COLLÈGE DE FRANCE
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Chaire de Physique de la Matière Condensée

Des oxydes supraconducteurs aux atomes froids

- la matière à fortes corrélations quantiques -

Cycle 2009-2010
Cours 5 – 2 juin 2010

Antoine Georges

Cours 5: *Introduction* à la structure et aux propriétés électroniques des **oxydes de métaux de transition**

Séminaire:

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Véronique BROUET
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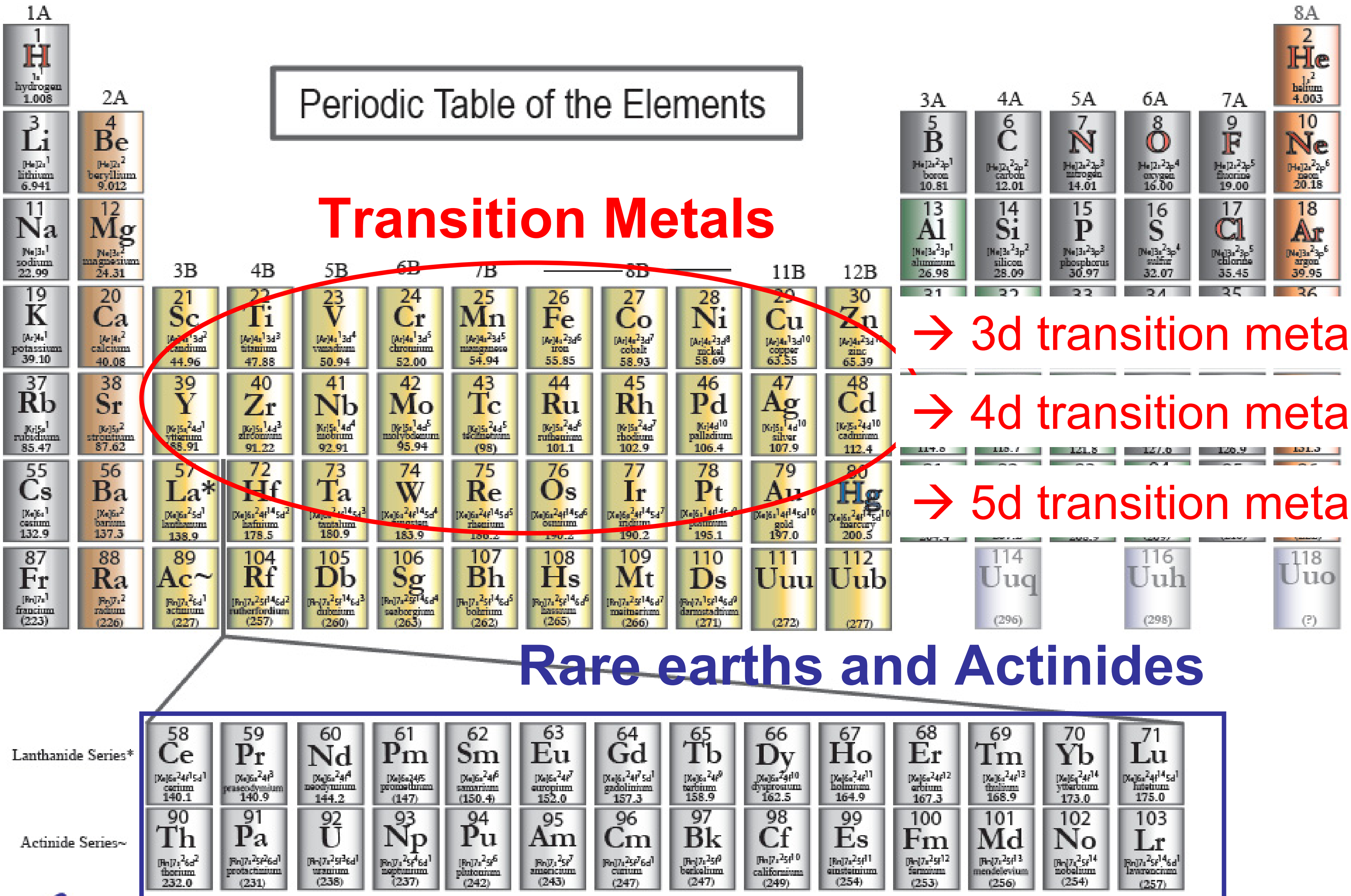
Les nouveaux supraconducteurs au fer vus par photoémission résolue en angle

Why study transition-metal oxides ?

- TMOs (and materials with strong electronic correlations in general) do `BIG THINGS' !
- Many of these `big things' raise a number of intriguing fundamental questions
- Some of these `big things' may even be useful for applications…
- The structures are beautiful and have a certain degree of controllability, and the diversity of phenomena is amazing

OUTLINE

- Some of the `big things' that oxides do…
- Some structures
- `Mott phenomenon' is of key importance
- Atomic orbitals. Why localized ? Crystal-field splitting.
- Some notions of electronic structure
- Interactions
- Mott and charge-transfer insulators



Periodic Table of the Elements

1A	2A	3B	4B	5B	6B	7B	8B			11B	12B	3A	4A	5A	6A	7A	8A
1 H hydrogen 1.008																	2 He helium 4.003
3 Li lithium 6.941	4 Be beryllium 9.012											5 B boron 10.81	6 C carbon 12.01	7 N nitrogen 14.01	8 O oxygen 16.00	9 F fluorine 19.00	10 Ne neon 20.18
11 Na sodium 22.99	12 Mg magnesium 24.31											13 Al aluminum 26.98	14 Si silicon 28.09	15 P phosphorus 30.97	16 S sulfur 32.07	17 Cl chlorine 35.45	18 Ar argon 39.95
19 K potassium 39.10	20 Ca calcium 40.08	21 Sc scandium 44.96	22 Ti titanium 47.88	23 V vanadium 50.94	24 Cr chromium 52.00	25 Mn manganese 54.94	26 Fe iron 55.85	27 Co cobalt 58.93	28 Ni nickel 58.69	29 Cu copper 63.55	30 Zn zinc 65.39						
37 Rb rubidium 85.47	38 Sr strontium 87.62	39 Y yttrium 88.91	40 Zr zirconium 91.22	41 Nb niobium 92.91	42 Mo molybdenum 95.94	43 Tc technetium (98)	44 Ru ruthenium 101.1	45 Rh rhodium 102.9	46 Pd palladium 106.4	47 Ag silver 107.9	48 Cd cadmium 112.4	114.8	118.7	121.8	127.6	126.9	131.3
55 Cs cesium 132.9	56 Ba barium 137.3	57 La* lanthanum 138.9	72 Hf hafnium 178.5	73 Ta tantalum 180.9	74 W tungsten 183.9	75 Re rhenium 186.2	76 Os osmium 190.2	77 Ir iridium 190.2	78 Pt platinum 195.1	79 Au gold 197.0	80 Hg mercury 200.5	204.4	207.2	209.0	(209)	(210)	(222)
87 Fr francium (223)	88 Ra radium (226)	89 Ac~ actinium (227)	104 Rf rutherfordium (257)	105 Db dubnium (260)	106 Sg seaborgium (263)	107 Bh bohrium (262)	108 Hs hassium (265)	109 Mt meitnerium (266)	110 Ds darmstadtium (271)	111 Uuu (272)	112 Uub (277)		114 Uuq (296)		116 Uuh (298)		118 Uuo (?)

Transition Metals

→ 3d transition metals

→ 4d transition metals

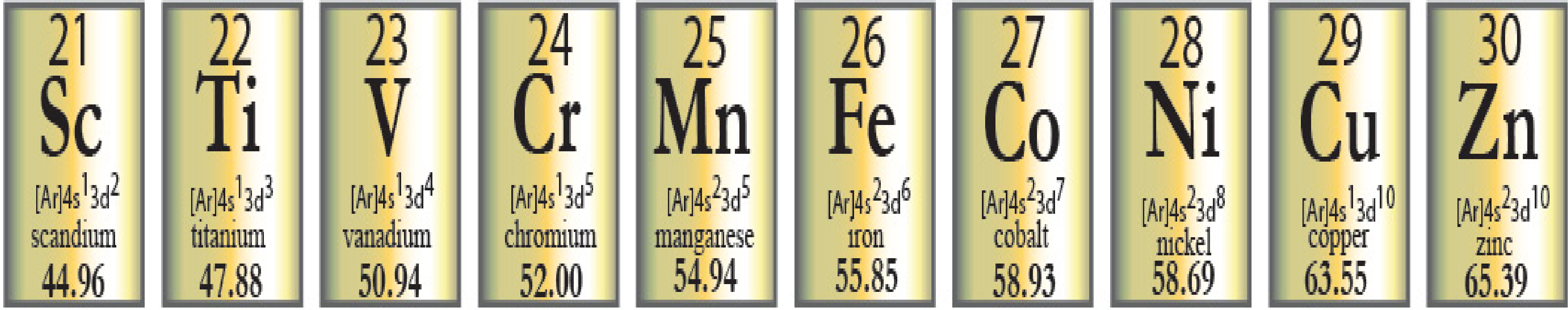
→ 5d transition metals

Rare earths and Actinides

Lanthanide Series*	58 Ce cerium 140.1	59 Pr praseodymium 140.9	60 Nd neodymium 144.2	61 Pm promethium (147)	62 Sm samarium (150.4)	63 Eu europium 152.0	64 Gd gadolinium 157.3	65 Tb terbium 158.9	66 Dy dysprosium 162.5	67 Ho holmium 164.9	68 Er erbium 167.3	69 Tm thulium 168.9	70 Yb ytterbium 173.0	71 Lu lutetium 175.0
Actinide Series~	90 Th thorium 232.0	91 Pa protactinium (231)	92 U uranium (238)	93 Np neptunium (237)	94 Pu plutonium (242)	95 Am americium (243)	96 Cm curium (247)	97 Bk berkelium (247)	98 Cf californium (249)	99 Es einsteinium (254)	100 Fm fermium (253)	101 Md mendelevium (256)	102 No nobelium (254)	103 Lr lawrencium (257)

Electronic configuration of neutral isolated atom:

8
O
[He]$2s^2 2p^4$
oxygen
16.00



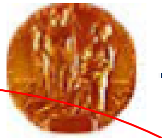
21	22	23	24	25	26	27	28	29	30
Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
[Ar]$4s^1 3d^2$	[Ar]$4s^1 3d^3$	[Ar]$4s^1 3d^4$	[Ar]$4s^1 3d^5$	[Ar]$4s^2 3d^5$	[Ar]$4s^2 3d^6$	[Ar]$4s^2 3d^7$	[Ar]$4s^2 3d^8$	[Ar]$4s^1 3d^{10}$	[Ar]$4s^2 3d^{10}$
scandium	titanium	vanadium	chromium	manganese	iron	cobalt	nickel	copper	zinc
44.96	47.88	50.94	52.00	54.94	55.85	58.93	58.69	63.55	65.39


K.A. Müller

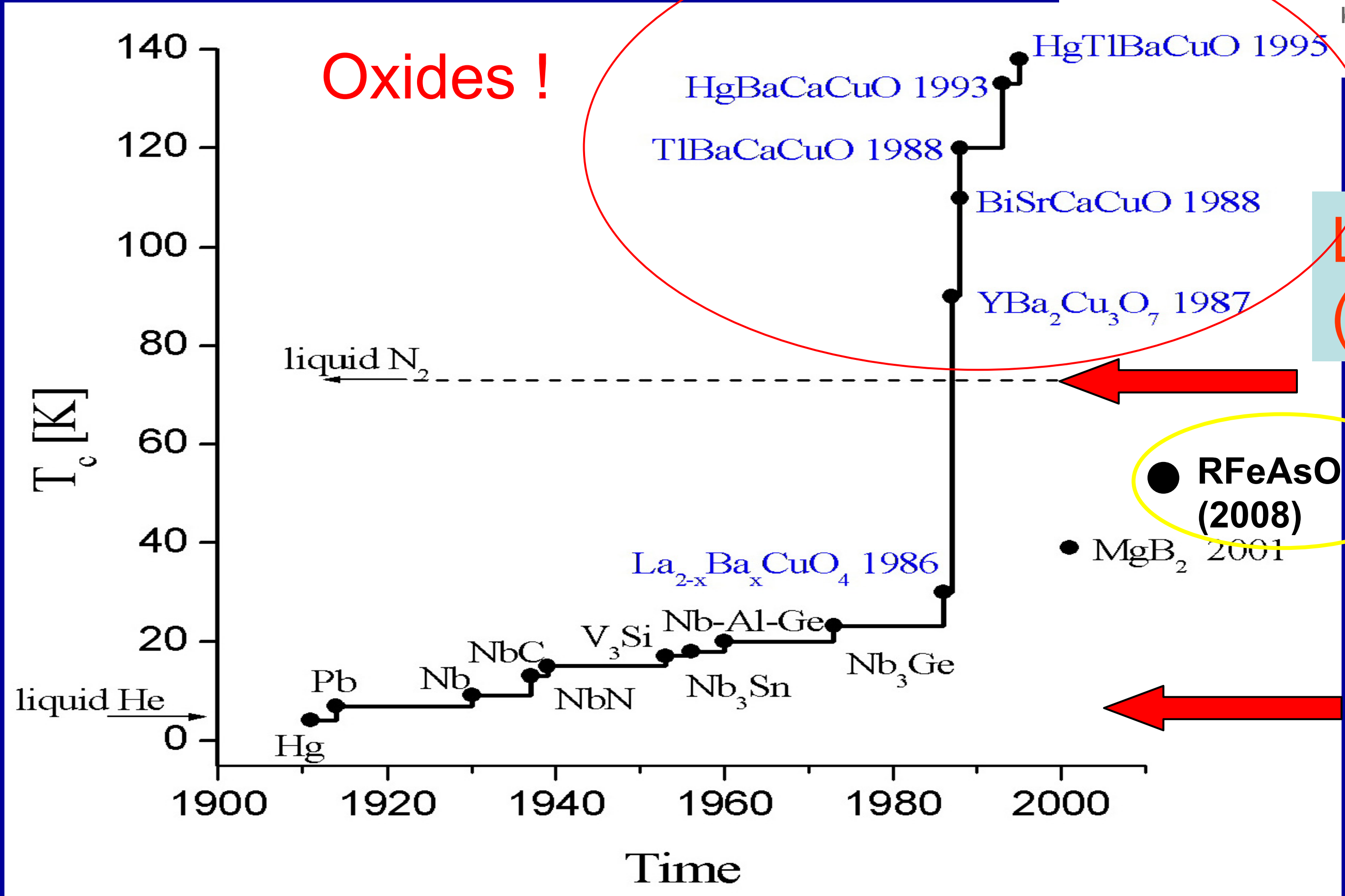
Big things/1

High-Tc superconductivity !


J.G. Bednorz


The Nobel Prize in Physics 1987

k-through in the discovery of superconductivity



Liquid nitrogen
(77 K)

Iron pnictides

Liquid Helium
(4 K)

Big things/2

METAL- -INSULATOR TRANSITIONS

V_2O_3

with pressure / substitutions on V-site: A time-honoured Example displaying a rich variety of phenomena

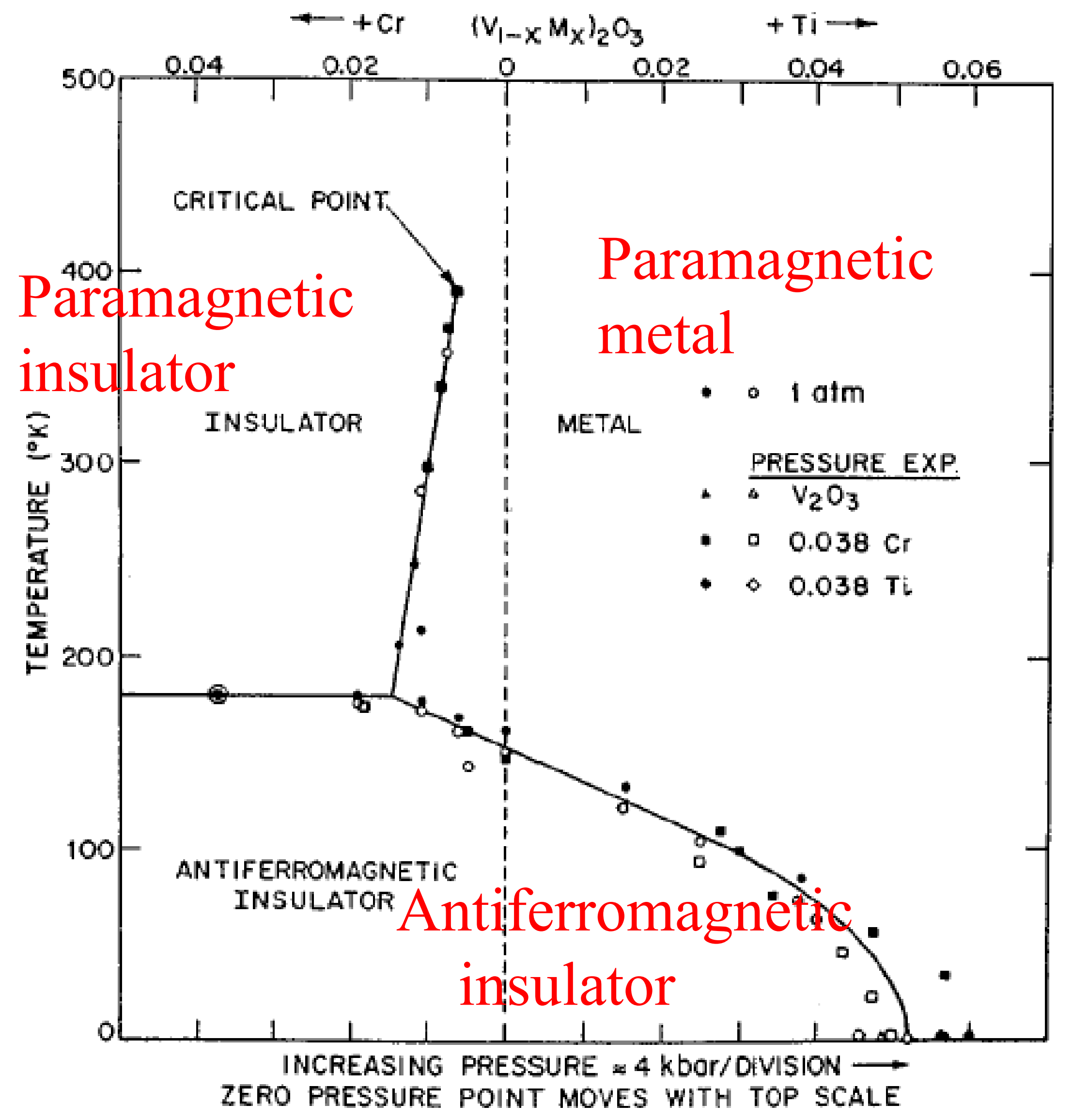
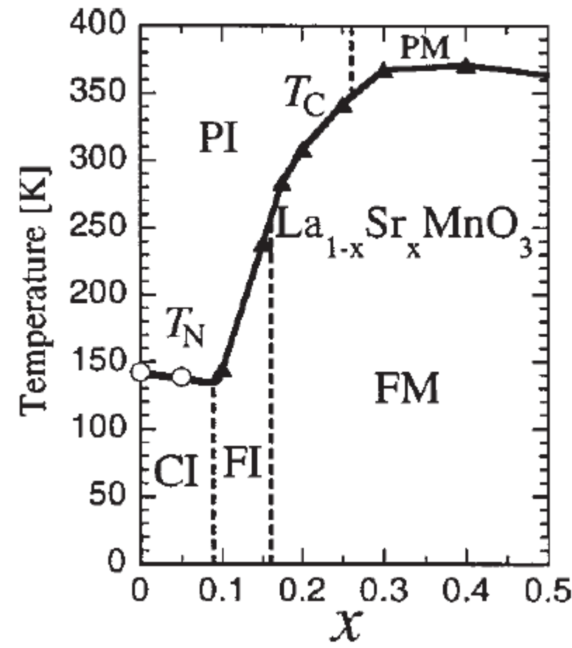
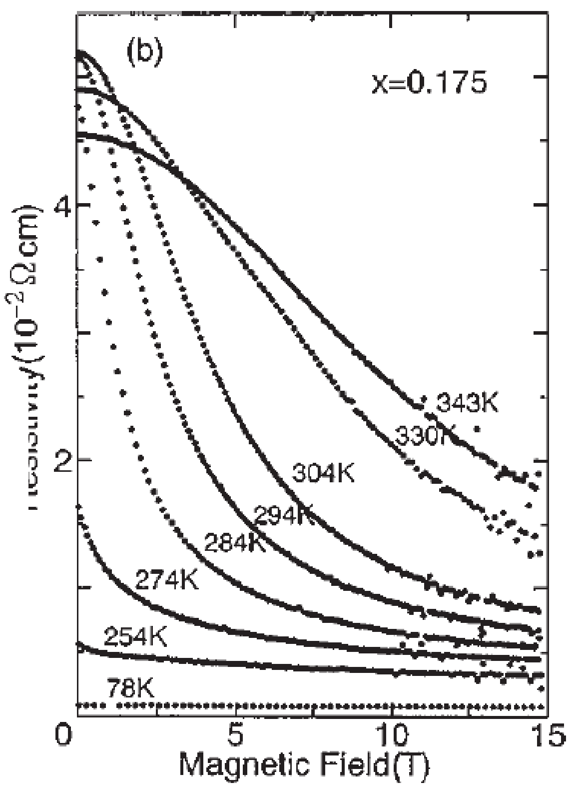


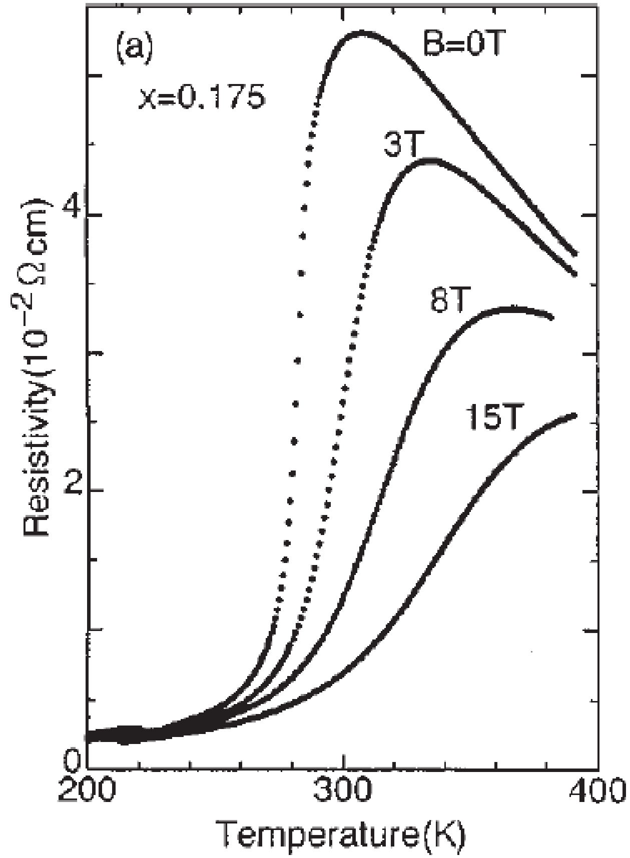
FIG. 70. Phase diagram for doped V_2O_3 systems, $(V_{1-x}Cr_x)_2O_3$ and $(V_{1-x}Ti_x)_2O_3$. From McWhan *et al.*, 1971, 1973.

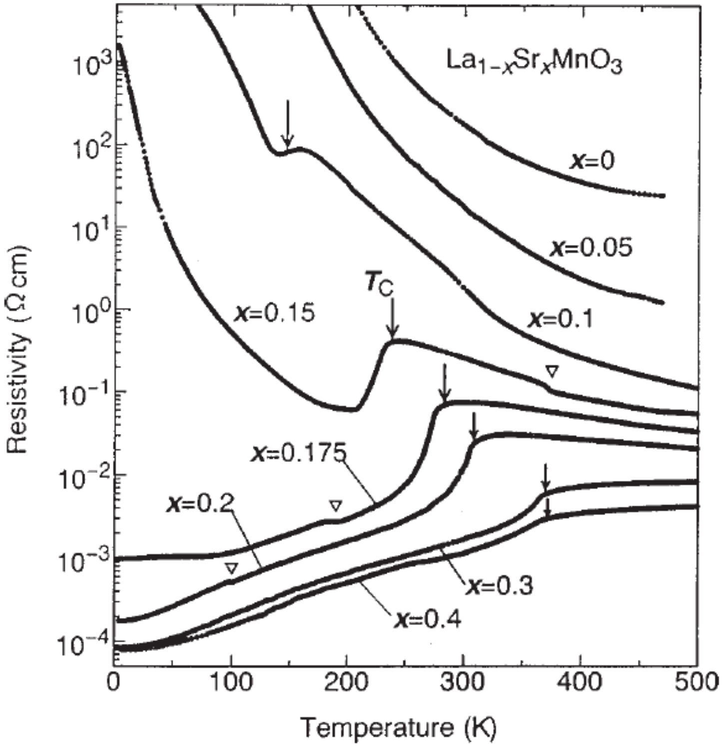
Big things/3

“Colossal” Magnetoresistance: $La_{1-x}Sr_xMnO_3$!







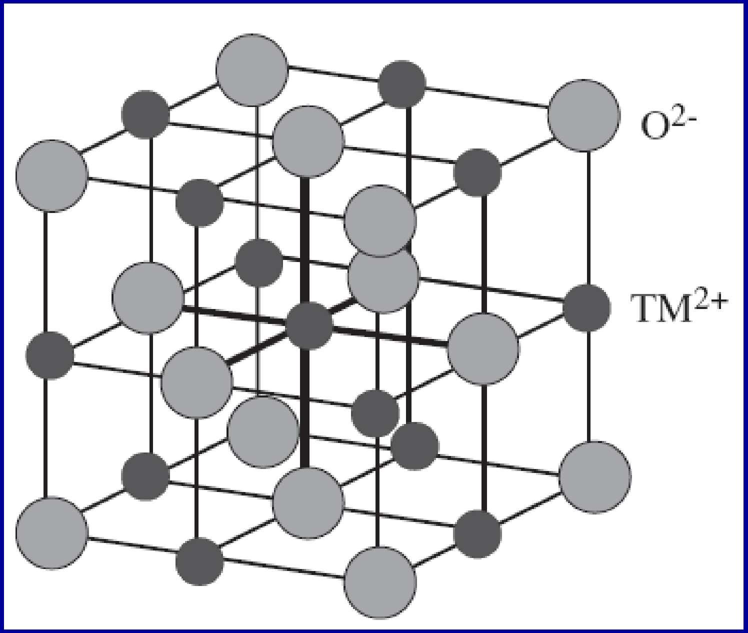


Large thermopower (Seebeck coefficient) of cobaltates, etc...

2. Structures

2.1 Monoxides **MO**: not much controllability…

NaCl structure



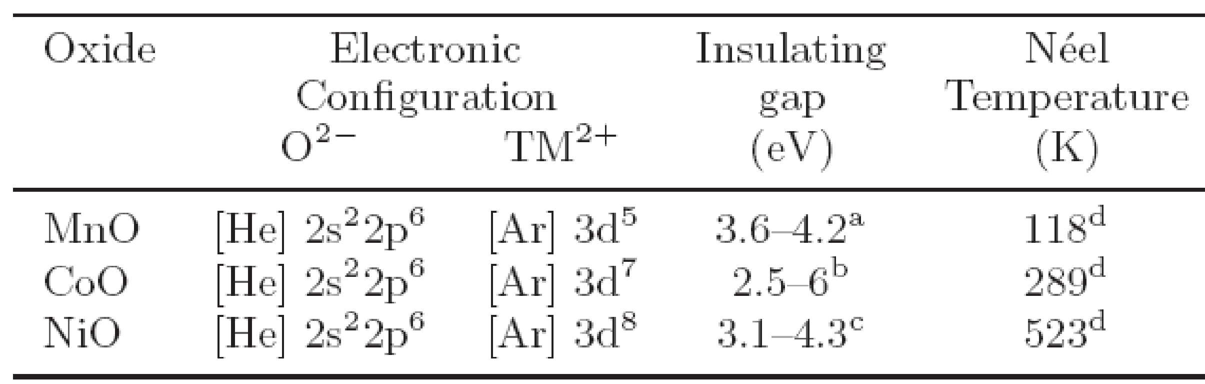
Nominal valences:
(quite ionic)
- Oxygen takes 2 electrons
- M gives out two electrons:
  → M^{2+}

TiO, VO: ~ metals (O-deficient)

MnO, CoO, NiO: Mott (or charge-transfer) magnetic insulators

– see below

(historic example: NiO)



Oxide	Electronic Configuration O^{2-}	Electronic Configuration TM^{2+}	Insulating gap (eV)	Néel Temperature (K)
MnO	[He] $2s^2 2p^6$	[Ar] $3d^5$	3.6–4.2[a]	118[d]
CoO	[He] $2s^2 2p^6$	[Ar] $3d^7$	2.5–6[b]	289[d]
NiO	[He] $2s^2 2p^6$	[Ar] $3d^8$	3.1–4.3[c]	523[d]

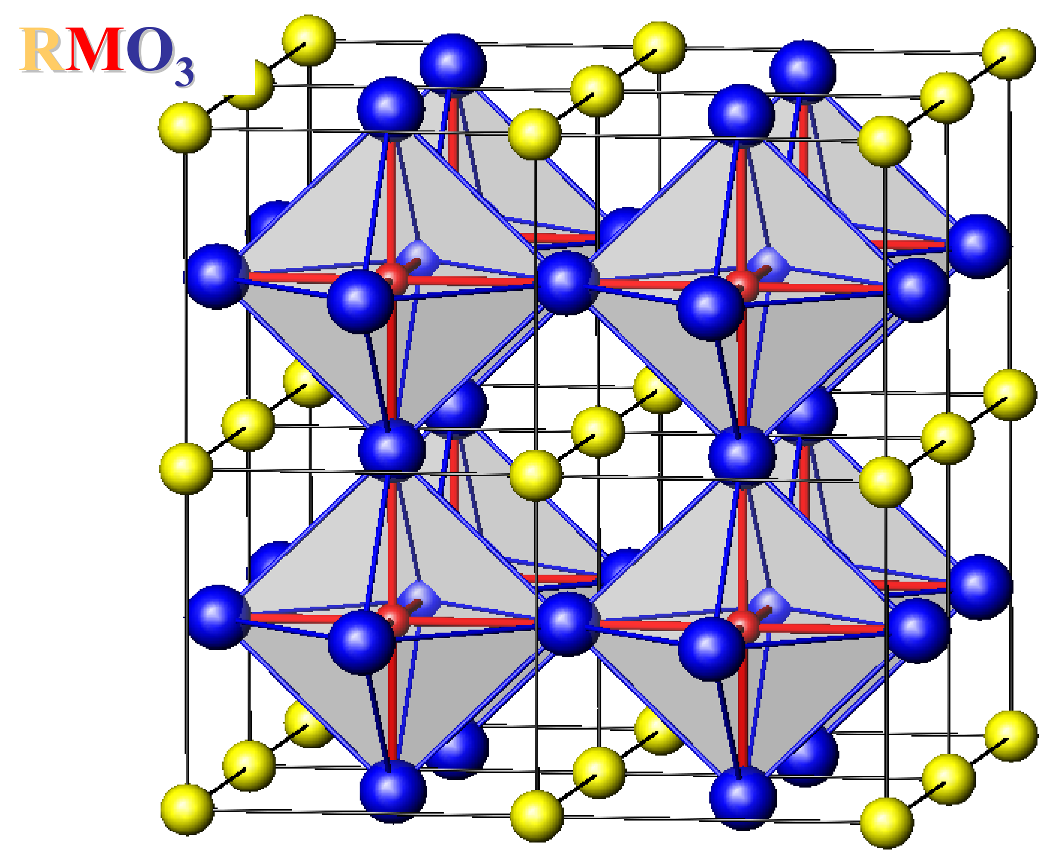
Ternary compounds (and more): the simple (and beautiful, too) perovskite structure and its descendants…

For example: $SrVO_3$

Perfectly cubic <u>perovskite</u> RMO_3 :

- transition-metal Ion M at center of oxygen octahedra
→MO_6 structural units

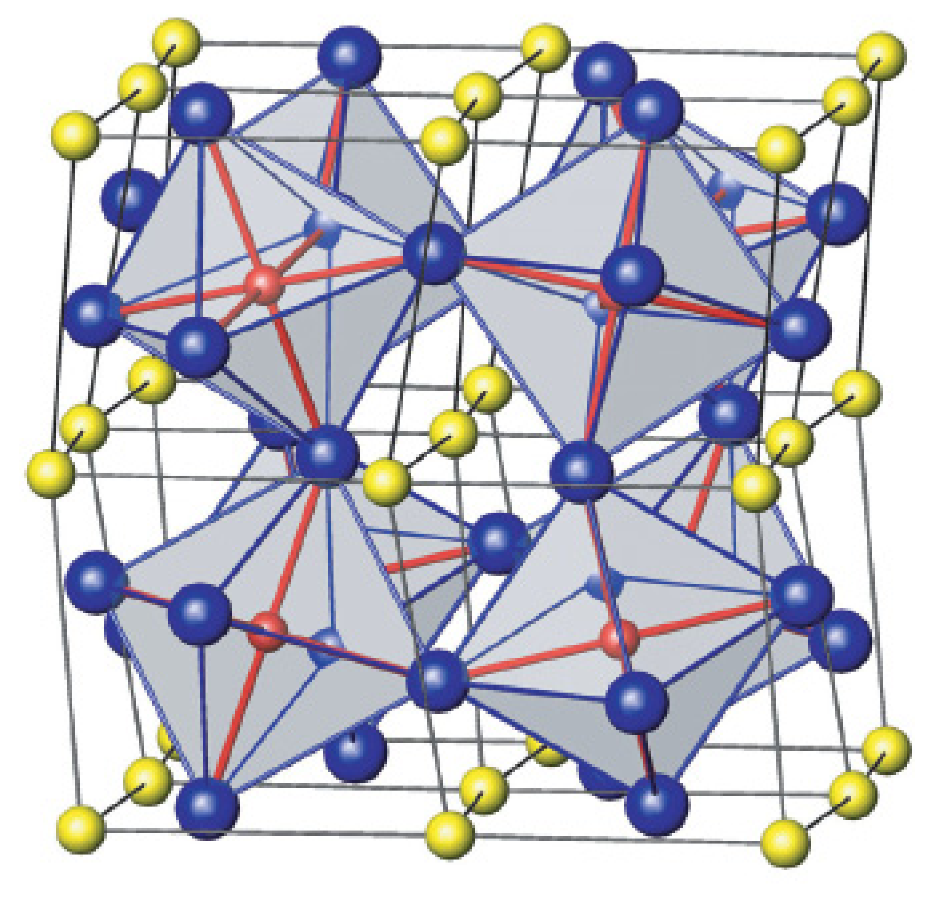
- e.g. rare-earth ions R form simple cubic lattice



[L.A Perovski 1792-1856
Oural mountains
discovery of CaTiO3 G.Rose, 1839]

Distorted perovskites

Depending on the ionic radii of the 3 ions, the material often Adopts a structure which breaks perfect cubic symmetry and Can be viewed as a distorted perovskite.



Example:

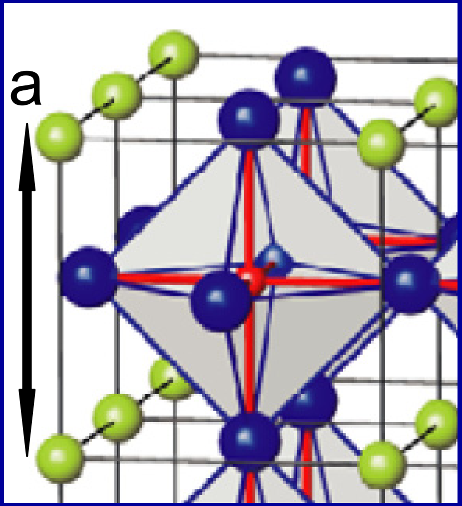
`$GdFeO_3$' distortion

- Octahedra remain perfect (no or very small Jahn-Teller)
- Rotation of octahedra along [010] and [001]
- Orthorombic symmetry
- 4 M-atoms per unit cell, all equivalent by symmetry
- M-O-M angle becomes π-θ

Other possible distortions e.g rhomboedric, rotation [111]

RMO_3 : ``tolerance factor''

- Consider close packing by hard spheres of radii r_R, r_M, r_O (ionic radii)
- Call a length of cubic cell



$$d(O-R)=\frac{a}{\sqrt{2}}\ ,\ d(O-M)=\frac{a}{2}$$

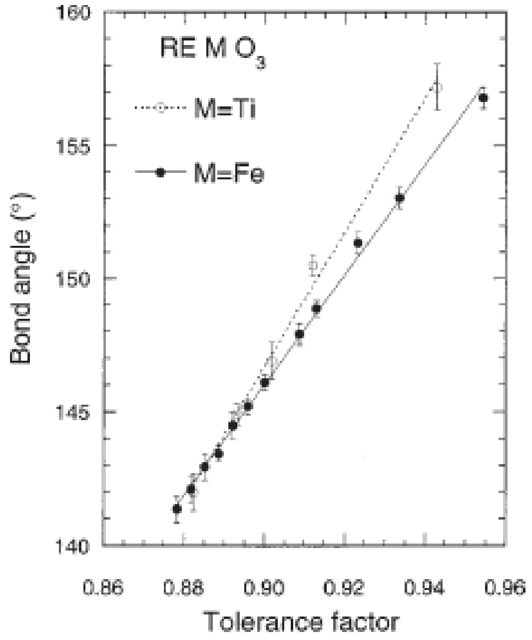


FIG. 62. The metal-oxygen-metal bond angles in an orthorhombically distorted perovskite ($GdFeO_3$-type) as a function of tolerance factor.

- Ideal packing will have:

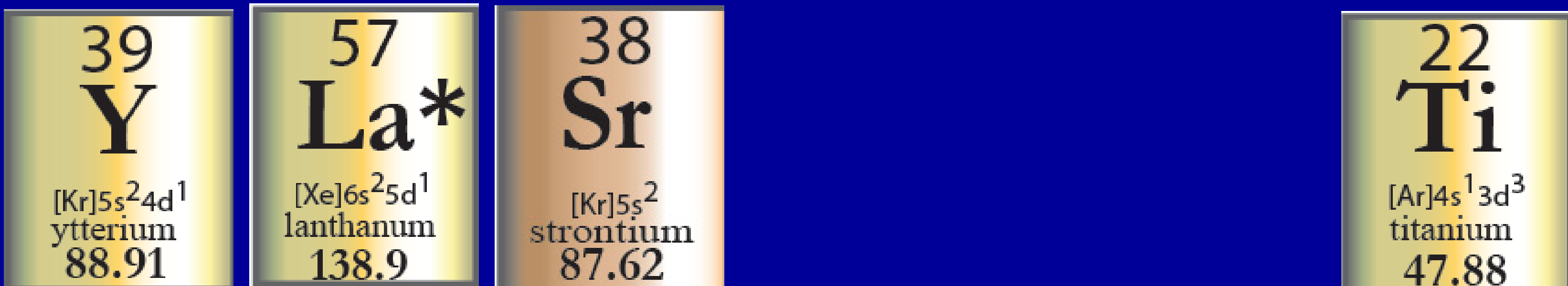
$$t\equiv\frac{r_R+r_O}{\sqrt{2}(r_M+r_O)}=1$$

* t=1: ideal cubic perovskite
* t<1: deforms to rhomboedral, then orthorombic
* t too small (<0.86): unstable

All this offers control on the material:

- Substitutions on R-site allow for a control of the (nominal) valence of M-ion
- e.g: $LaTiO_3$→La^{3+} [Xe], Ti^{3+} : [Ar]$3d^1$ config.
- SrTiO3→Sr^{2+} [Xe], Ti^{4+} : [Ar]$3d^0$ config.
- Iso-valent substitutions on R-site allow for a control of the distortion, hence of:

- Bandwidth (see below)
- And importantly of the splitting between d-levels



Controlling dimensionality: the Ruddlesden-Popper series $R_{n+1}M_nO_{3n+1}$ (`layered perovskite')

Unit-cell

n=2

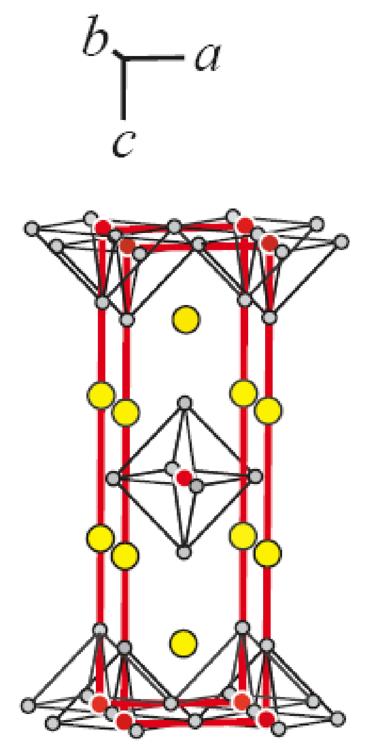
n=3

$Sr_3Ru_2O_7$

I4/mmm

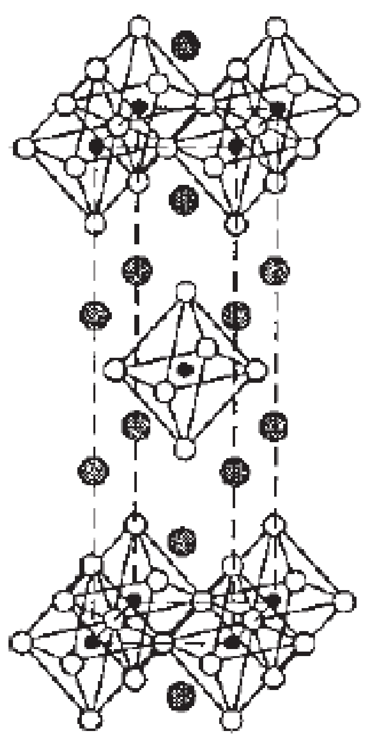
MO$_2$ layer →

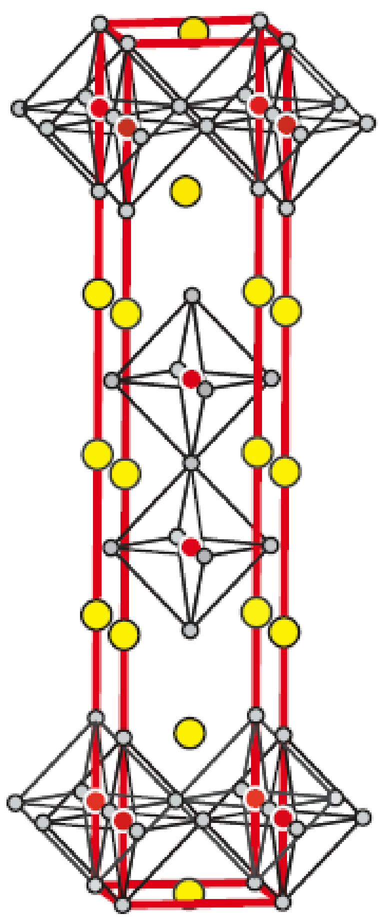
MO$_2$ layer →



I4/mmm

Sr_2RuO_4



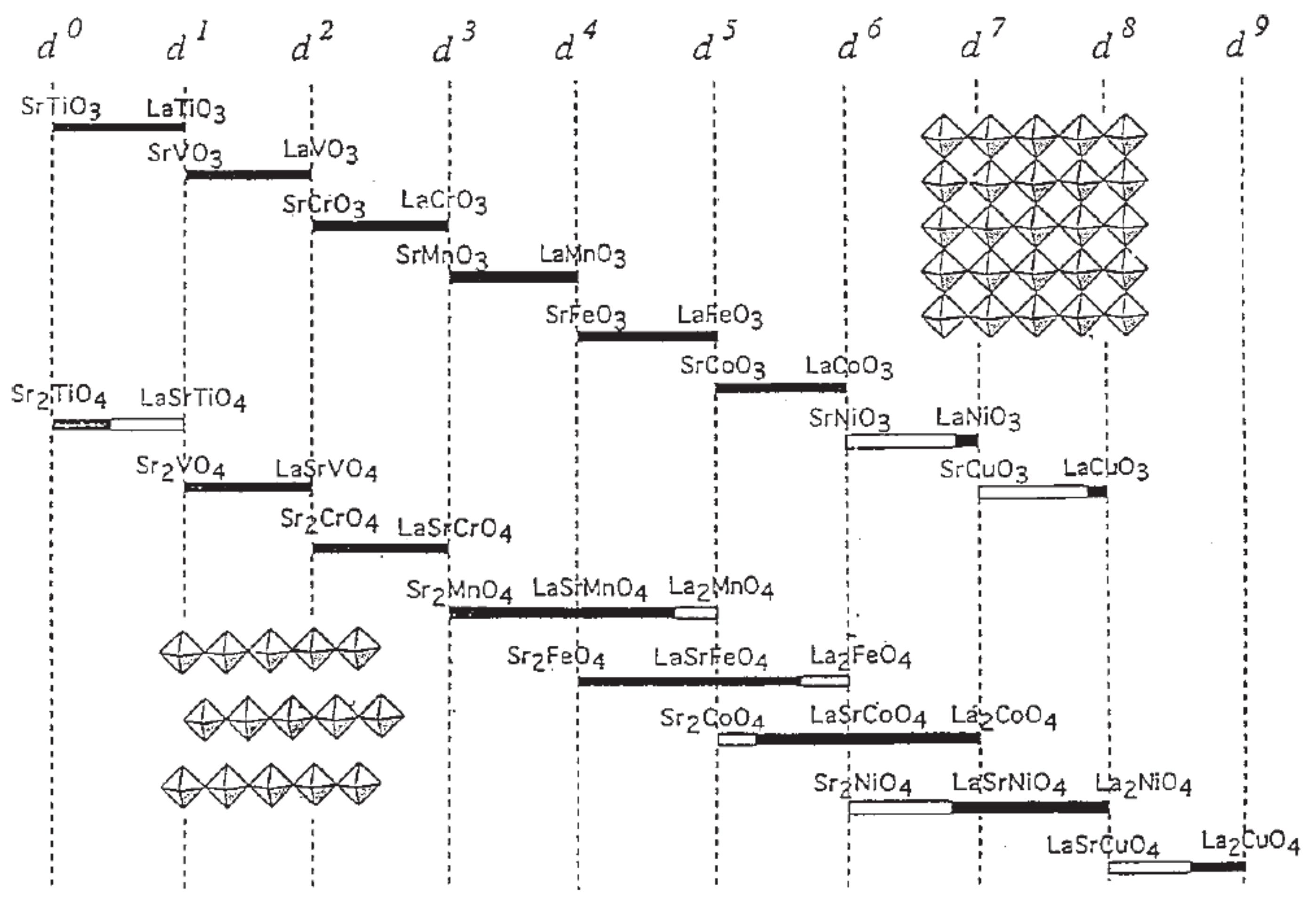


Increasing n : ``from d=2 to d=3''

Usual perovskite RMO_3 corresponds to n→infinity

Some examples:

alloying on R-site changes nominal valence of M



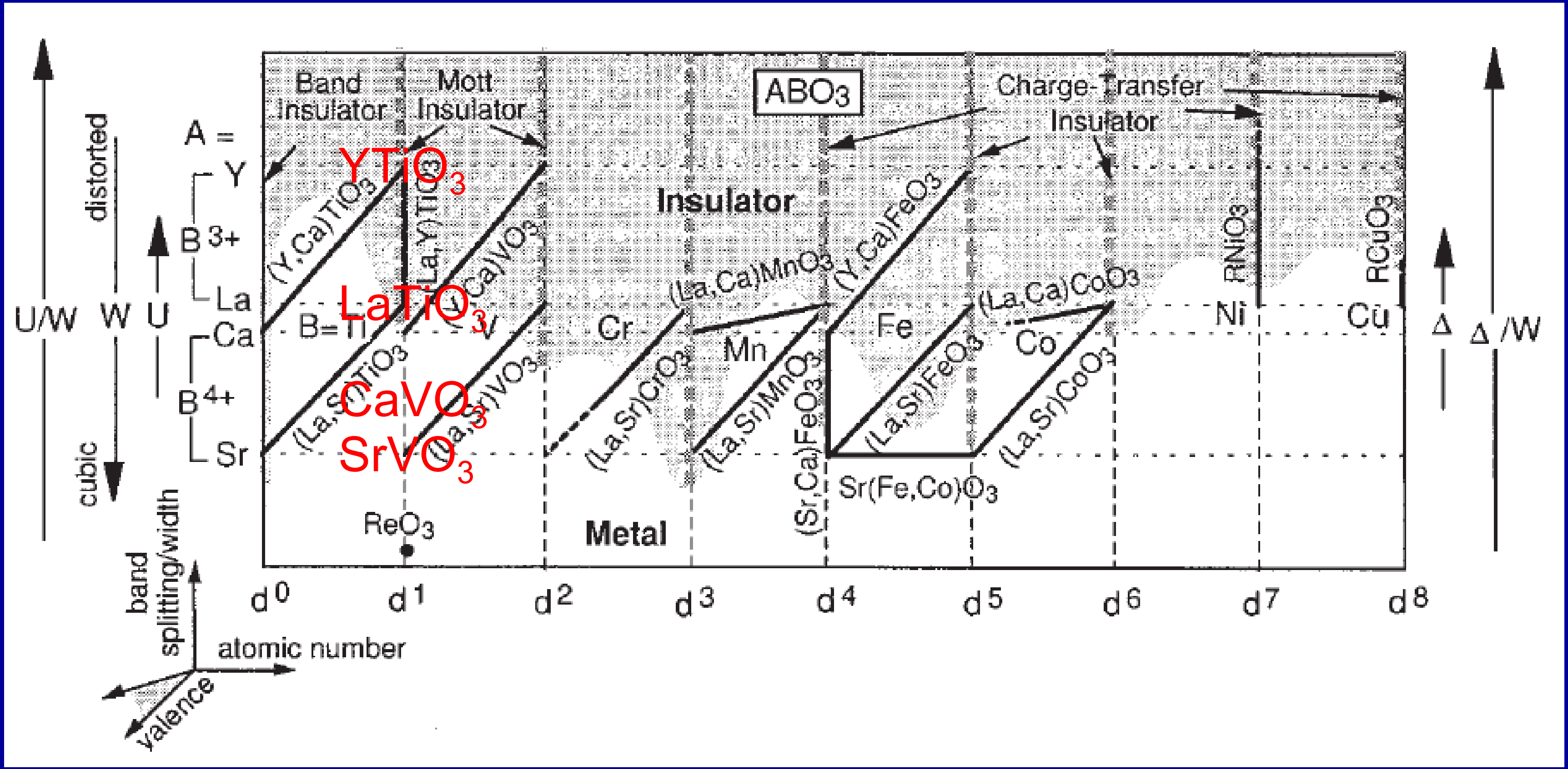
$Sr_{n+1}M_nO_{3n+1}$: $2(n+1)+4n-2(3n+1)=0$ →M remains 4+ for all n

e.g. M=Ti 3d^1 shell (titanates); M=Ru 4d^4 shell (ruthenates)

$La_{n+1}M_nO_{3n+1}$: La^{3+} →nominal valence of M is $(3n-1)/n$ +

e.g. $(La,Ba)_2CuO_4$ first discovered hi-Tc SC

3. The Mott phenomenon plays a key role

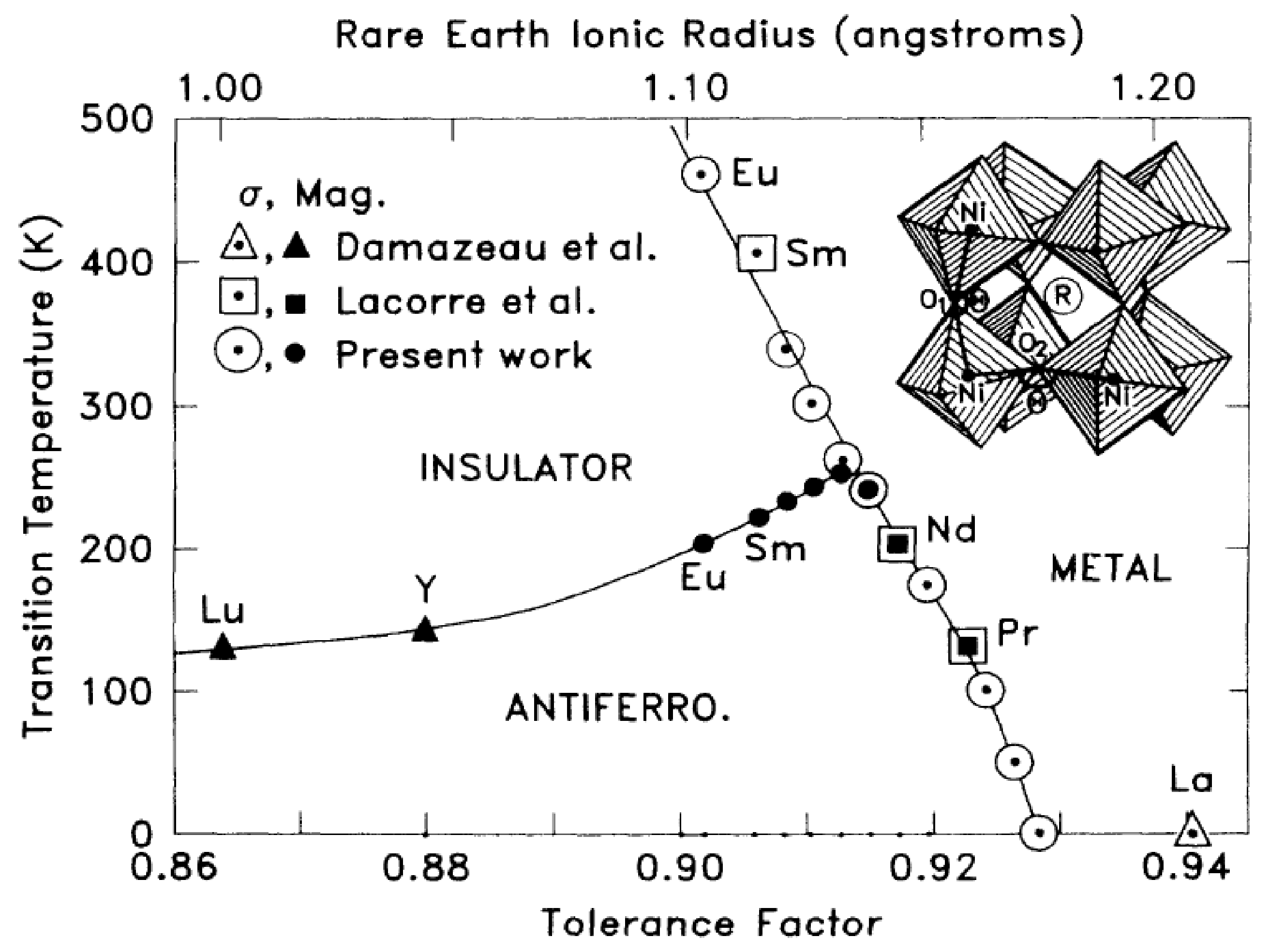


\`\`Atsushi Fujimori’s map of RMO_3 perovskites’’

J.Phys Chem Sol. 53 (1992) 1595

Partially filled d-shells… and yet often insulators

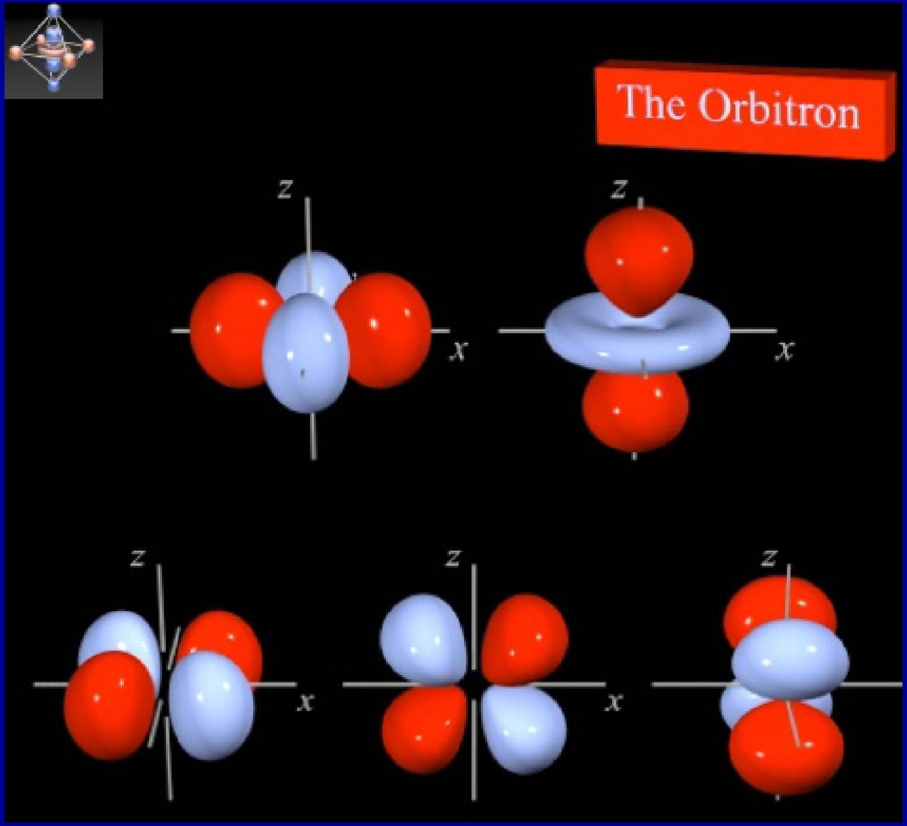
The $RNiO_3$ $3d^7$ compounds



Torrance at al. Phys Rev B 45 (1992) 8209

4. Orbitals: from the isolated atom to the solid - crystal-field splitting – (Bethe, van Vleck)

Cubic-symmetry adapted 3d-orbitals:



3d orbitals are quite localized:
- No nodes in radial part
- Large centrifugal barrier $l(l+1)/r^2$

$$d_{x^2-y^2}\ ,\ d_{3z^2-r^2}$$

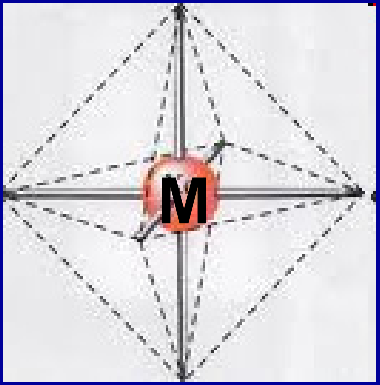
→ The e_g doublet

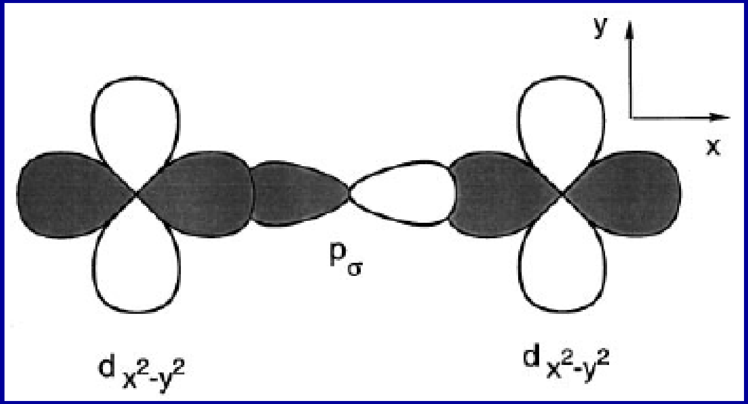
$$d_{xy}\ ,\ d_{xz}\ ,\ d_{yz}$$

→ The t_{2g} triplet

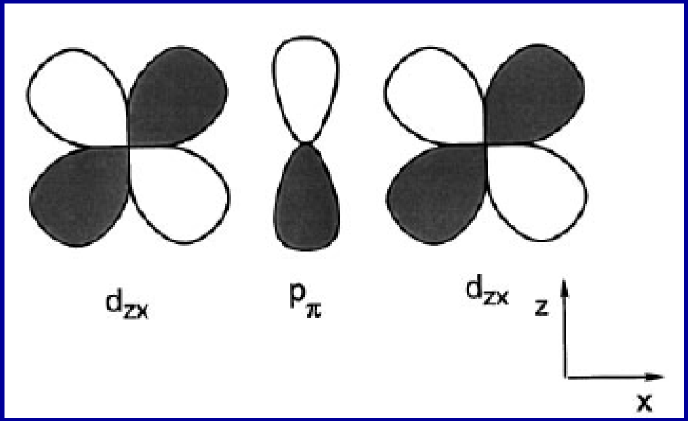
http://winter.group.shef.ac.uk/orbitron

Crystal-field splitting in octahedral environment :





eg orbitals point towards oxygen atoms(sigma-bonding)
→feel larger Coulomb potential
→ pushed to higher energy



t2g orbitals point away from oxygen atoms(pi-bonding)
→feel smaller Coulomb potential
→ lower energy than eg

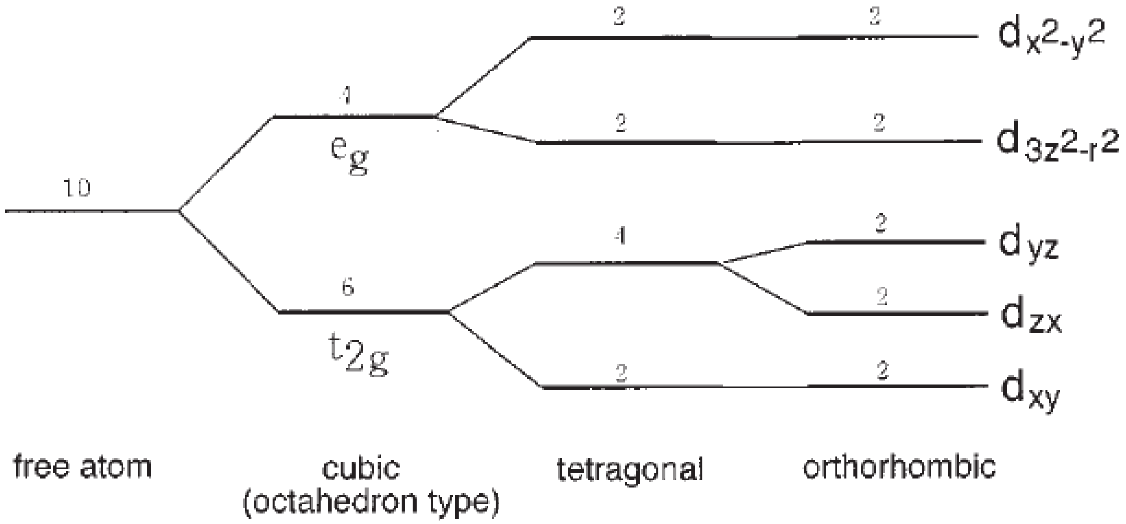


FIG. 2. Crystal-field splitting of $3d$ orbitals under cubic, tetragonal, and orthorhombic symmetries. The numbers cited near the levels are the degeneracy including spins.

Lowering further the crystal symmetry (distort from cubic)
Induces additional lifting of degeneracy

Tetrahedral environment (MO_4):
eg has lower energy, t2g higher

A crystal-field theory primer…

Hydrogen atom wave-functions with $l = 2$ (d-shell). Spherical coordinates: $\vec{r} = r\,(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\phi)$.

$$\psi_m(\theta,\phi) = R(r)\,Y_2^m(\theta,\phi)$$

with:

$$Y_2^0 \sim 3\cos^2\theta - 1\ ,\ Y_2^{\pm1} \sim \sin 2\theta\, e^{\pm i\phi}\ ,\ Y_2^{\pm2} \sim \sin^2\theta\, e^{\pm 2i\phi}$$

Cubic harmonics, transforming under irreducible representations of cubic group:

$$xy\ :\ \chi_{xy}(\theta,\phi) \sim \frac{xy}{r^2} \sim \sin\theta\cos\phi\sin\theta\sin\phi \sim \sin^2\theta\sin 2\phi \sim Y_2^{+2} - Y_2^{-2}$$

Similarly:

$$\chi_{xz} \sim Y_2^{+1} + Y_2^{-1}\ ,\ \chi_{yz} \sim Y_2^{+1} - Y_2^{-1}\ ,\ \chi_{x^2-y^2} \sim Y_2^{+2} + Y_2^{-2}\ ,\ \chi_{3z^2-r^2} \sim Y_2^0$$

MO_6 octahedron: Potential created by point charge on O-sites at center of cube, d being distance to center:

$$V(\vec{r}) \equiv \frac{Ze^2}{4\pi\varepsilon_0}\sum_{i=1}^{6}\frac{1}{||\vec{r} - \vec{R}_i||} \qquad (3.1)$$

Expand:

$$\frac{4\pi\varepsilon_0}{Ze^2}V(r) = \frac{6}{d} + \frac{7\sqrt{\pi}}{3}\frac{r^4}{d^5}\left[Y_4^0(\theta,\phi) + \sqrt{\frac{5}{14}}(Y_4^4(\theta,\phi) + Y_4^{-4}(\theta,\phi))\right] + \cdots \tag{3.2}$$

Treat second term as perturbation $\delta V(r,\theta,\phi)$: breaks spherical symmetry. Because of proper choice of cubic orbital above:

$$\begin{aligned} \langle\chi_m|\delta V|\chi_{m'}\rangle &= \Delta_t\,\delta_{mm'}\,\text{for}\,m = xy, xz, yz \\ &= \Delta_e\,\delta_{mm'}\,\text{for}\,m = x^2-y^2, 3z^2-r^2 \end{aligned}$$

with:

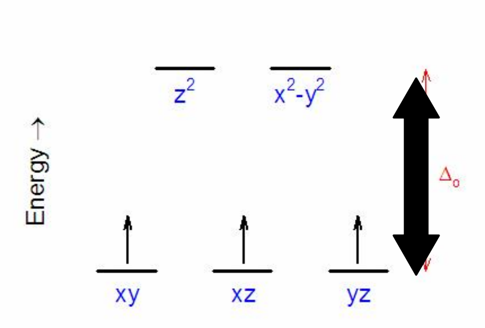
$$\boxed{\Delta_e - \Delta_t = 1.67\,\frac{Ze^2}{4\pi\varepsilon_0\,d^5}\int_0^\infty r^4 R(r)^2\,r^2 dr \equiv \text{“}10\,Dq\text{''}}$$

As is well-known, this explains e.g. why ruby is red/violet… Cf e.g: http://www.chm.davidson.edu/vce/CoordChem/CFT.html

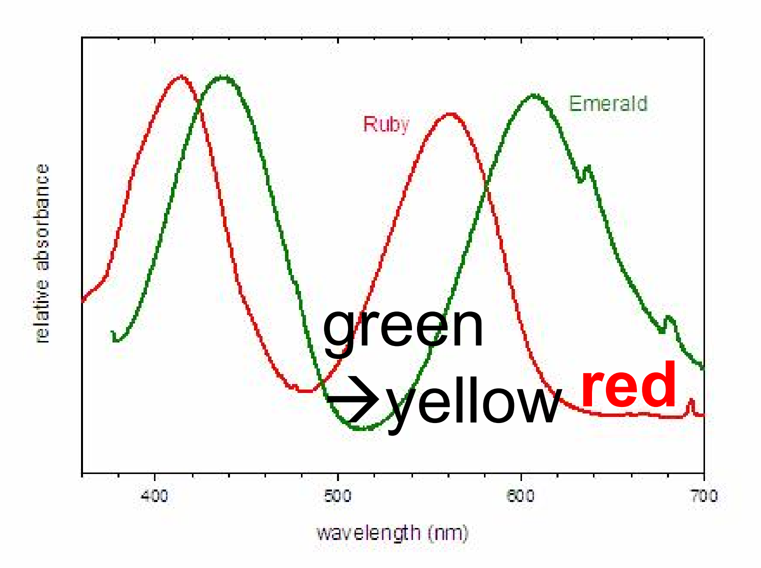
Ruby: small amount Of Cr $^{3+}$ impurities Substituting Al^{3+} in Al_2O_3 (corundom), a large-gap transparent insulator

Cr3+ ($3d^3$) 3 electrons in t_{2g} shell

$$\Delta_0 = 2.21\,\mathrm{eV} \to \lambda \simeq 561\,\mathrm{nm}$$

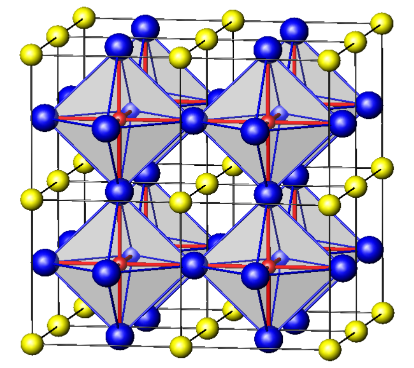


absorption of most visible wavelength beyond red

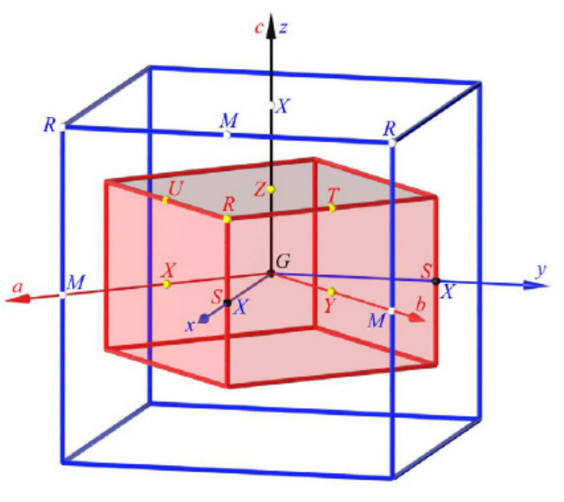


5. From the atom to the full solid: energy bands of oxides

(or: how to make sense of a plate of spaghettis…)



A simple case: cubic $SrVO_3$



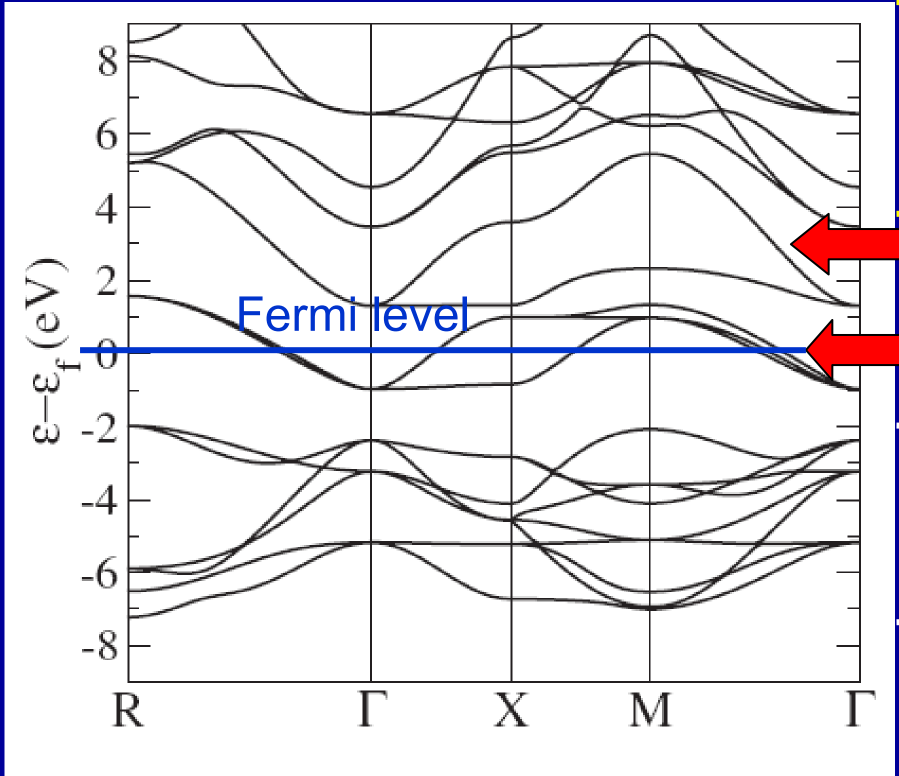


FIG. 1. LDA band structure for $SrVO_3$.

Sr 5s and 4d

2 V-eg bands

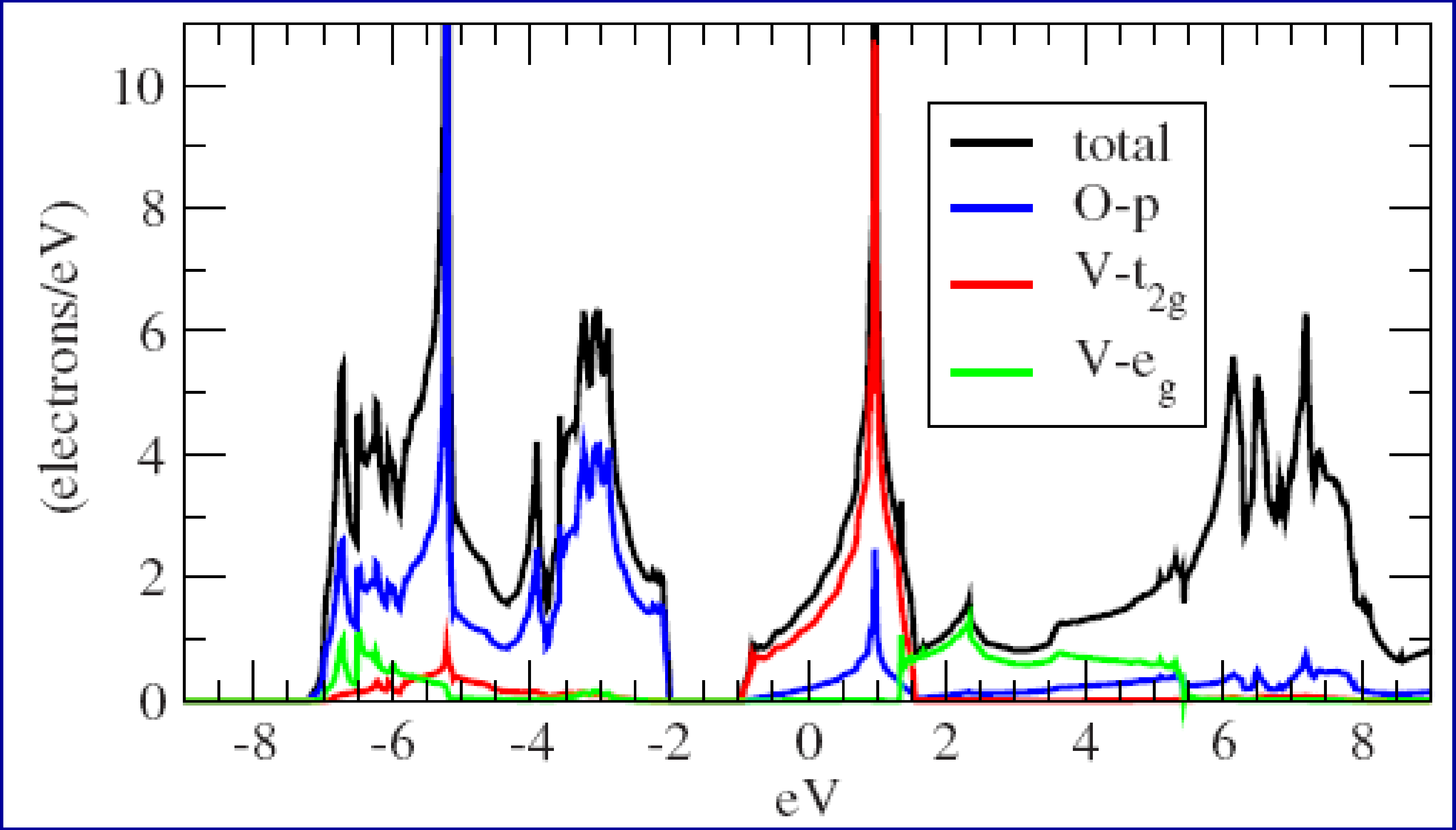
3 V-t2g bands

9=3*3 Oxygen bands

Pavarini et al.
PRL 92 (2004) 176403
New J.Phys 7 (2005) 188
Amadon et al.
PRB 77 (2008) 205112

Density of states:

(orbitally-resolved, i.e projected on ~ atomic orbitals)



Strong mixing of V-eg states with oxygen

t2g bandwidth ~ 2.6 eV

To understand orbital character better, plot `fat bands':

Project Bloch functions onto atomic-like orbitals and plot matrix element at each k-point: $|\langle\psi_{\mathbf{k}\nu}|\phi_{lm}\rangle|^2$

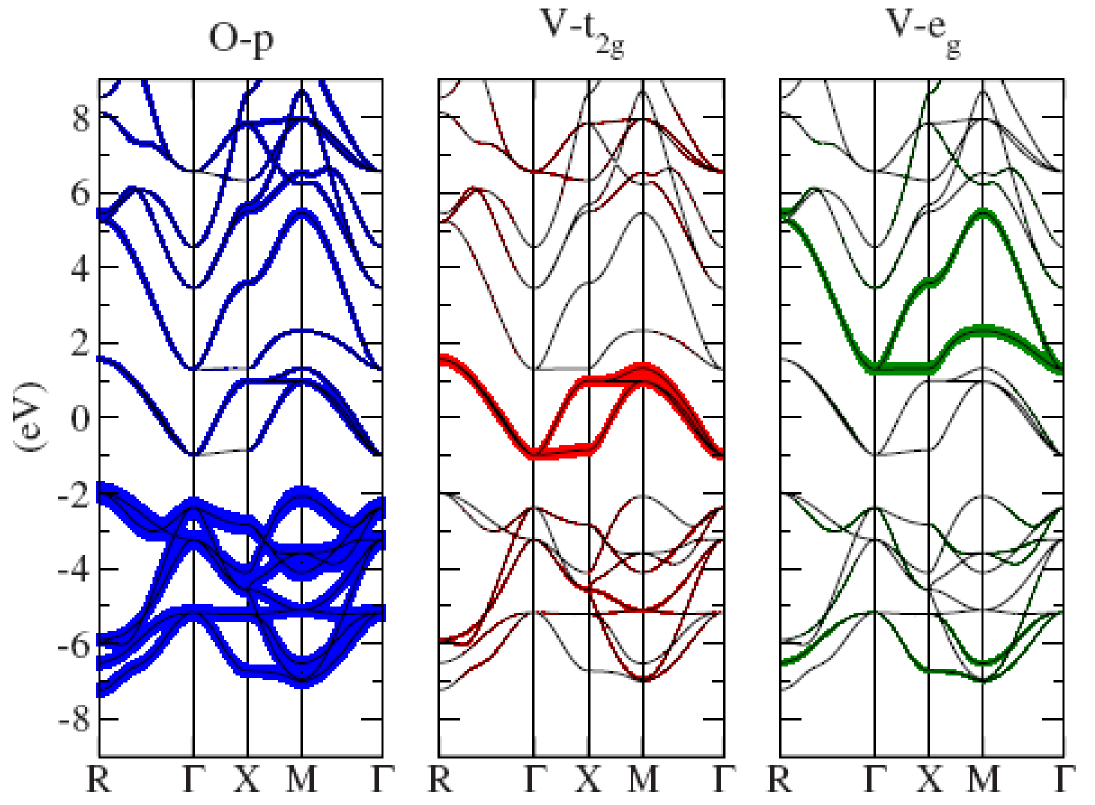


FIG. 3. (Color online) LDA band structure for $SrVO_3$ computed in PAW, with "fatbands" to show the amplitude of the projection of each band on a given atomic orbital (O p, V t_{2g}, and V e_g).

Mixing of oxygen with d-states obvious, especially for eg

Summarize key infos from band-structure, in this (quite) simple case:

- t_{2g} manifold of 3 bands well-separated from oxygen (below) and e_g bands (above)
- t2g bands occupied by 1 electron in total (as requested)
- t2g bandwidth around 2.6 eV
- Distance between center of t2g and center of oxygen band: about 6.5 eV (only 1eV from top of O to bootom of t2g though) → `charge-transfer energy' is large
- Bandstructure (LDA) is that of a METAL
- Effective mass (from specific heat) is found to be roughly a factor of 2 larger than the one from LDA

More on the bandwidth: hopping is *via oxygen*

- Each Vanadium is in a cage of 6 oxygens

→Direct d-d hopping is difficult, hence direct t_{dd} is small
(this is one of the two main differences between a pure Transition metal and its oxide, the other one being that the 4s orbital is empty in the oxyde → oxydes have narrow bands)

- Hopping of electrons on V-sites occurs through hybridization between O p-orbitals and V d-orbitals, with amplitude t_{pd}

-Roughly, when the charge-transfer energy Δ is large, the amplitude of the effective d-d hopping is of order:

$$t_{\text{eff}}^{dd} \sim t_{pd}^2/\Delta$$

Hence, theorist’s model of an oxide:

(1 electron part of the hamiltonian, for interactions, see later)

$$-t_{pd}\sum_{\langle ij\rangle}(d_i^\dagger p_j+\text{h.c.})+\Delta\sum_{i}(d_i^\dagger d_i-p_i^\dagger p_i)+\text{p}-\text{p hoppings}+\cdots$$

p-d hopping

Charge-transfer energy

Other stuff

Here, I didn’t write orbital indices, which are of course crucial in the real world !

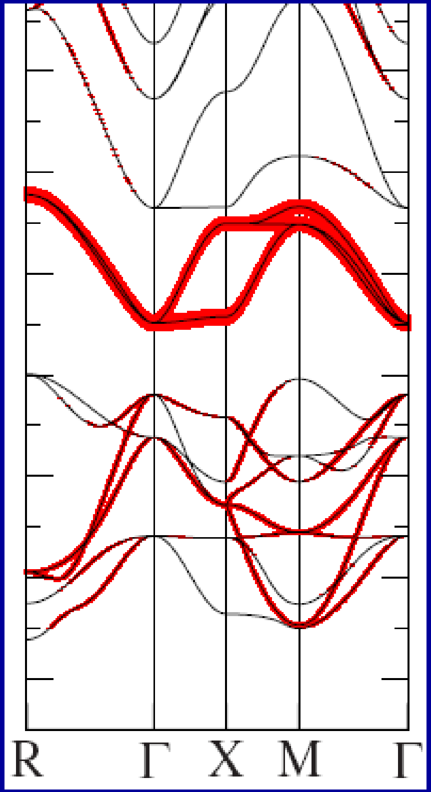
For large Δ, and t $_{pp}$=0, we may even want to `integrate out’ the oxygens to get a tight-binding model for the d-bands only:

$$-t_{dd}^{\text{eff}}\sum_{\langle ij\rangle}(d_i^\dagger d_j+\text{h.c.})$$

$$t_{\text{eff}}^{dd}\sim t_{pd}^2/\Delta$$

To give a realistic meaning to this, use Wannier functions:

1) Decide for which bands (or rather: for which energy window) an effective model will be constructed



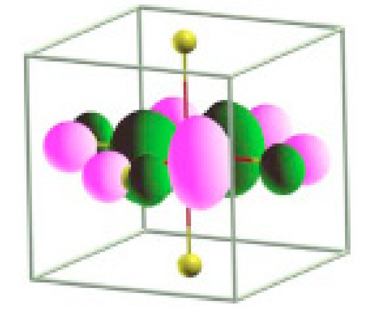
V-t_{2g} states only
(3 bands)

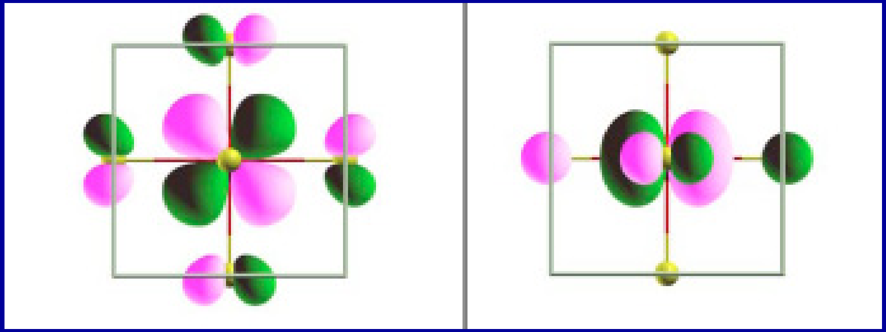
V-t2g and eg states
And O –states
(14 bands)

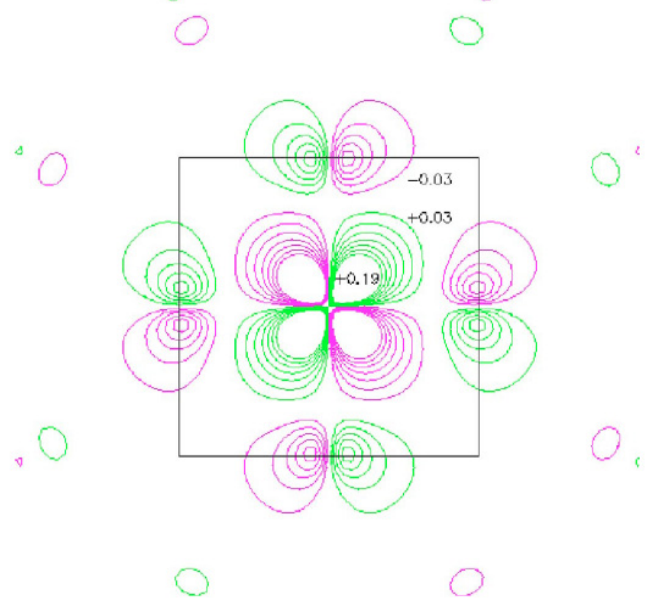
Small energy window
→Wannier functions will leak on oxygen sites to capture V-O hybridization

Large energy window
→Wannier functions are quite localized and atomic-like

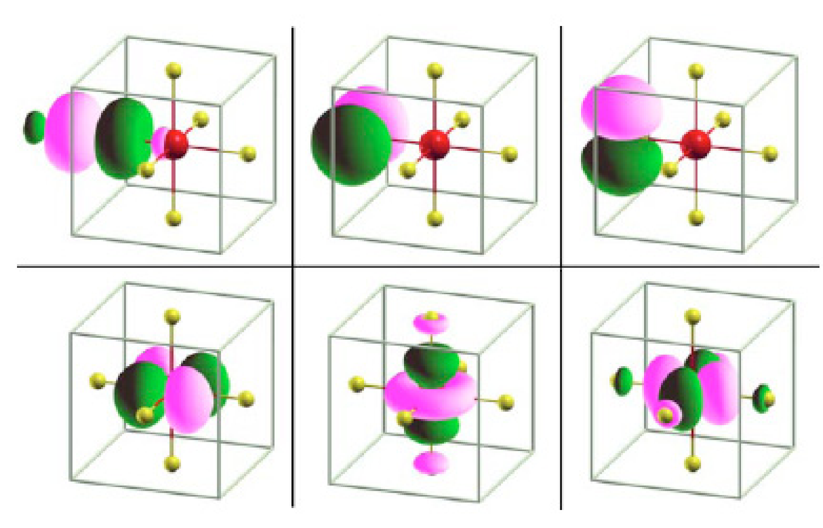
t2g only: extended Wanniers







V t2g+eg and O: localized Wanniers



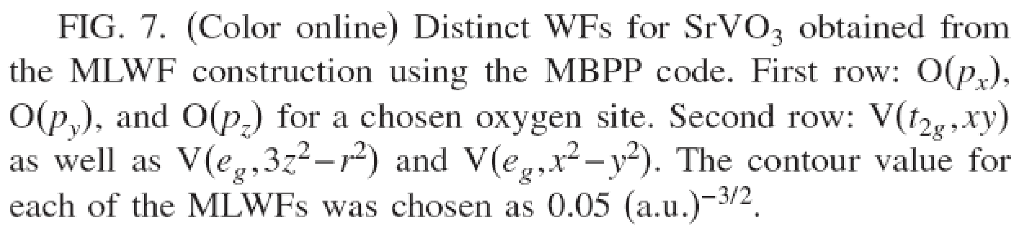


FIG. 7. (Color online) Distinct WFs for $SrVO_3$ obtained from the MLWF construction using the MBPP code. First row: $O(p_x)$, $O(p_y)$, and $O(p_z)$ for a chosen oxygen site. Second row: $V(t_{2g},xy)$ as well as $V(e_g,3z^2-r^2)$ and $V(e_g,x^2-y^2)$. The contour value for each of the MLWFs was chosen as 0.05 $(\text{a.u.})^{-3/2}$.

F.Lechermann et al.
Phys Rev B 74 (2006) 125120

Hopping integrals between Wannier functions (ab-initio tight-binding description)

An example (!): $CaVO_3$ – slight distortion from cubic symmetry

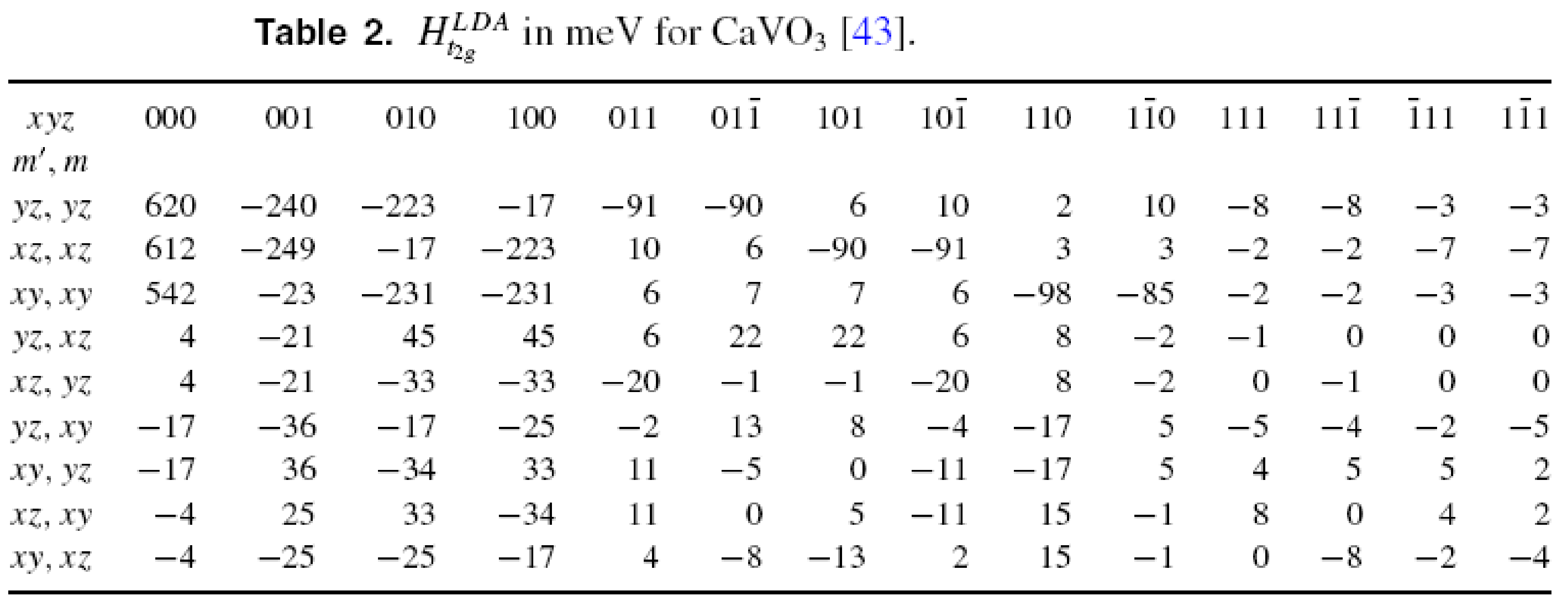
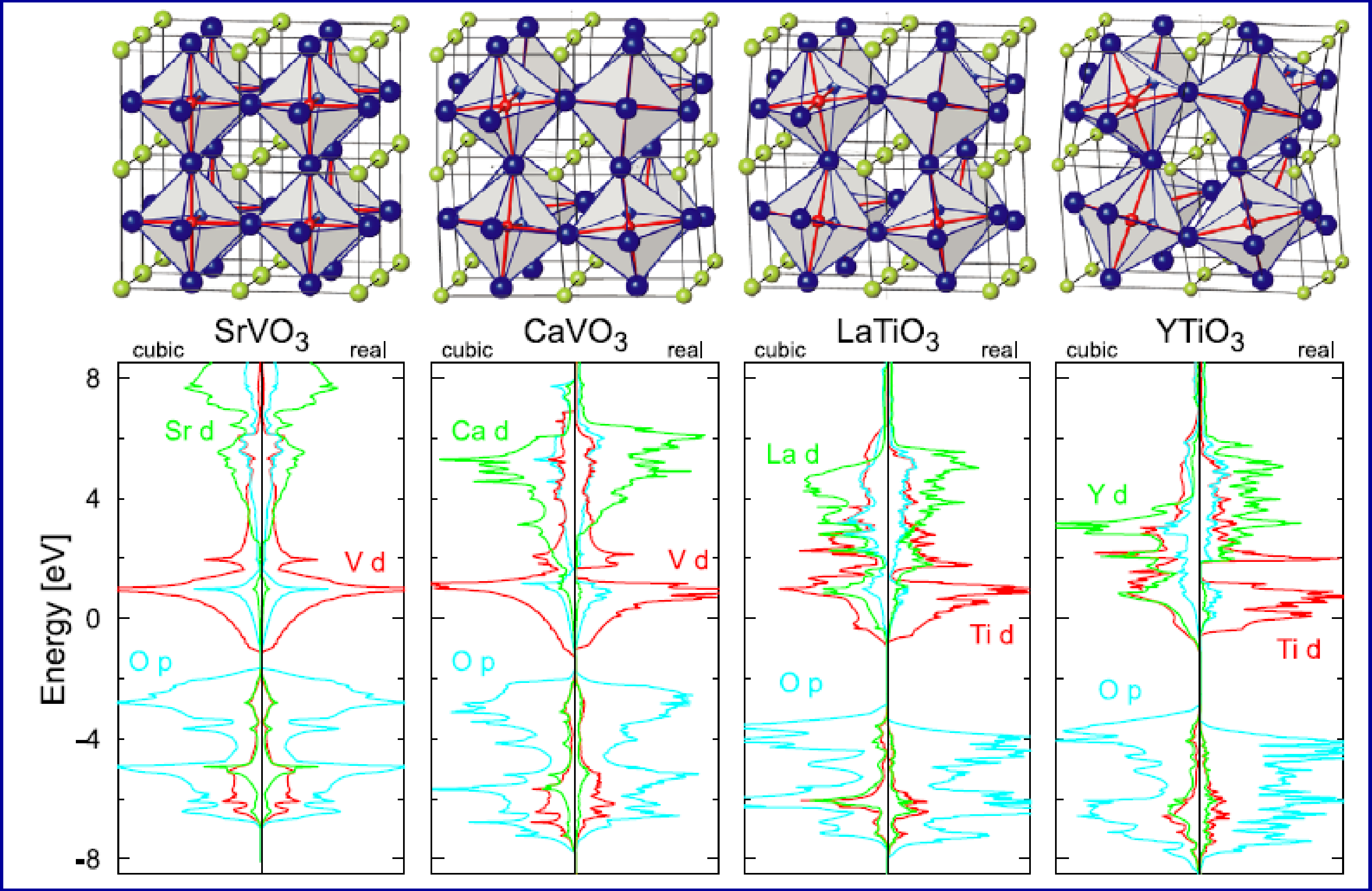


Table 2. $H^{LDA}_{t_{2g}}$ in meV for $CaVO_3$ [43].

xyz	000	001	010	100	011	$01\bar{1}$	101	$10\bar{1}$	110	$1\bar{1}0$	111	$11\bar{1}$	$\bar{1}11$	$1\bar{1}1$
m', m														
yz, yz	620	−240	−223	−17	−91	−90	6	10	2	10	−8	−8	−3	−3
xz, xz	612	−249	−17	−223	10	6	−90	−91	3	3	−2	−2	−7	−7
xy, xy	542	−23	−231	−231	6	7	7	6	−98	−85	−2	−2	−3	−3
yz, xz	4	−21	45	45	6	22	22	6	8	−2	−1	0	0	0
xz, yz	4	−21	−33	−33	−20	−1	−1	−20	8	−2	0	−1	0	0
yz, xy	−17	−36	−17	−25	−2	13	8	−4	−17	5	−5	−4	−2	−5
xy, yz	−17	36	−34	33	11	−5	0	−11	−17	5	4	5	5	2
xz, xy	−4	25	33	−34	11	0	5	−11	15	−1	8	0	4	2
xy, xz	−4	−25	−25	−17	4	−8	−13	2	15	−1	0	−8	−2	−4

Effect**s** of the orthorombic distortion: $SrVO_3$, $CaVO_3$,$LaTiO_3$,$YTiO_3$ (all d^1, ***ALL METALS in LDA !)***



Left panels: hypothetical cubic; Right panel: real structure

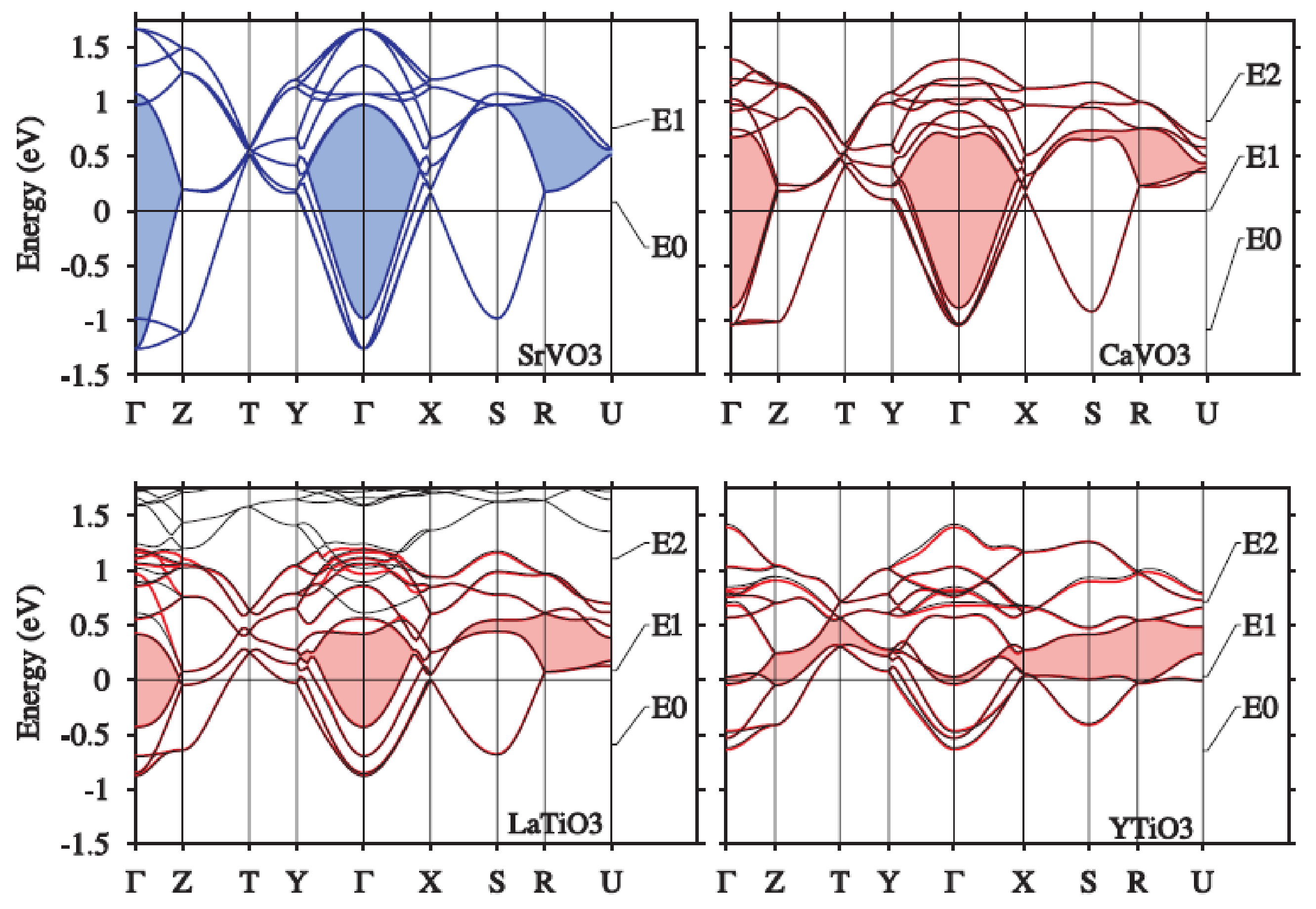


Figure 10. Low-energy LDA bandstructures of $SrVO_3$, $CaVO_3$, $LaTiO_3$, and $YTiO_3$. The cubic bands for $SrVO_3$ (figure 3) have been folded into the orthorhombic BZ (figure 9). The black bands were obtained with a large NMTO basis, while the coloured ones were obtained with the truly-minimal B $d(t_{2g})$ basis. The two are indistinguishable, except for $LaTiO_3$ where the bottom of the La 5*d*-band overlaps the top of the Ti t_{2g}-band because the older structural data [44] was used here. With the recent, slightly more distorted structure [12], O-A covalency removes this overlap as discussed in section 2 and figure 1, and as shown in figures 4, 12, and 17. In order to emphasize the development of the bandstructure along the series, the gap between the lower 1/3 and the upper 2/3 of the bands has been shaded.

Distortion: covalency between O and cation (Sr,La)

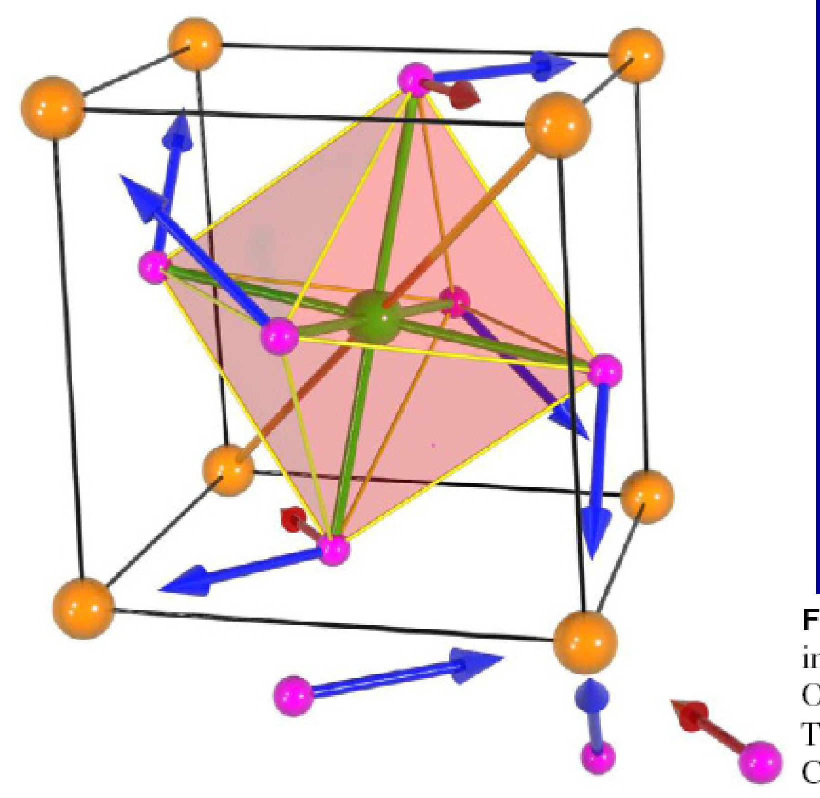


Figure 7. Schematic representation of the O-A covalent bonds shown for $LaTiO_3$ in figures 5 and 6: O1 binds to *two* while O2 binds to *one* of the four A-neighbours. One of the two O1-A bonds is relatively weak and is indicated by a short, red arrow. The resulting $GdFeO_3$-type distortion shortens the O-A bonds correspondingly. In $CaVO_3$, $LaTiO_3$, and $YTiO_3$, the shortest O1-A bond is shortened by respectively 10, 17, and 28% with respect to the average, the 2nd-shortest O1-A bond by respectively 4, 11, and 23%, and the shortest O2-A bond by respectively 12, 16, and 22%. The oxygen coordination of the A-ion is reduced from 12 to 4, with two of the near oxygens being in the horizontal, flat face of the distorted A-cube, and the two others in *one* of the vertical, buckled faces. The A-B-A diagonal (orange bar) lying in the plane of the short, red arrows is shortened by respectively 3, 7, and 9% of the average. The unit shown is the front bottom left one (subcell 1) seen in e.g. figure 2.

The two effects of distortion:

- 1) Reduction of total t2g bandwidth:

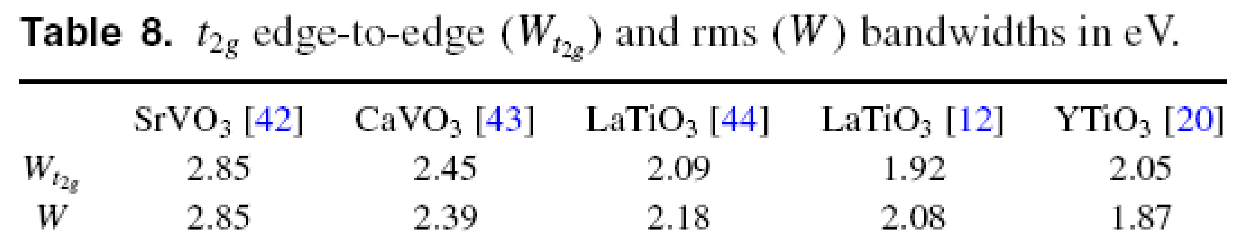


Table 8. t_{2g} edge-to-edge ($W_{t_{2g}}$) and rms (W) bandwidths in eV.

	SrVO$_3$ [42]	CaVO$_3$ [43]	LaTiO$_3$ [44]	LaTiO$_3$ [12]	YTiO$_3$ [20]
$W_{t_{2g}}$	2.85	2.45	2.09	1.92	2.05
W	2.85	2.39	2.18	2.08	1.87

This is because the O-M-O bond is no longer straight
→ pi-bonding less efficient

-2) Splitting between t2g orbitals (lifting of orbital degeneracy)

(140,200) meV for LaTiO3 ; (200,330) meV for YTiO3

→***Both effects*** are responsible for the Mott insulating state of LaTiO3 and YTiO3

(Some) Bibliography

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- N.Tsuda et al. *Electronic conduction in oxides*, Springer 2000
- N.F. Mott *Metal-insulator transitions, 2nd ed, Taylor&Francis 2000*
- M.Imada, A.Fujimori and Y.Tokura*, Metal-insulator transitions,* Rev. Mod. Phys. 70 (1998) 1039.
- W.A. Harrison *Electronic structure and the properties of solids*, Dover, 1989

Next week (lecture 6) :

More on the Mott transition in oxides
(theory and experiments) …