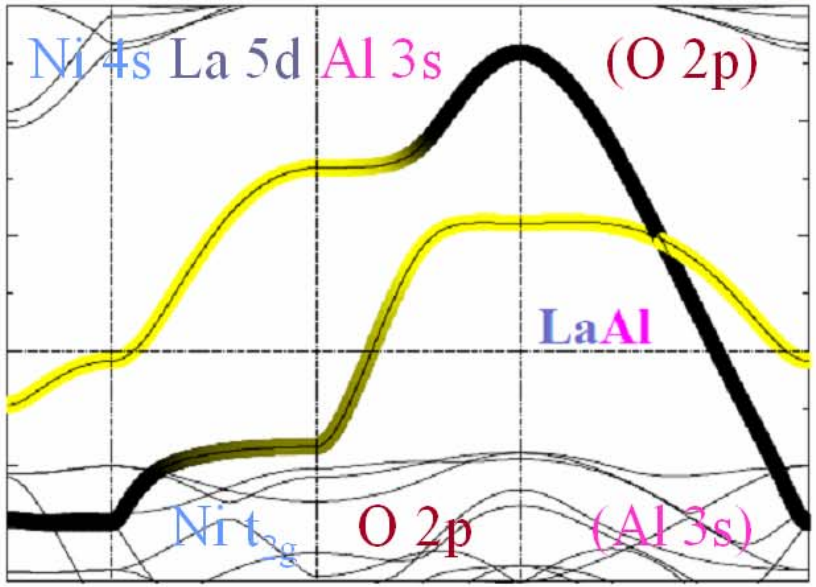
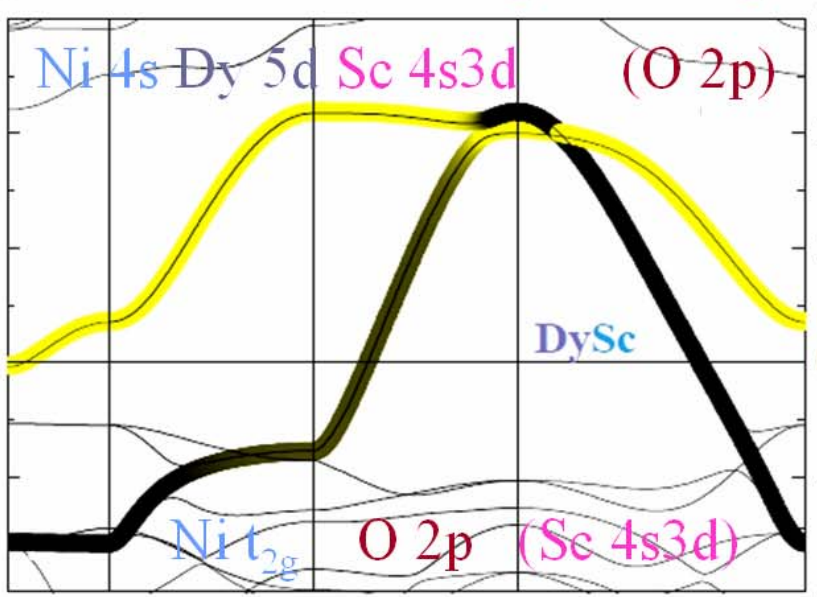
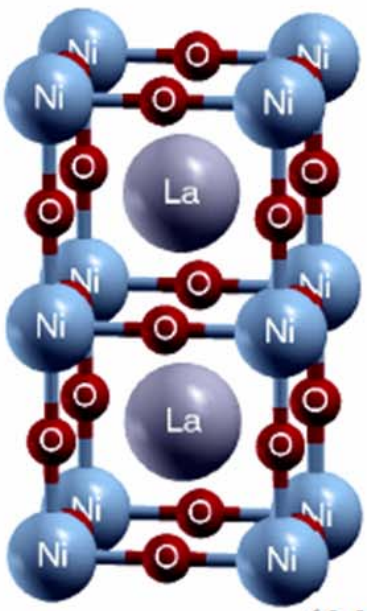
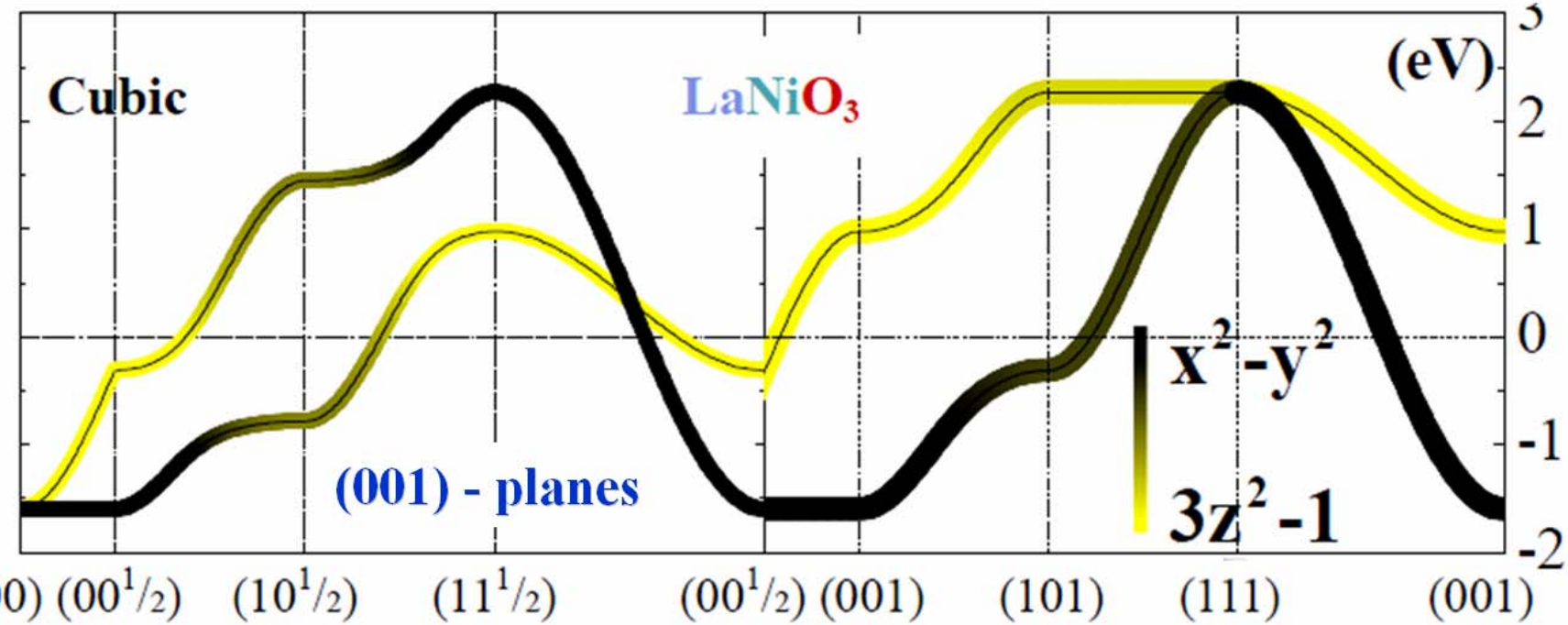


$LaNiO_3/DyScO_3$



Γ Z R A Z Γ Z R A Z





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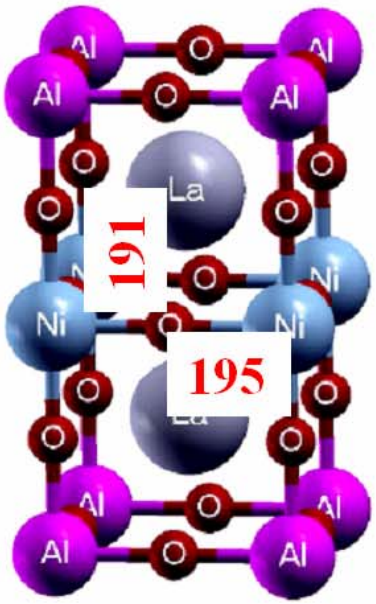
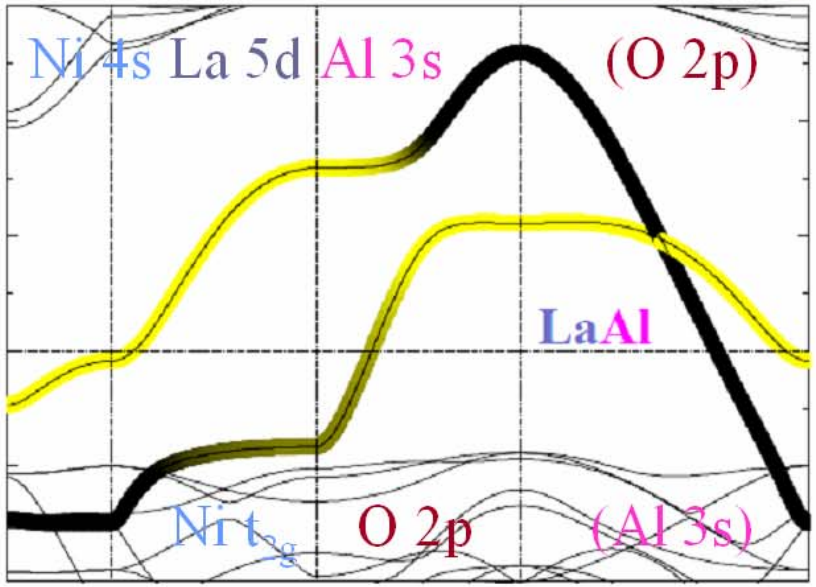
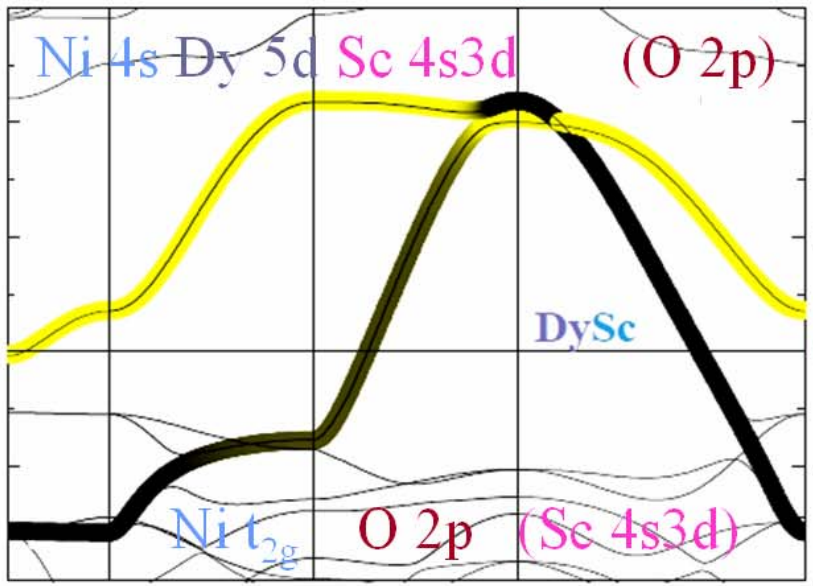
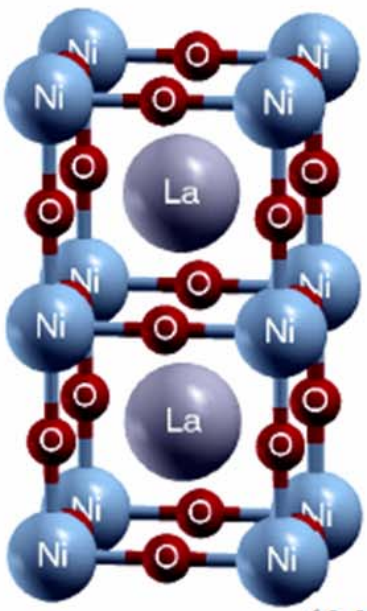
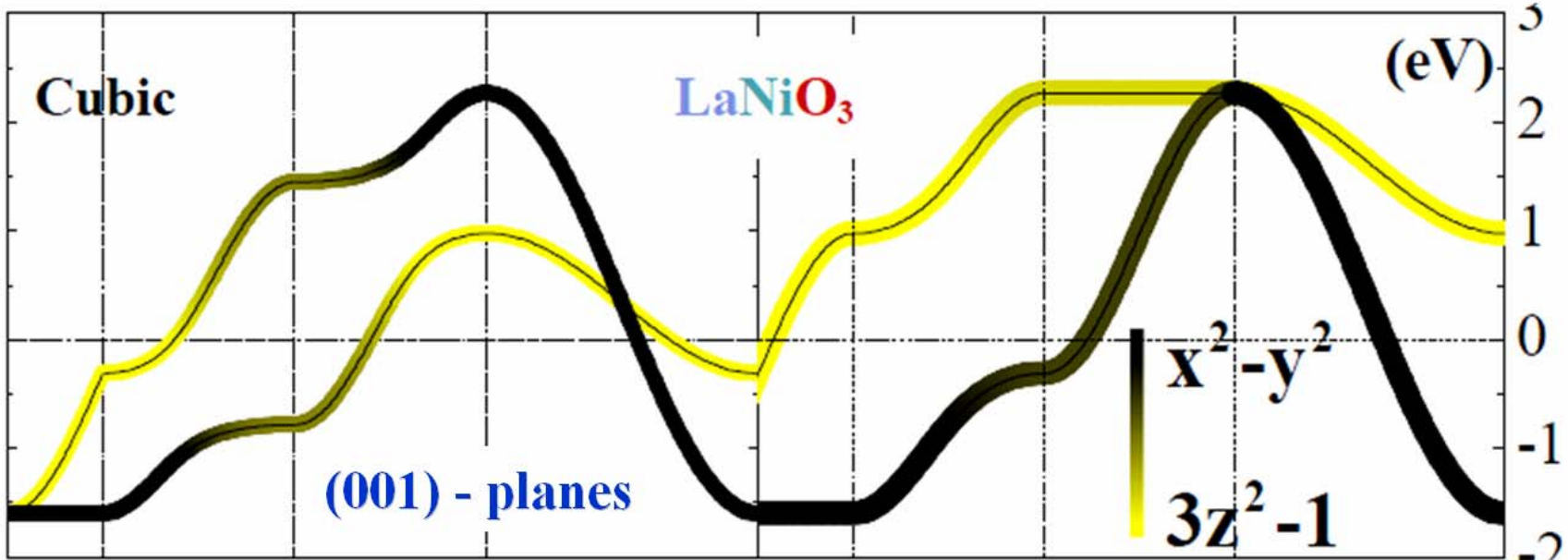




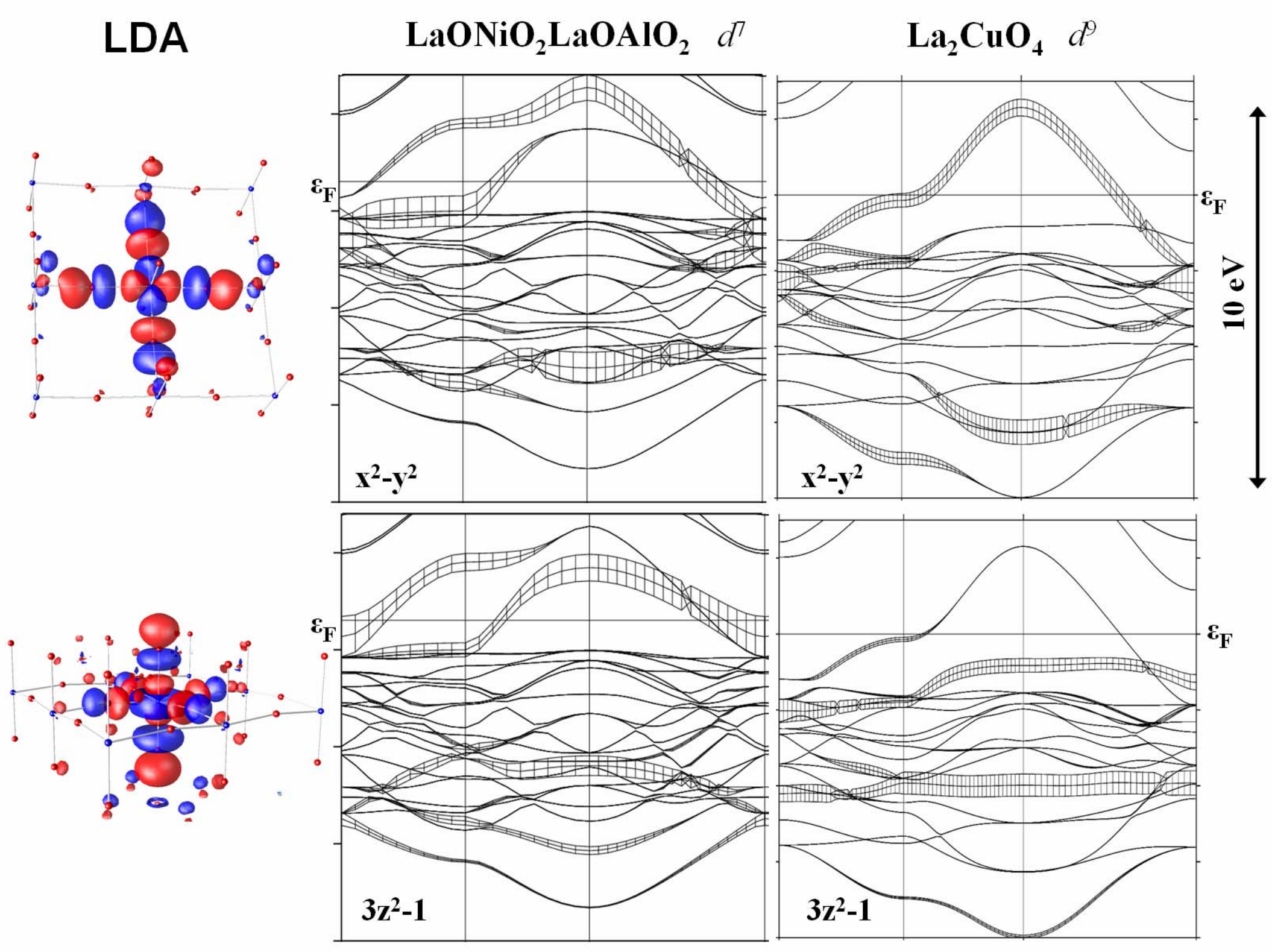


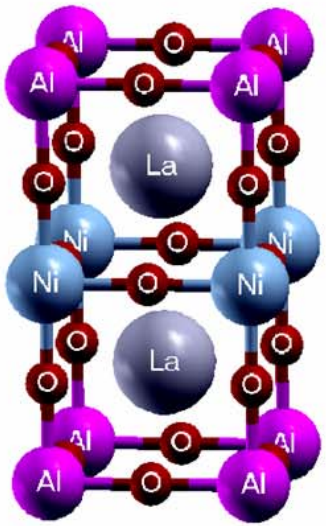
Γ Z R A Z Γ Z R A Z

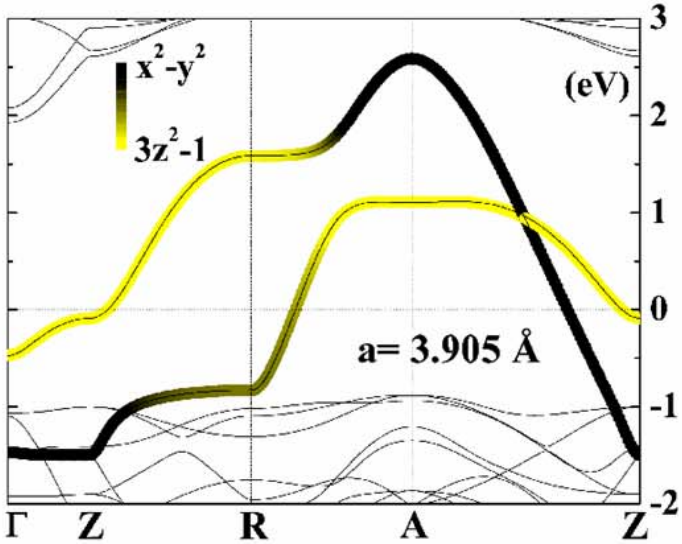


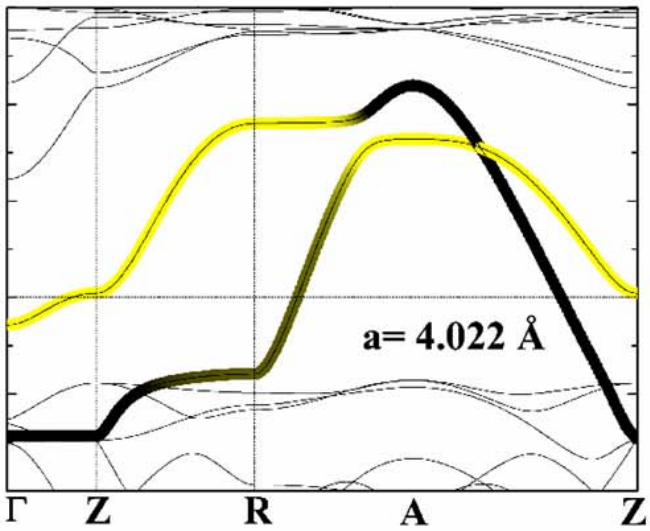


(000) (00^1/$_2$) (10^1/$_2$) (11^1/$_2$) (00^1/$_2$) (001) (101) (111) (001)


LDA
LaONiO2LaOAlO2 d7
La2CuO4 d9
εF
εF
x2-y2
x2-y2
10 eV
εF
εF
3z2-1
3z2-1

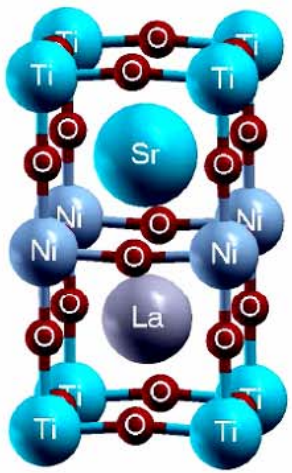


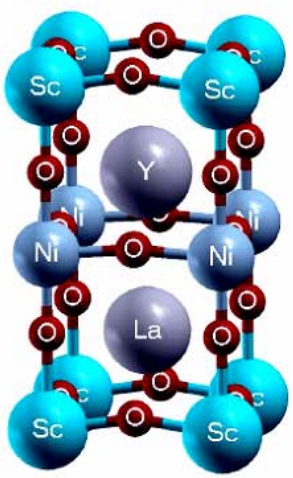


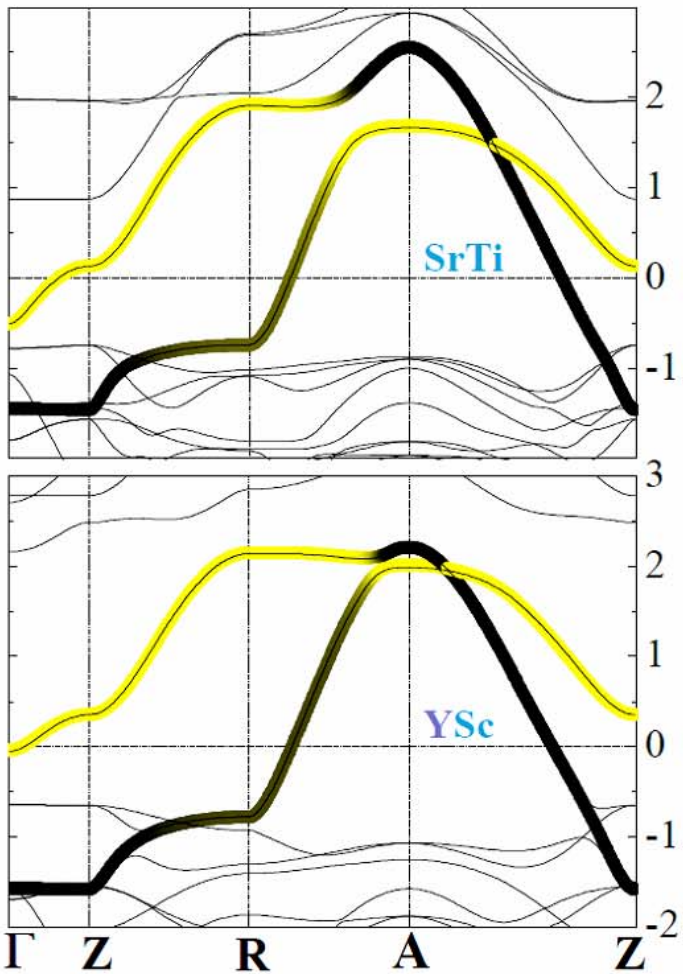


Control by lattice constant of the substrate

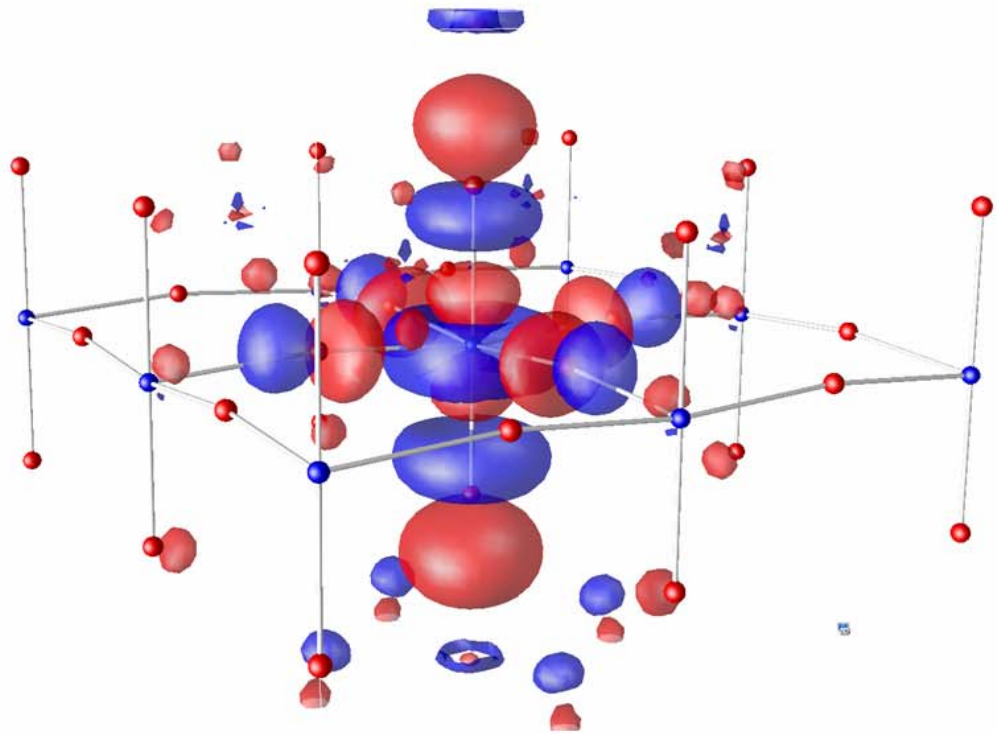
1-sheet FS:
5.7<*U*< 6.5 eV







Control by the chemistry (Al, Ti, Sc) of the insulating layers



LDA

LDA+DMFT

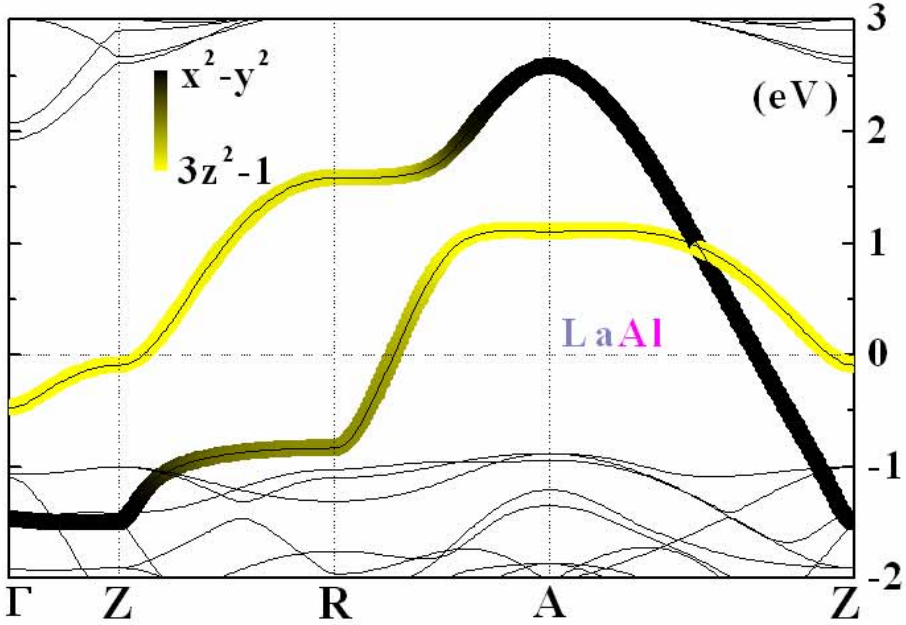
Undoped

U = 6.7 eV

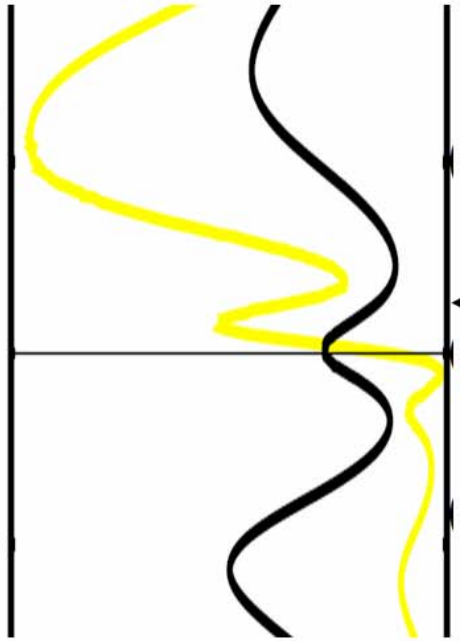
J = 0.7 eV,

T = 1100 K

Band structure



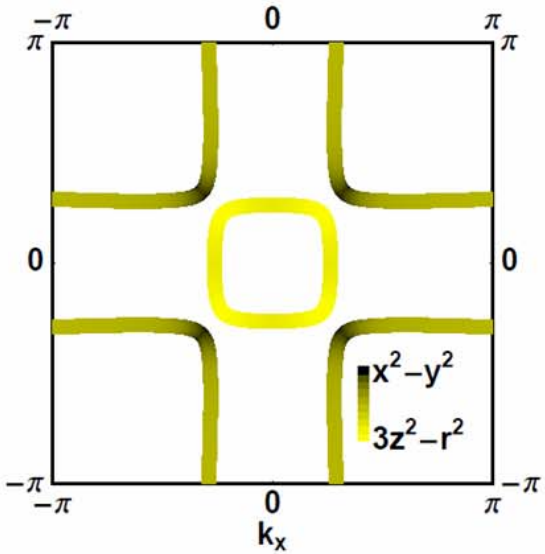
Spectral-density

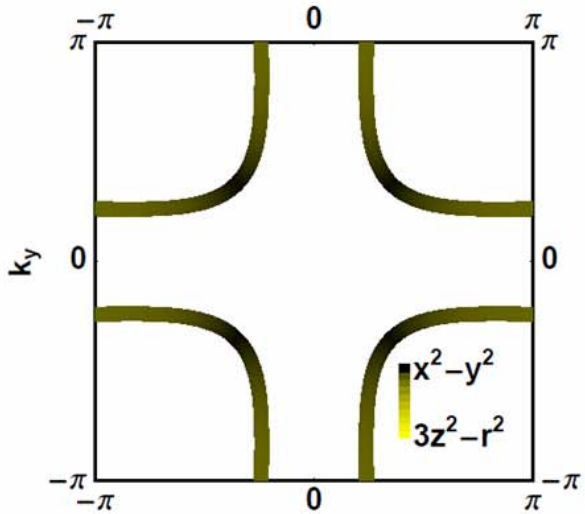


0 < U < 6.4 eV

two FS sheets.

Fermi surface





6.4 < U < 7.4

one FS sheet.

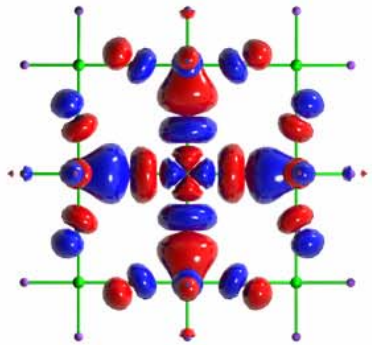
7.4 < U

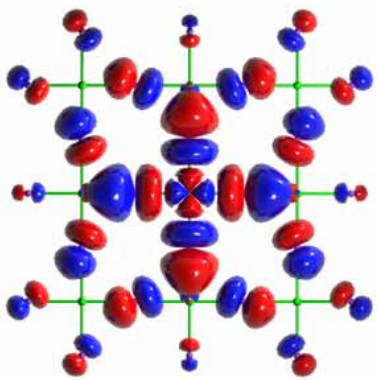
no FS; Mott ins.

The Coulomb correlations enhance the crystal-field splitting and simplifies the Fermi surface to one sheet when $\varepsilon_{3z^2-1}(\Gamma) > \varepsilon_F$, i.e. with a shape ($r \sim ½$), like that in the cuprates with the highest T_{cmax}

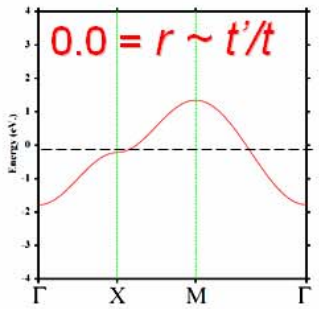
Cuprates $3d^{9-x} = 3d_{x^2-y^2}{}^{1-x}$

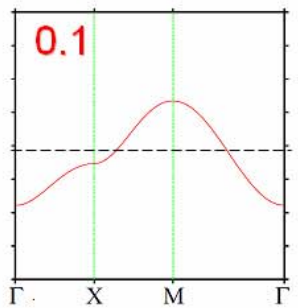
Conduction band LDA

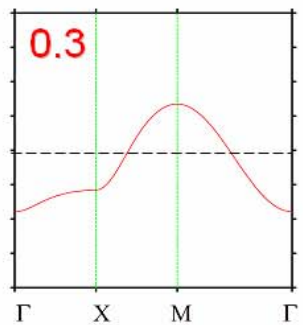


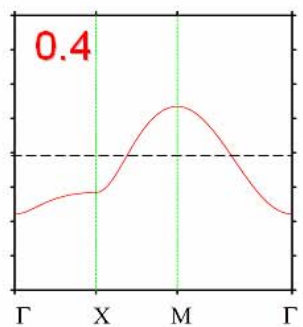


T. Saha-Dasgupta and OKA 2002





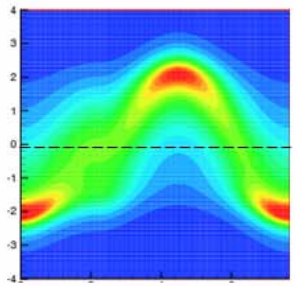


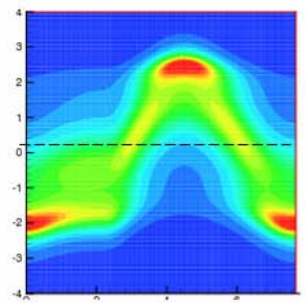


One-band Hubbard model LDA+DMFT

U =2.1 eV

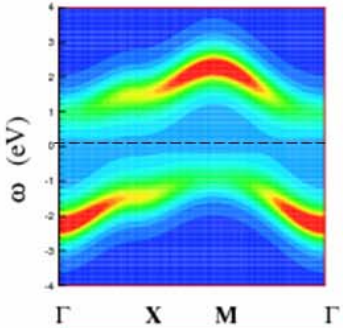
undoped

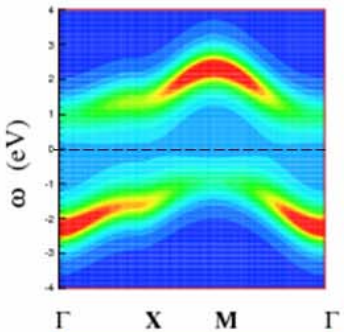


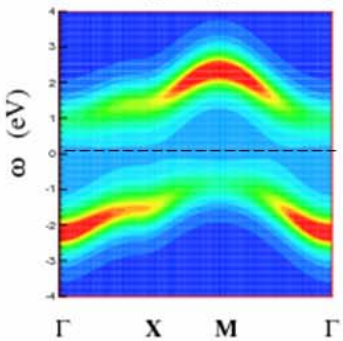


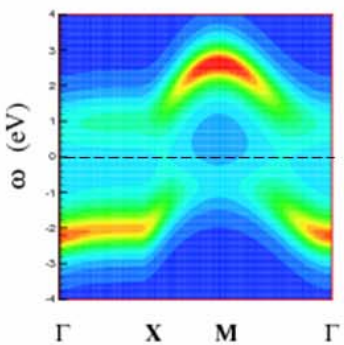
U = 3.0 eV

undoped

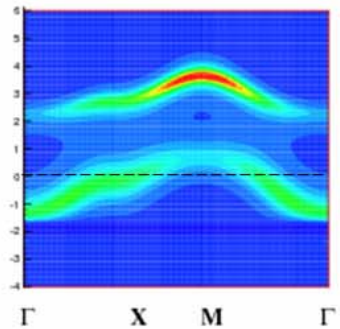


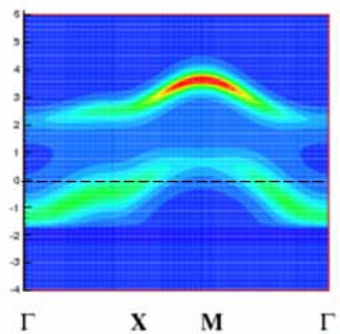


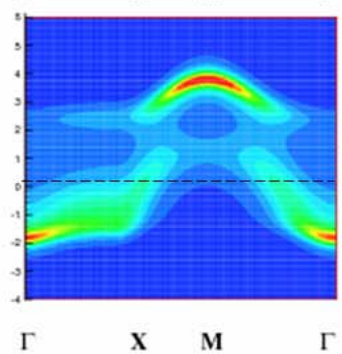


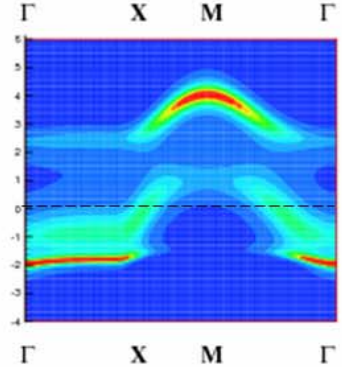


10% doped









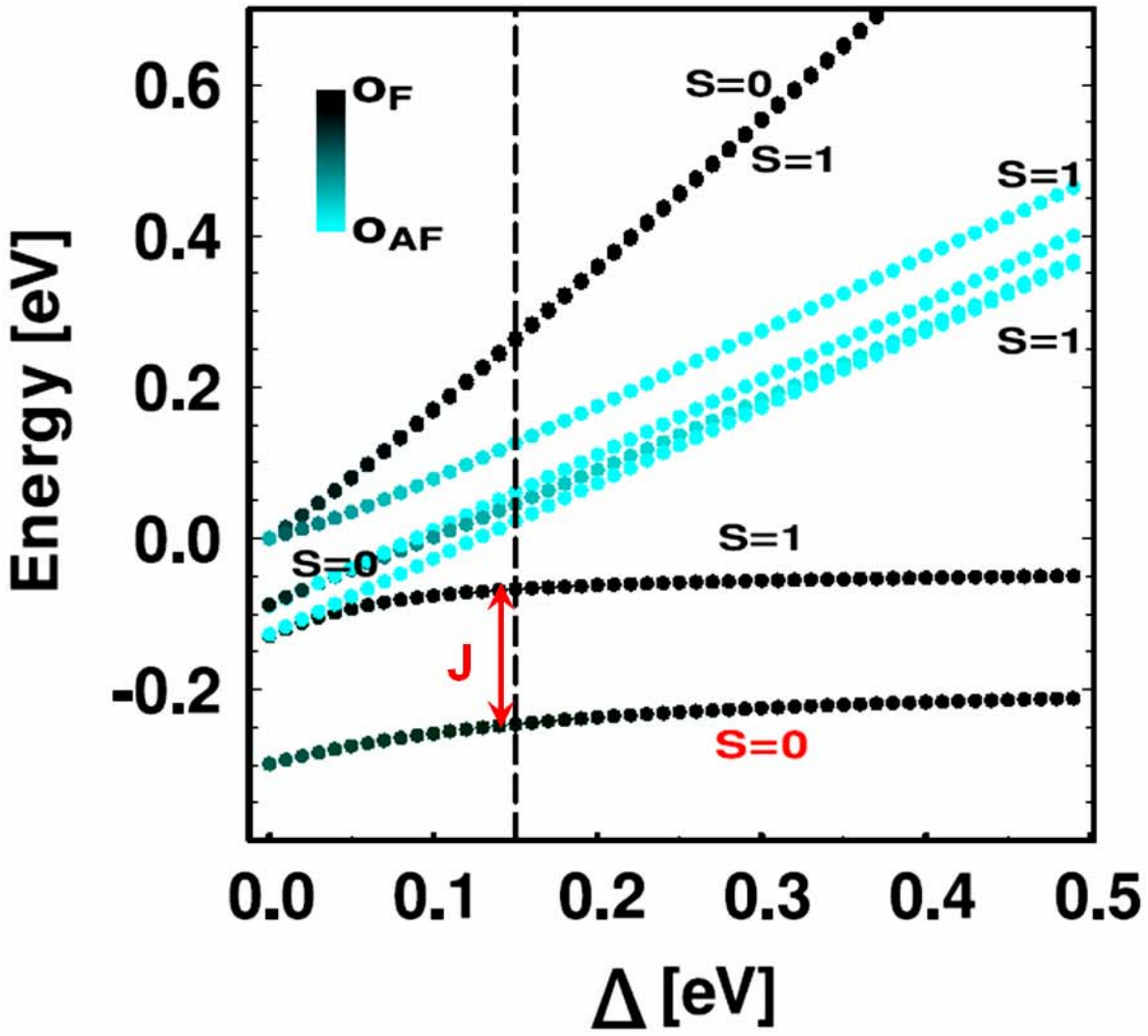


FIG. 3 (color online). Energy levels for the unstrained two-site model with $U = 6.4$ eV as a function of the splitting Δ between the energies of the $3z^2 - 1$ and $x^2 - y^2$ Wannier orbitals. The LDA value of Δ is indicated by the dashed line. O_F (O_{AF}) denotes a configuration with the same (different) orbital(s) on the two sites.

Phase diagram of 3D $RNiO_3$ perovskites

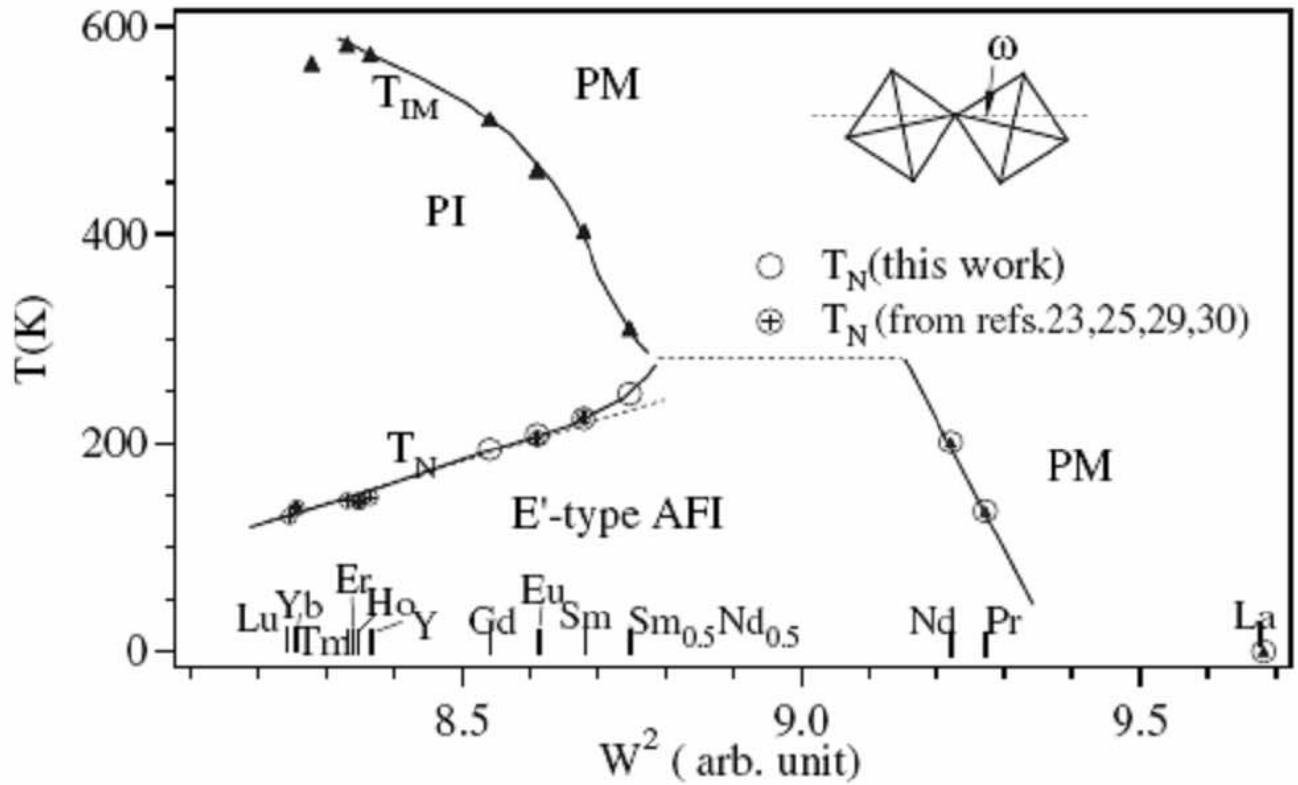
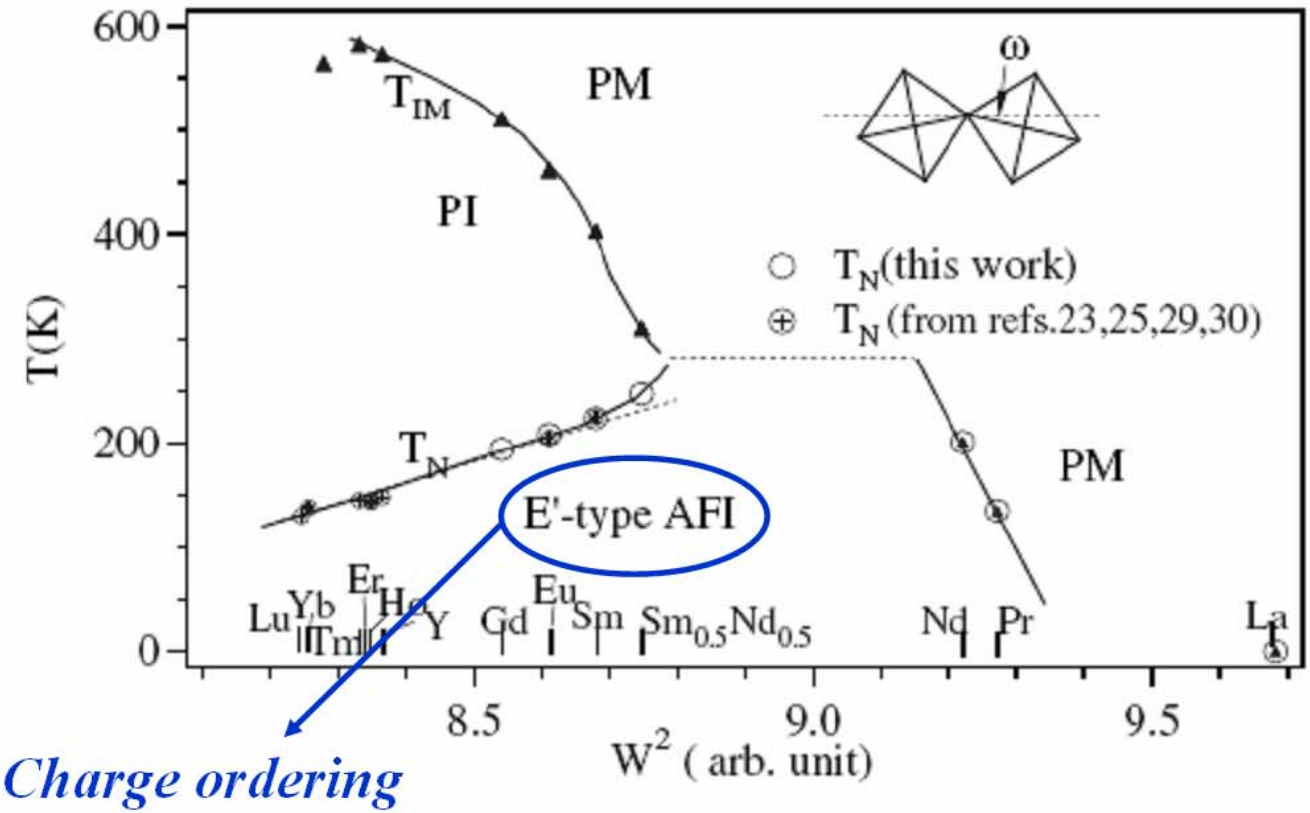


FIG. 5. The phase diagram of transition temperatures vs bandwidth W^2 at room temperature. T_{IM} and T_N are taken from Refs. [23,25,29,30]. Lines inside the figure are guides to the eyes. Inset: definition of the angle ω used to obtain $W \sim \cos\omega/(\text{Ni-O})^{3.5}$.

J.S. Zhou *et al.*, Phys. Rev. Lett. 95, 127204 (2005)

Phase diagram of 3D $RNiO_3$ perovskites



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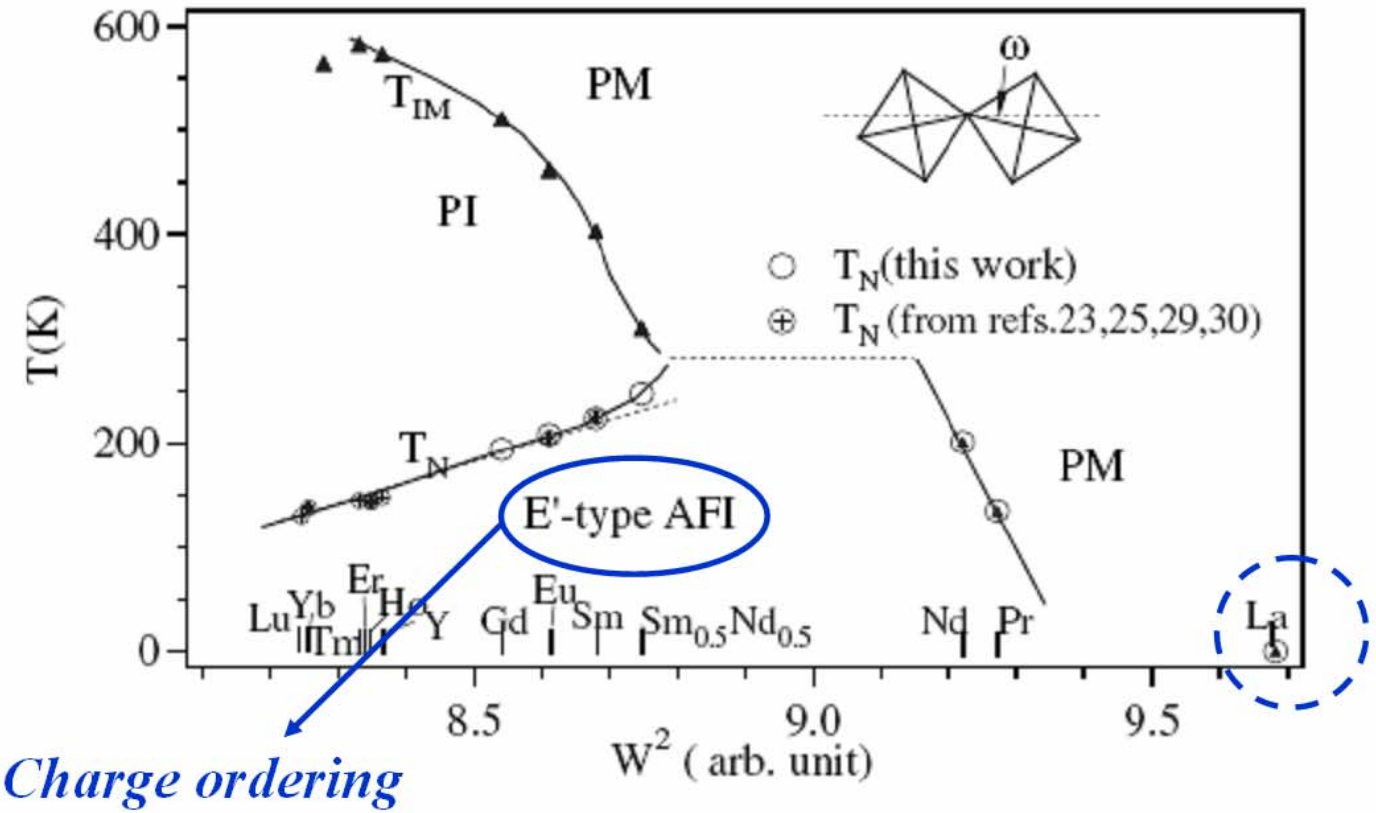

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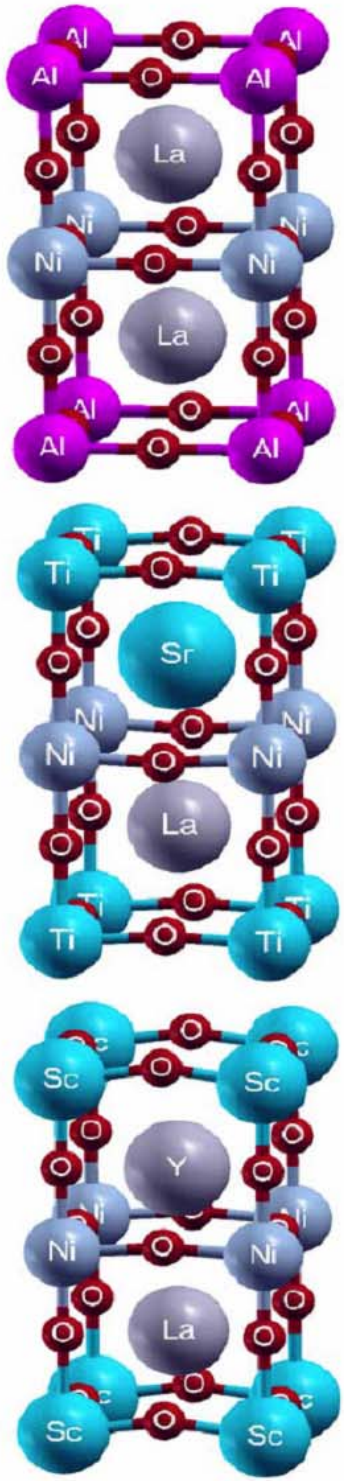
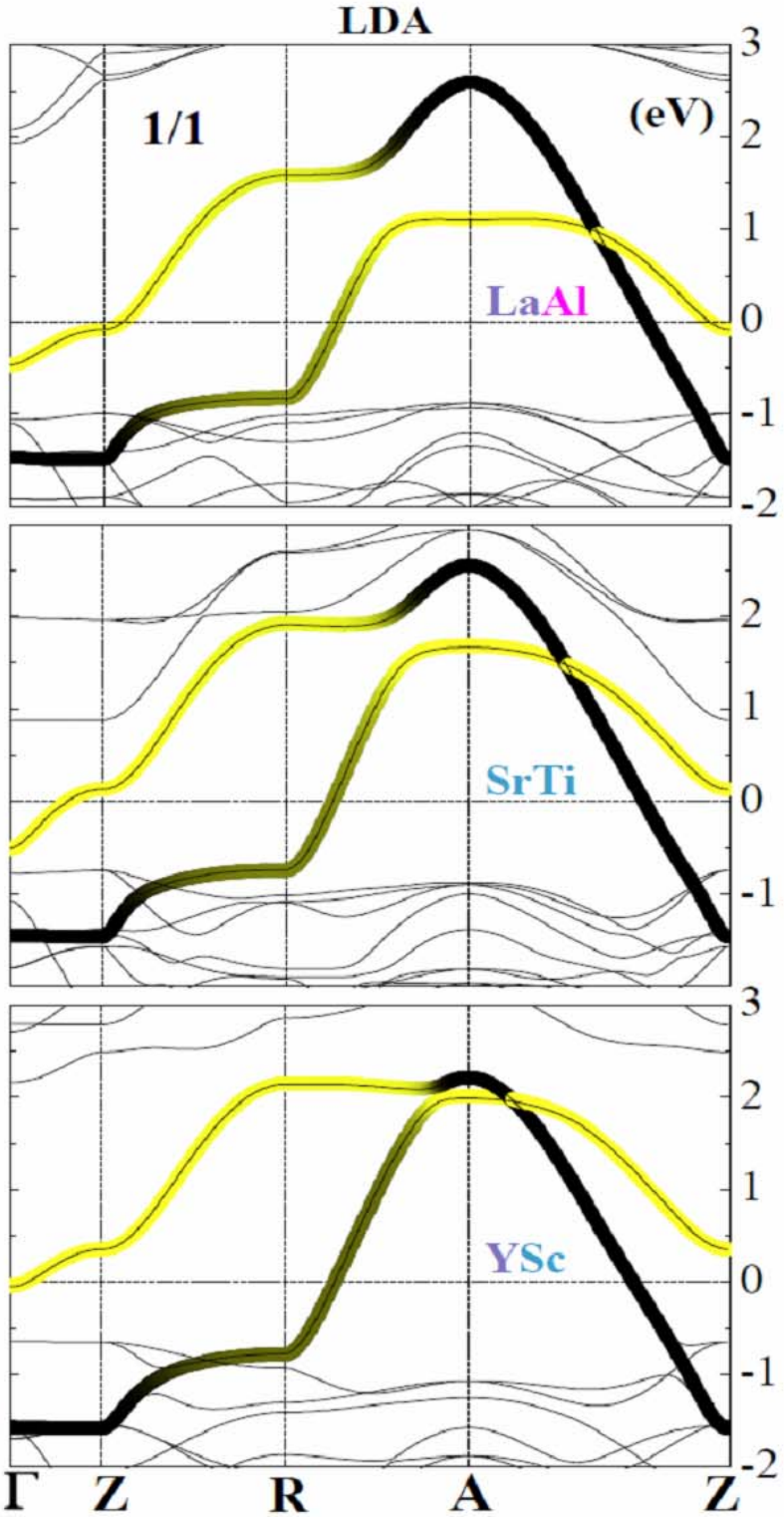
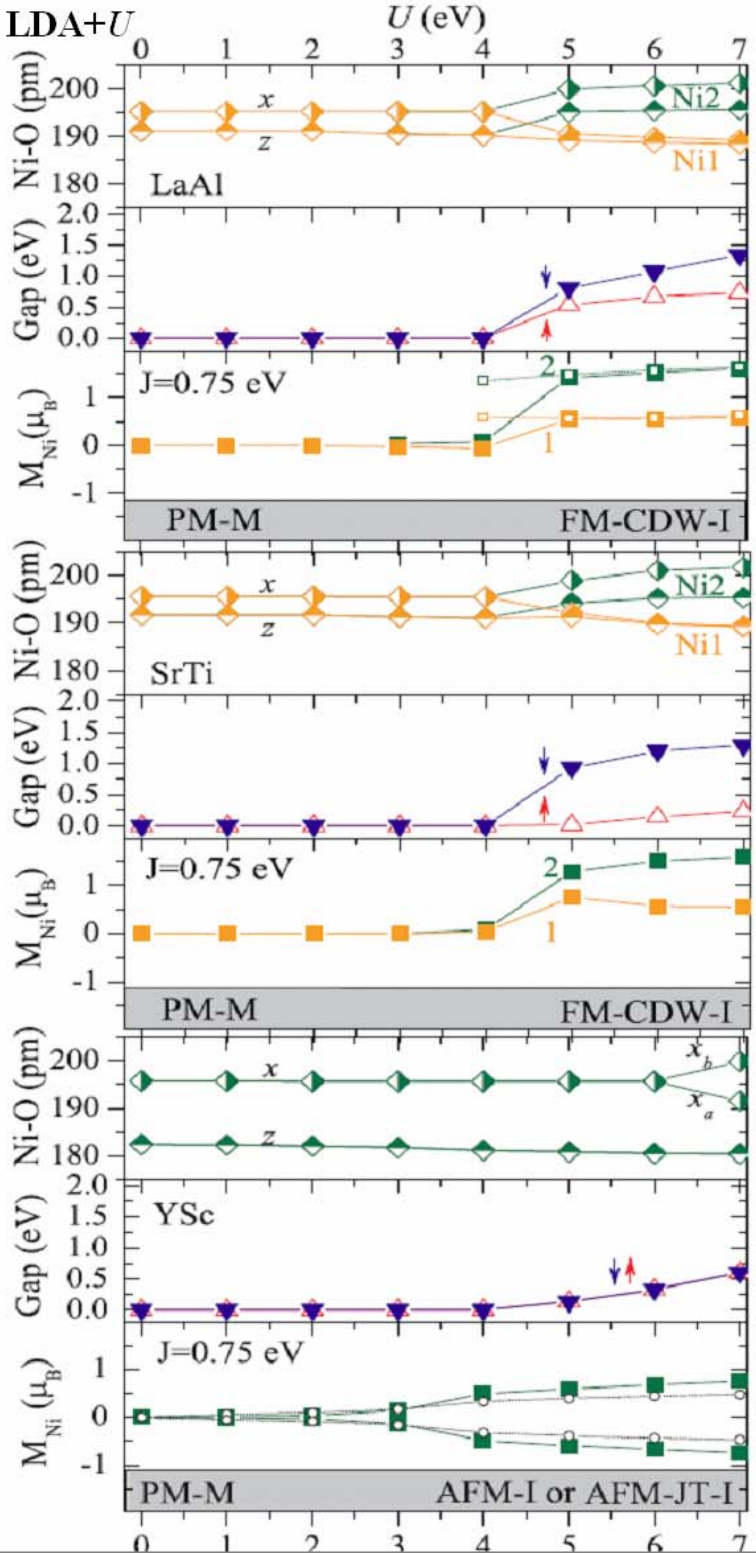
J.S. Zhou *et al.*, Phys. Rev. Lett. 95, 127204 (2005)

Chemical control is also a tool for avoiding charge disproportionation.







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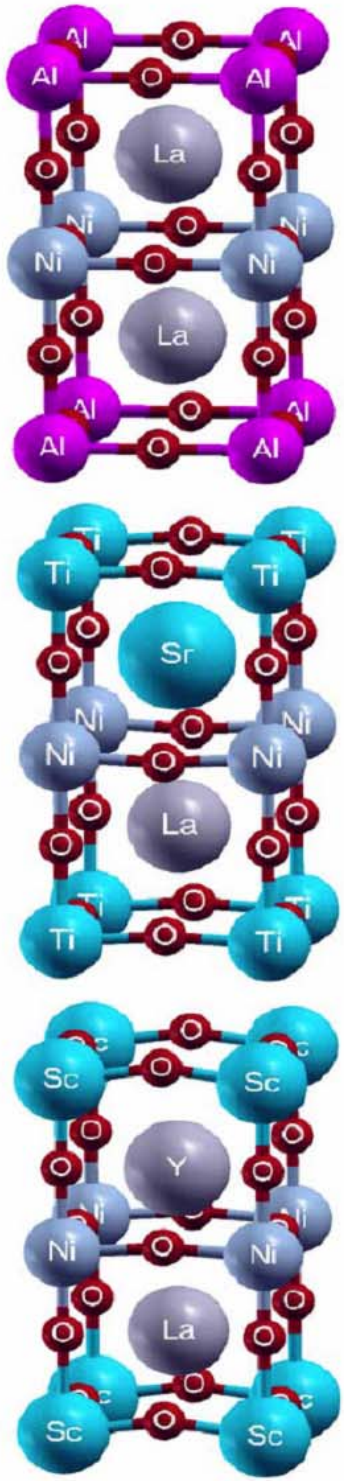

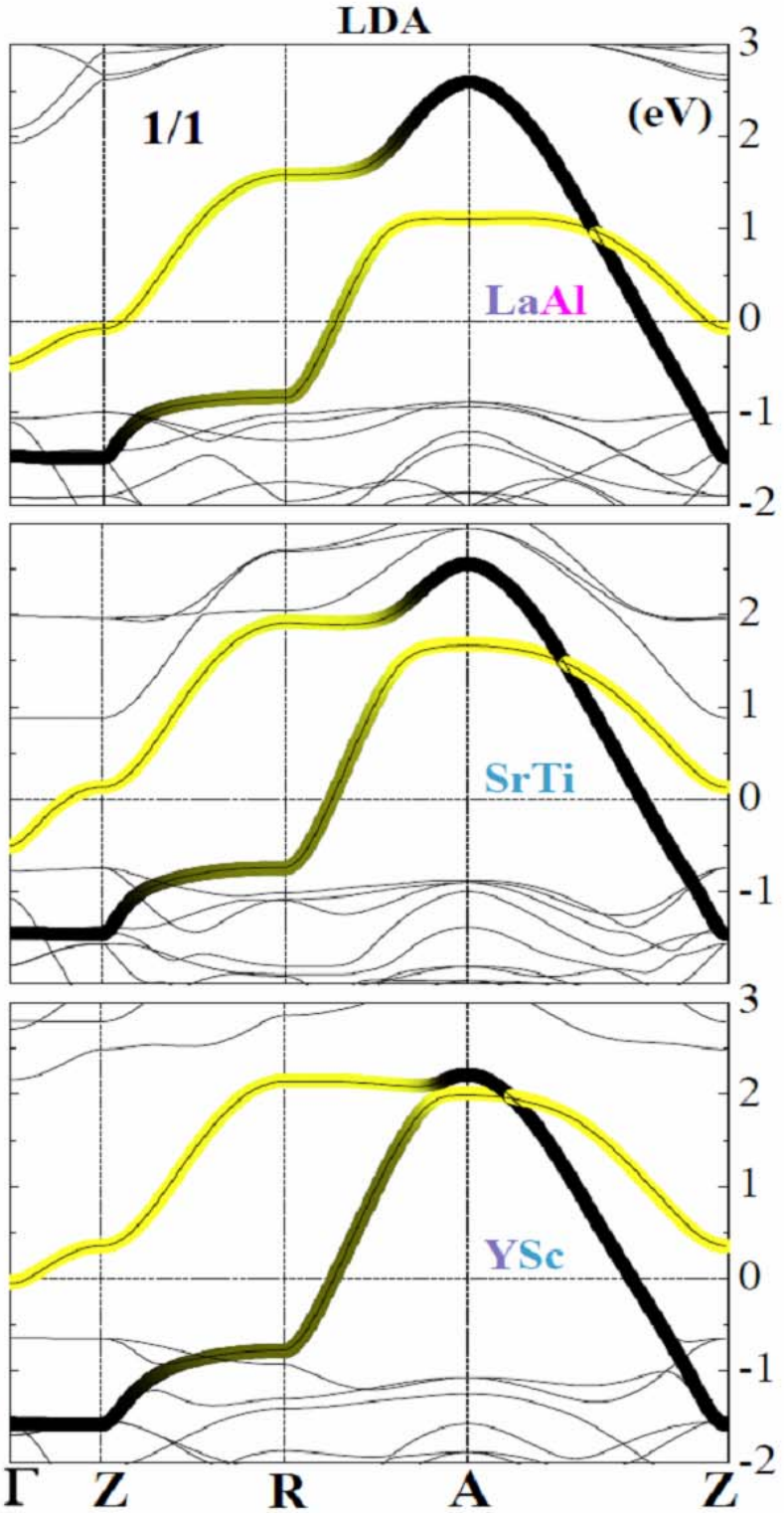

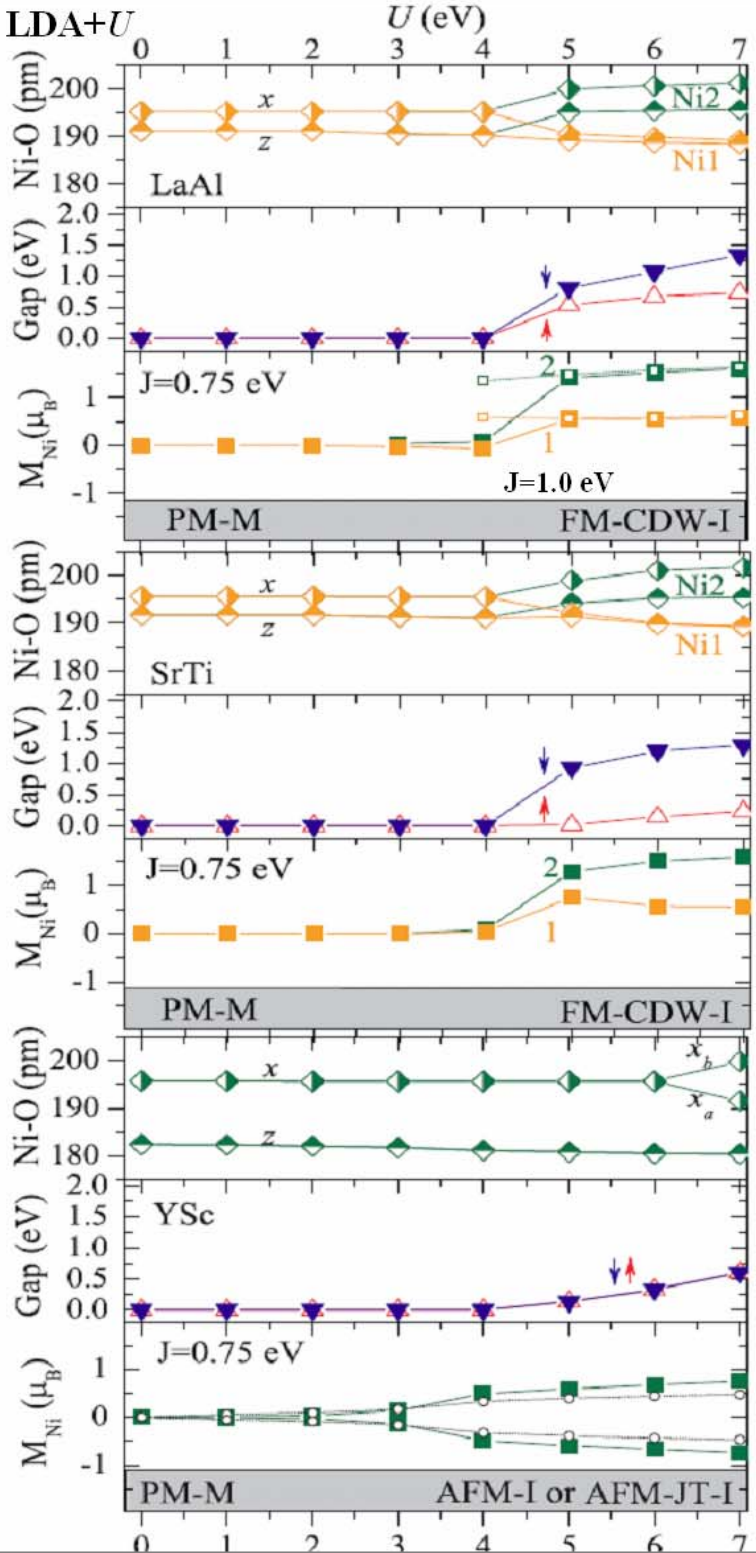

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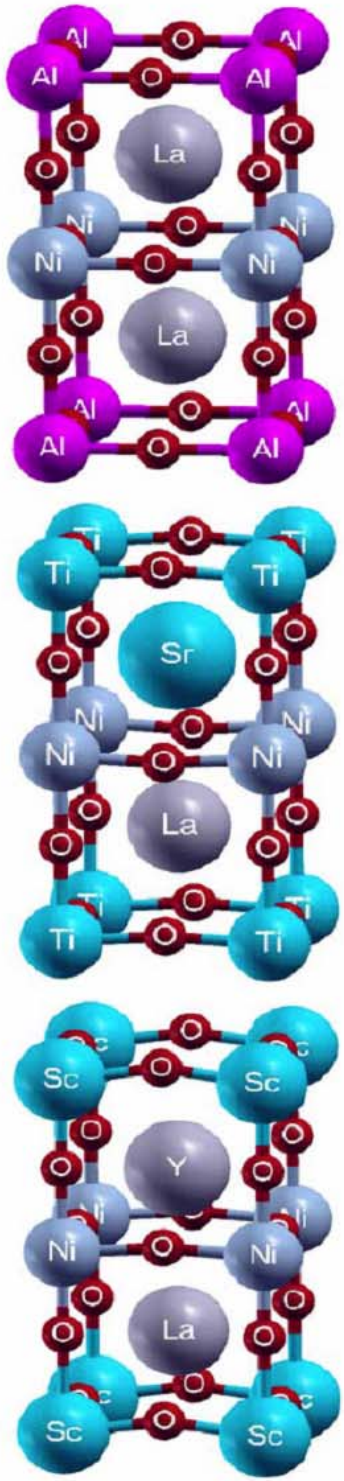
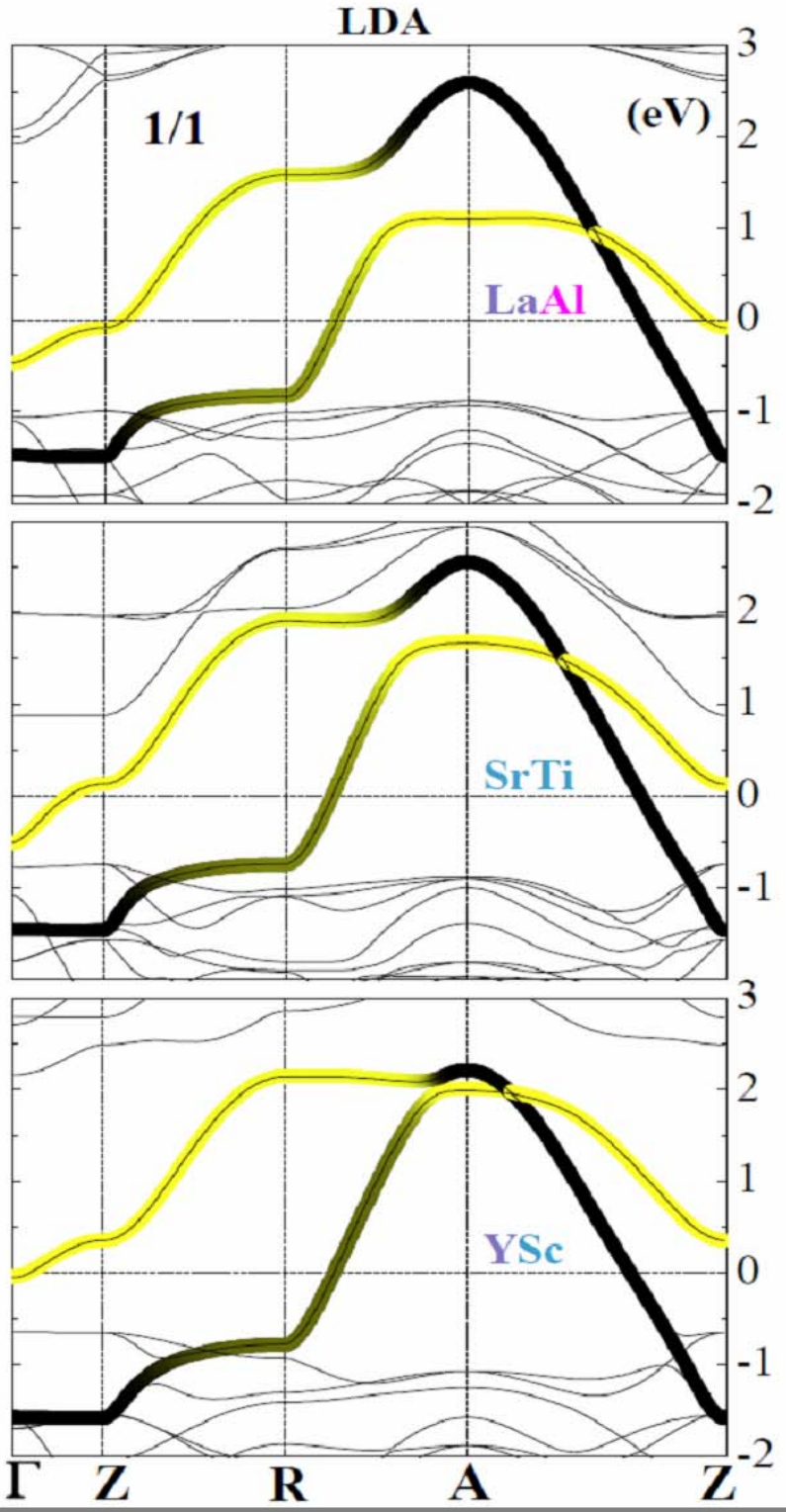
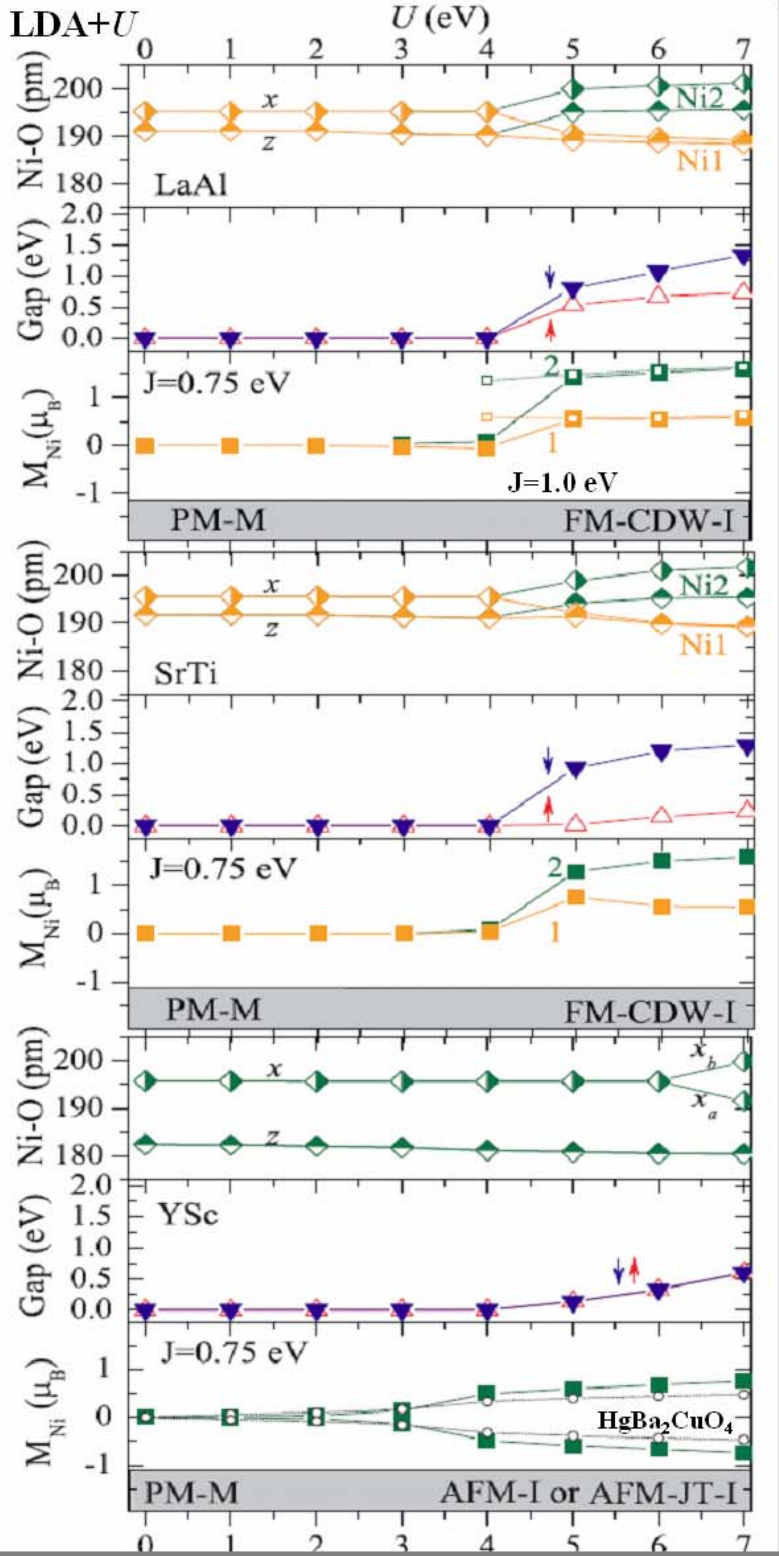
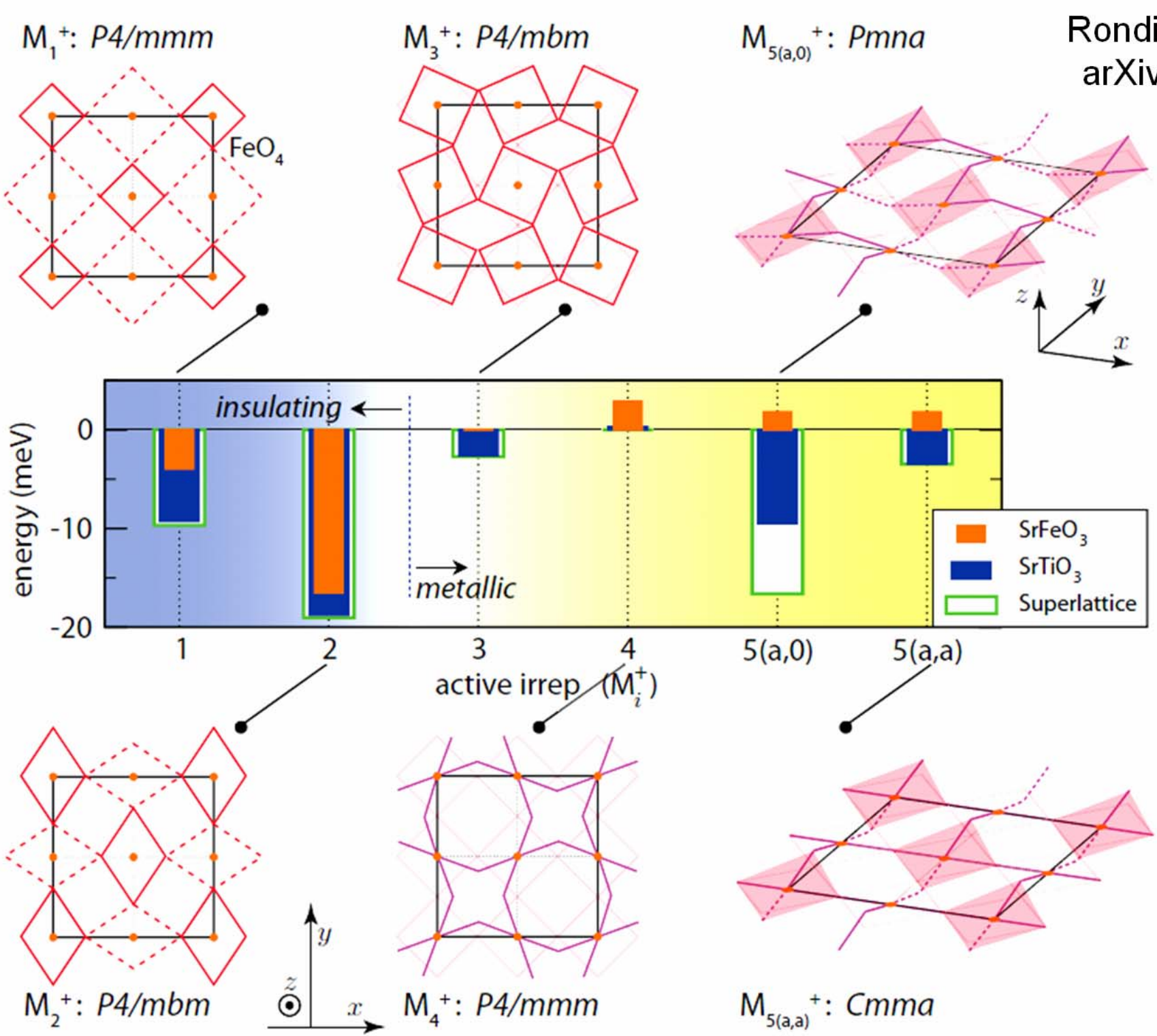
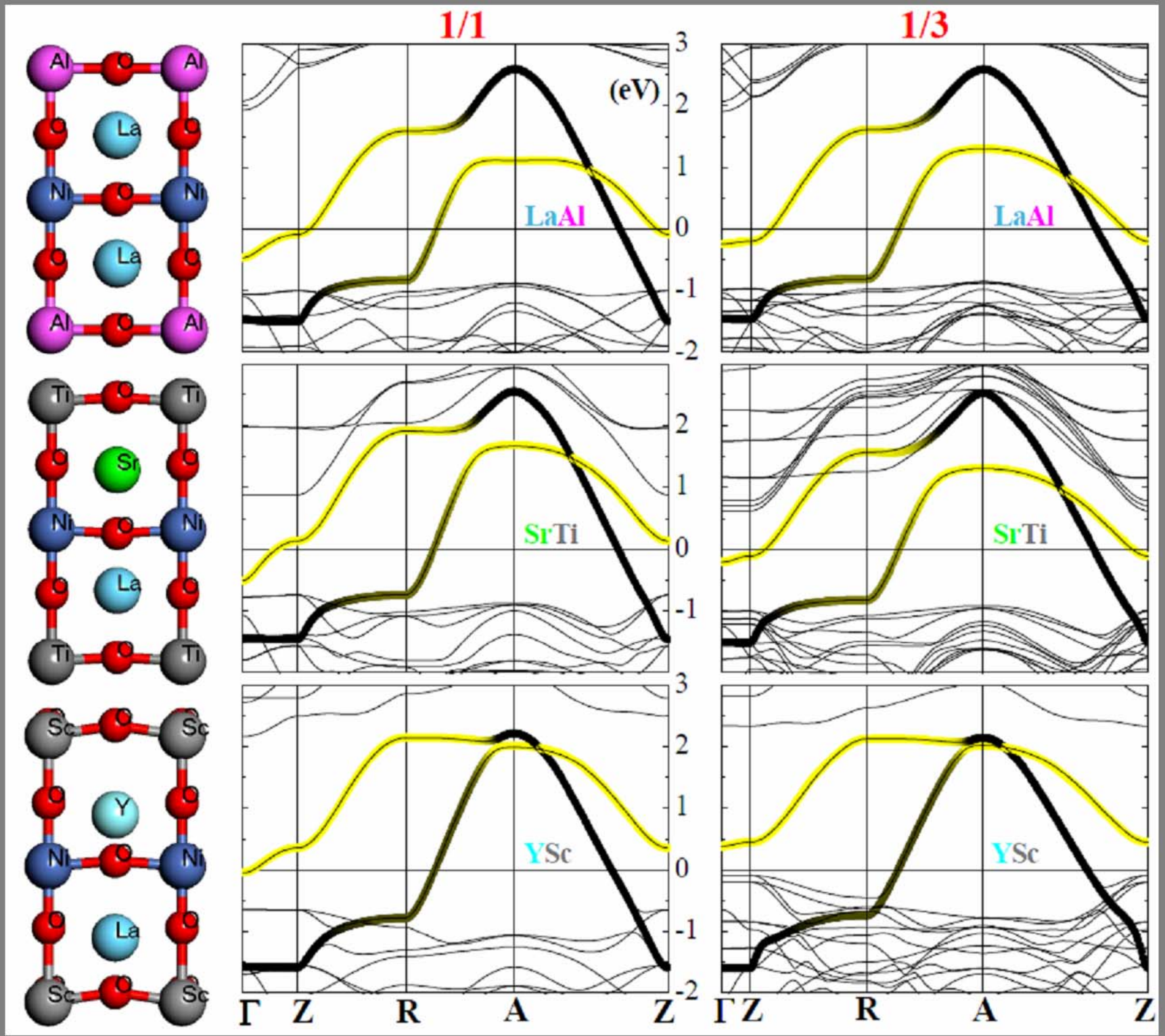







M1+: P4/mmm
M3+: P4/mbm
M5(a,0)+: Pmna
Rondinelli&Spaldin
arXiv: 0908.3502
d4
FeO4
z
y
x
insulating
metallic
energy (meV)
0
-10
-20
1
2
3
4
5(a,0)
5(a,a)
active irrep (Mi+)
SrFeO3
SrTiO3
Superlattice
M2+: P4/mbm
M4+: P4/mmm
M5(a,a)+: Cmma

Adding 2 insulating neighbor layers



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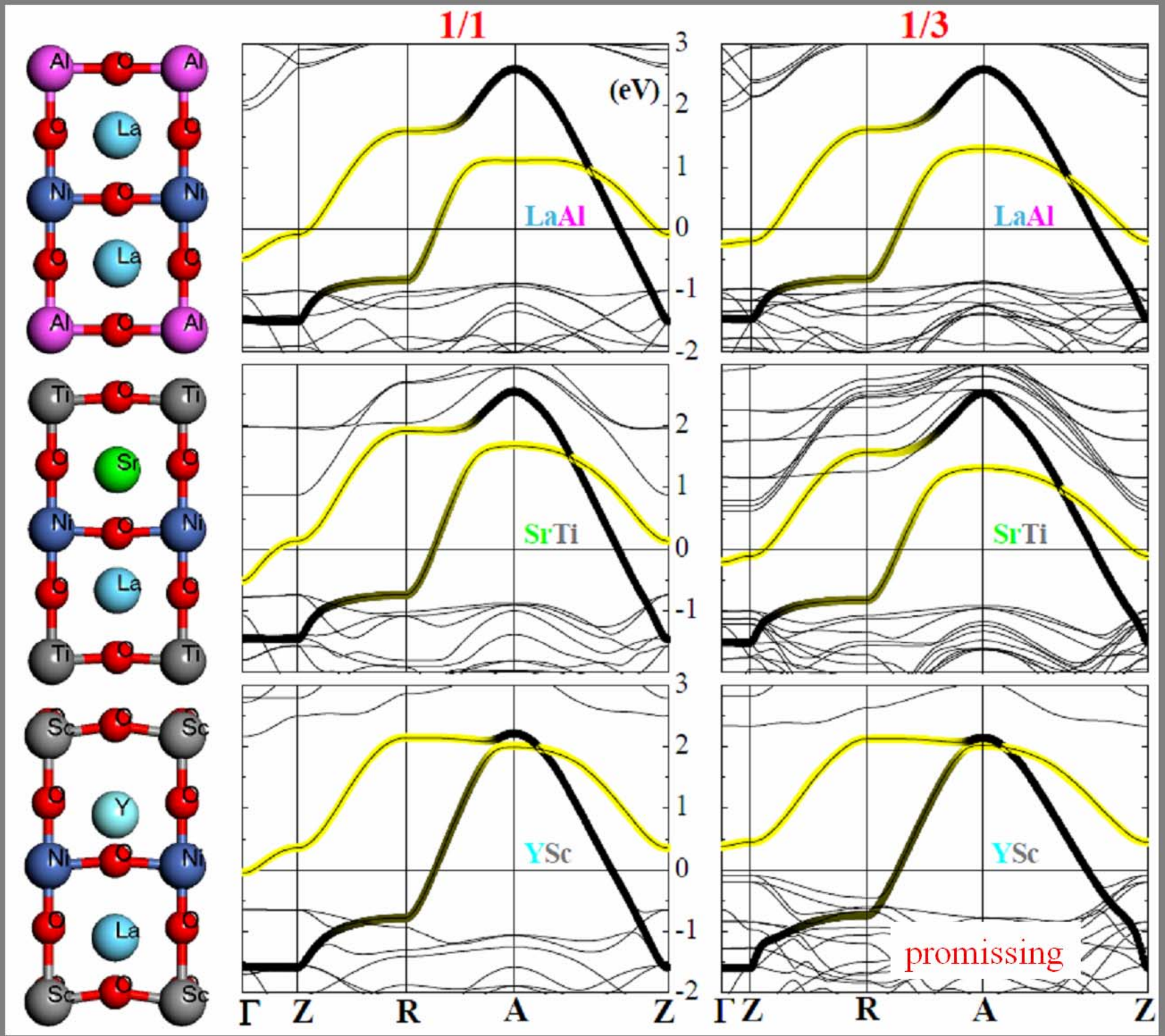
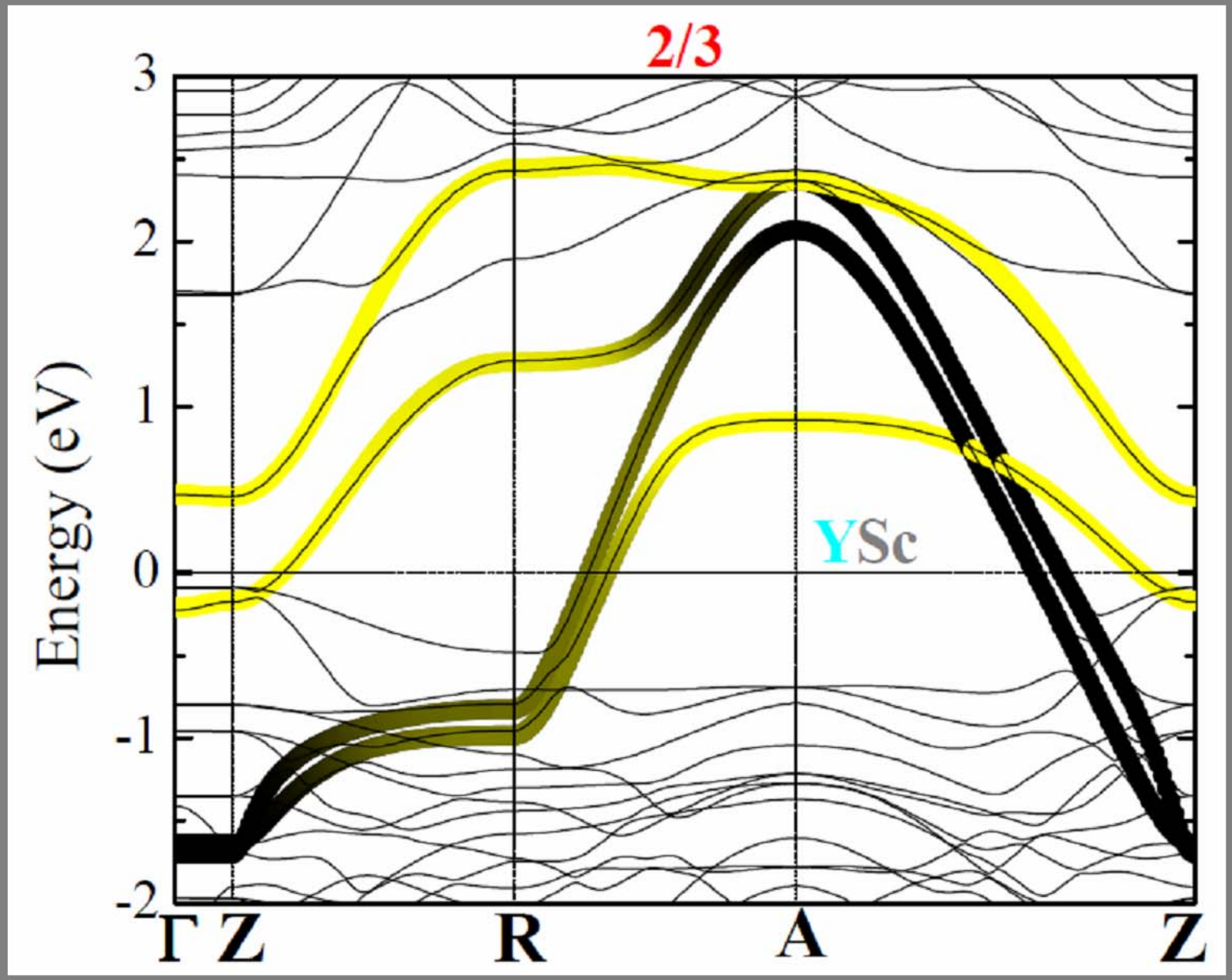


Adding also another NiO_2 layer (bilayer)



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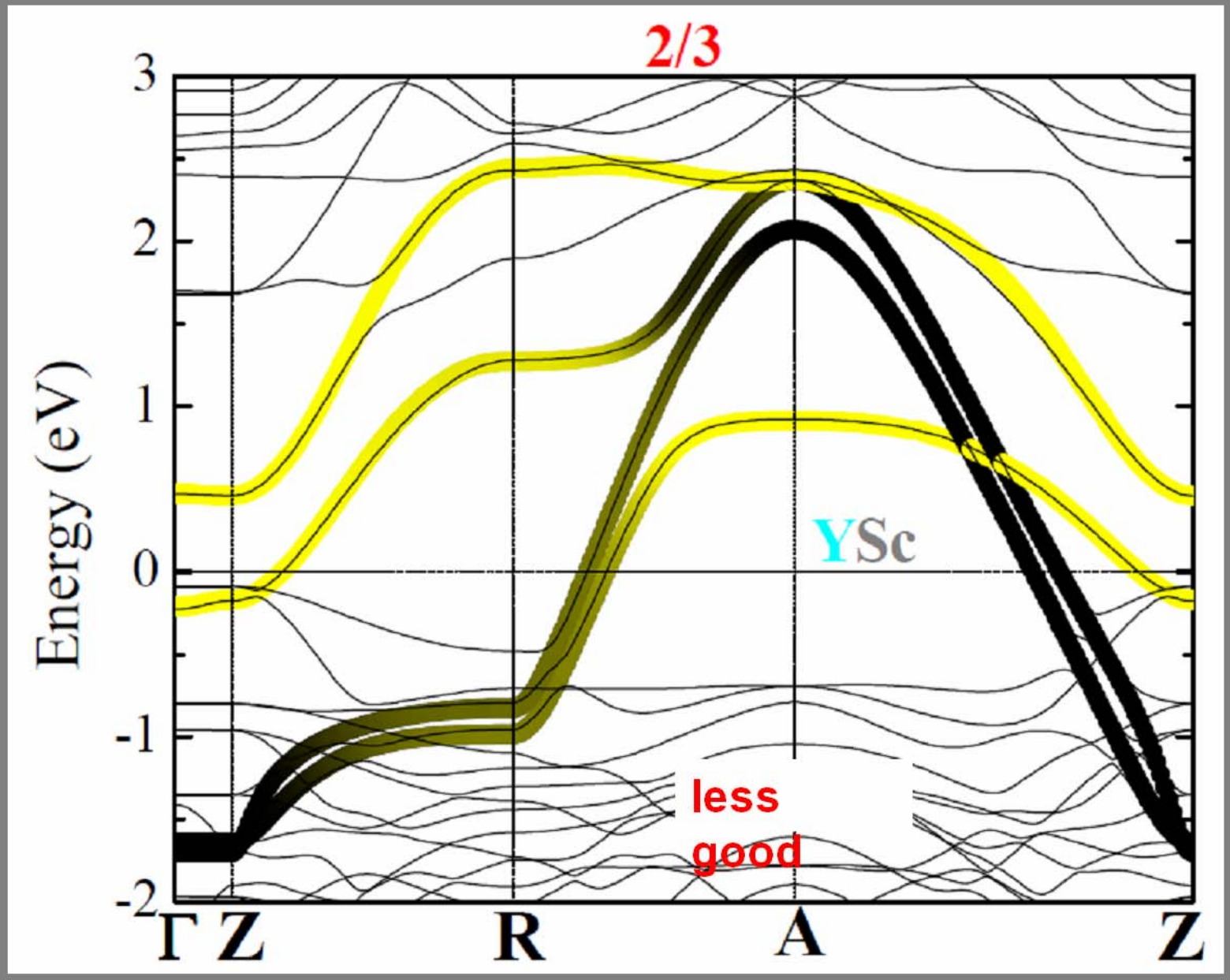

Instead of epitaxially made heterostructures, why not simply use the well-known nearly 2D bct bulk structure (e.g. $LaSrCuO_4$) ?

Instead of epitaxially made heterostructures, why not simply use the well-known nearly 2D bct bulk structure (e.g. $LaSrCuO_4$) ?

Electronic structure of possible nickelate analogs to the cuprates

V. I. Anisimov
Institute of Metal Physics, Ekaterinburg, GSP-170, Russia
and Theoretische Physik, ETH-Hönggerberg, CH-8093 Zürich, Switzerland

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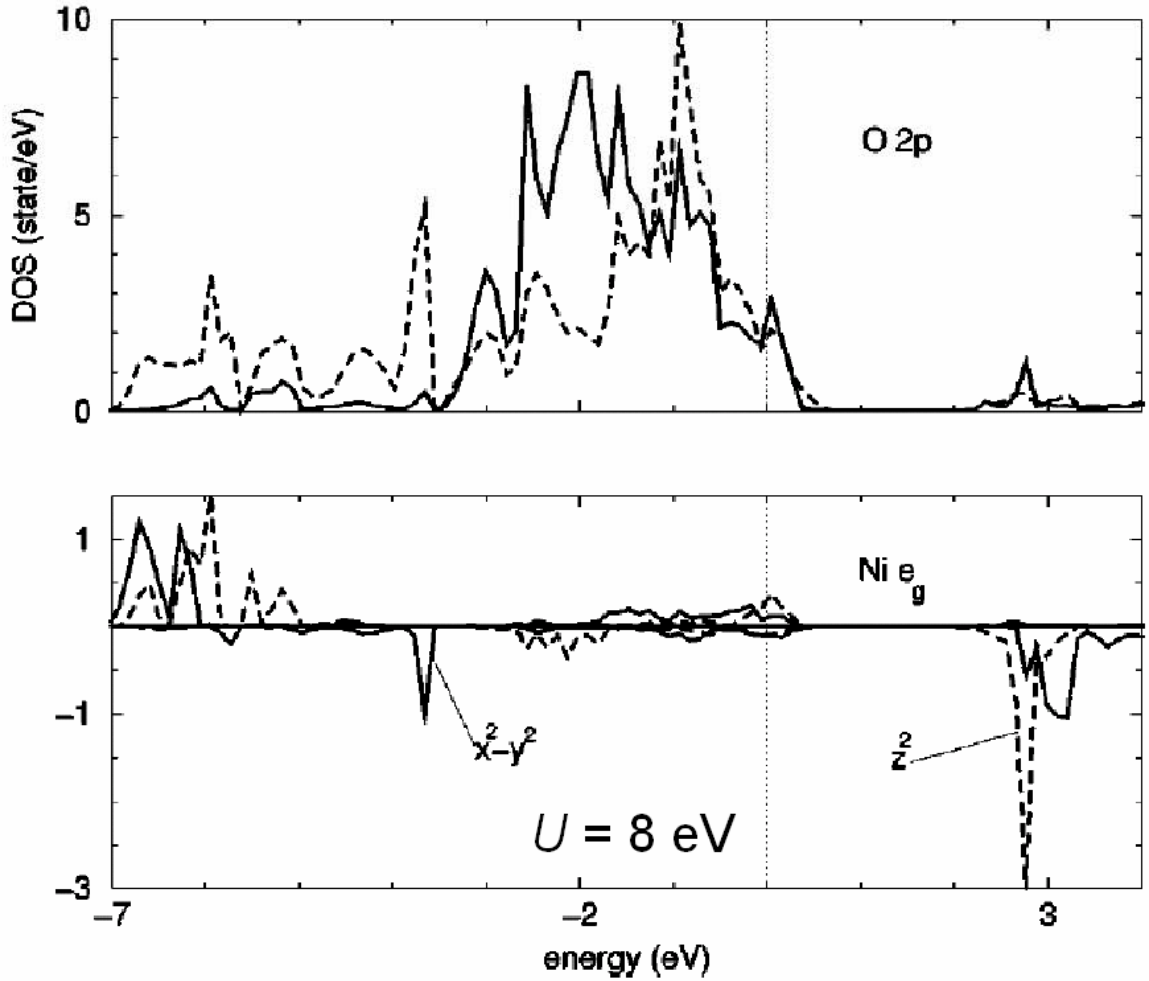
Theoretische Physik, ETH-Hönggerberg, CH-8093 Zürich, Switzerland
(Received 26 June 1998)

The electronic structure of various nickel oxides with nickel valence varying from 1+ to 3+ was investigated with the aim to find similarities and differences to the isoelectronic cuprates. Only if the Ni ions are forced into a planar coordination with the O ions can a $S=1/2$ magnetic insulator be realized with the difficult Ni^{+} oxidation state and possibly doped with low spin ($S=0$) Ni^{2+} holes directly analogous to the superconducting cuprates. The more common Ni^{3+} oxidation state cannot be used to make a parent magnetic insulator as it forms rather as localized $S=1$ Ni^{2+} embedded in a sea of itinerant O holes. Strong coupling of these holes to the localized spins via $2p$-$3d$ hybridization leads to a heavy-fermion system with a large Kondo

Instead of epitaxially made heterostructures, why not simply use the well-known nearly 2D bct bulk structure (e.g. $LaSrCuO_4$) ?



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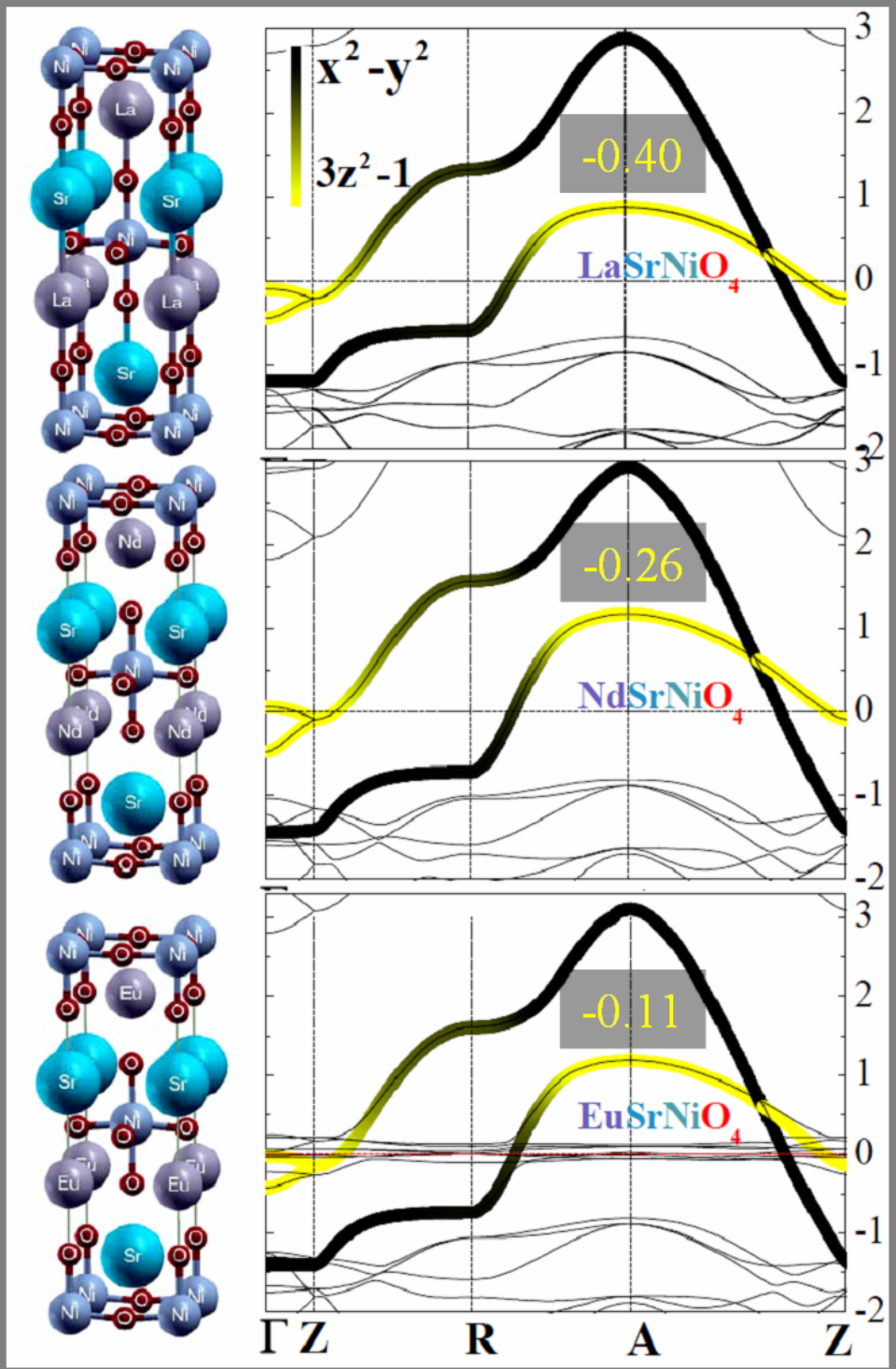
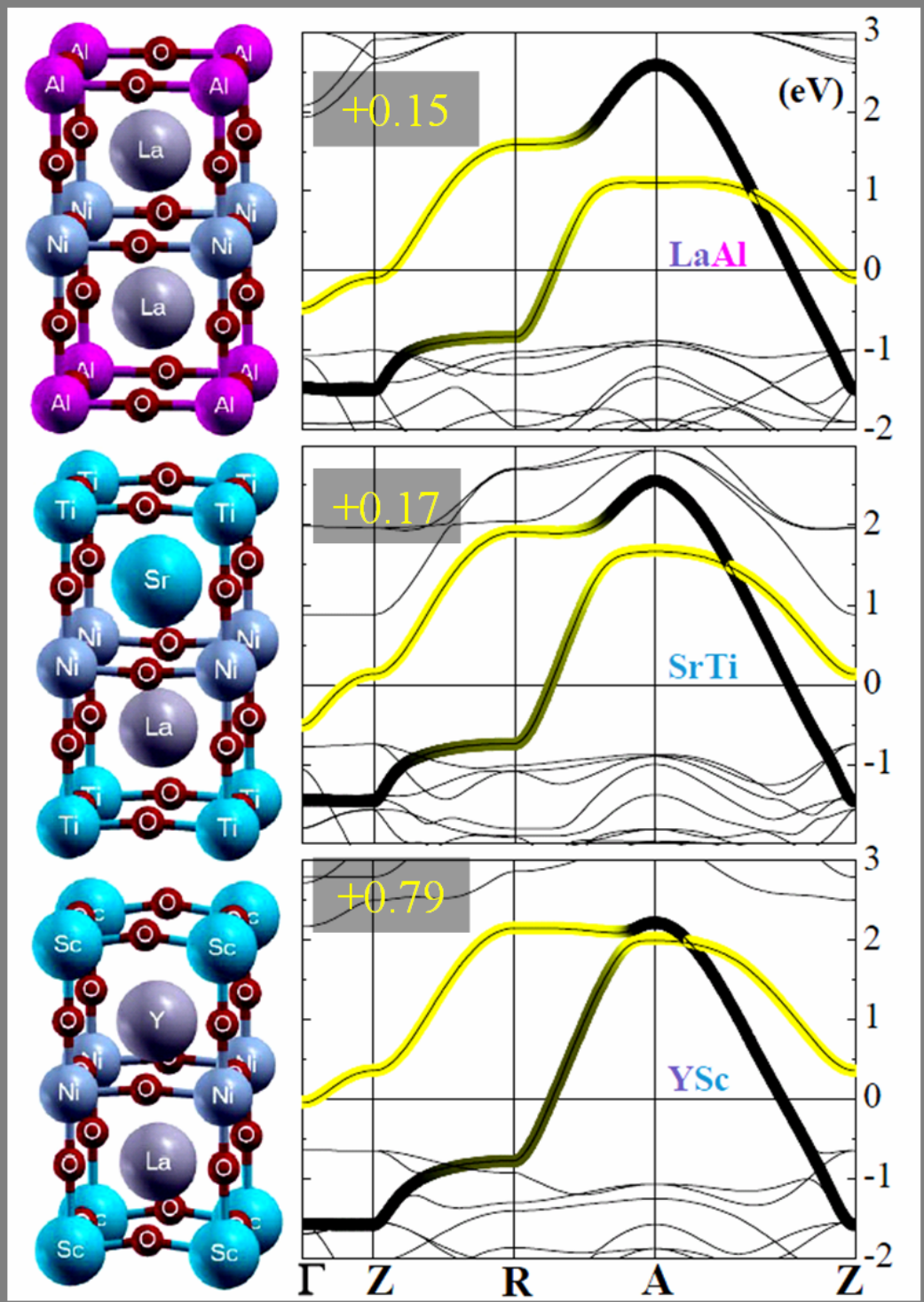
This is currently done in Tokura's group. From structures given to us by M. Ushida, we and R. Arita have made preliminary calculations:

Bulk 214 materials

$\varepsilon_{3z^2-1} - \varepsilon_{x^2-y^2}$

1/1 Heterostructures





For $LaSrNiO_4$ and $NdSrNiO_4$, our DMFT calculations indicate that, now, it is the band which is x^2-y^2-like along [110] which gets emptied. The resulting Fermi-surface has strong k_z-dispersion and is not like that of a HTSC cuprate, but seems consistent with ARPES.

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