COLLÈGE DE FRANCE
1530

Chaire de Physique de la Matière Condensée

Cuprates supraconducteurs : où en est-on ?

Antoine Georges

Cycle 2010-2011
Cours 1 – 9/11/2010

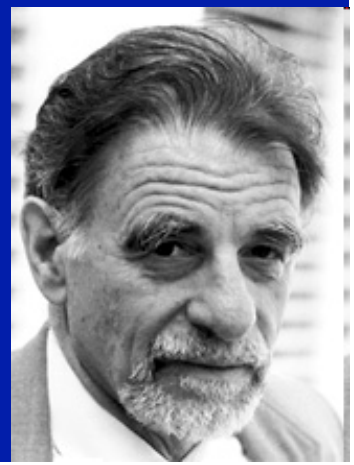
Some introductory remarks

- ***An amazing discovery…***

Bednorz, J.G. et K.A. *Muller*,
Possible high-Tc superconductivity in the Ba-La-Cu-O system.
Zeitschrift fur Physik B-Condensed. Matter, 1986

The Nobel Prize in Physics 1987

"for their important break-through in the discovery of superconductivity in ceramic materials"



- ***A tremendous research effort, which has boosted most experimental techniques and triggered the development of new ones.***

Cf. e.g. 2011 Buckley prize of APS to ARPES pioneers
J.C. Campuzano, P.Johnson and Z.X. Shen

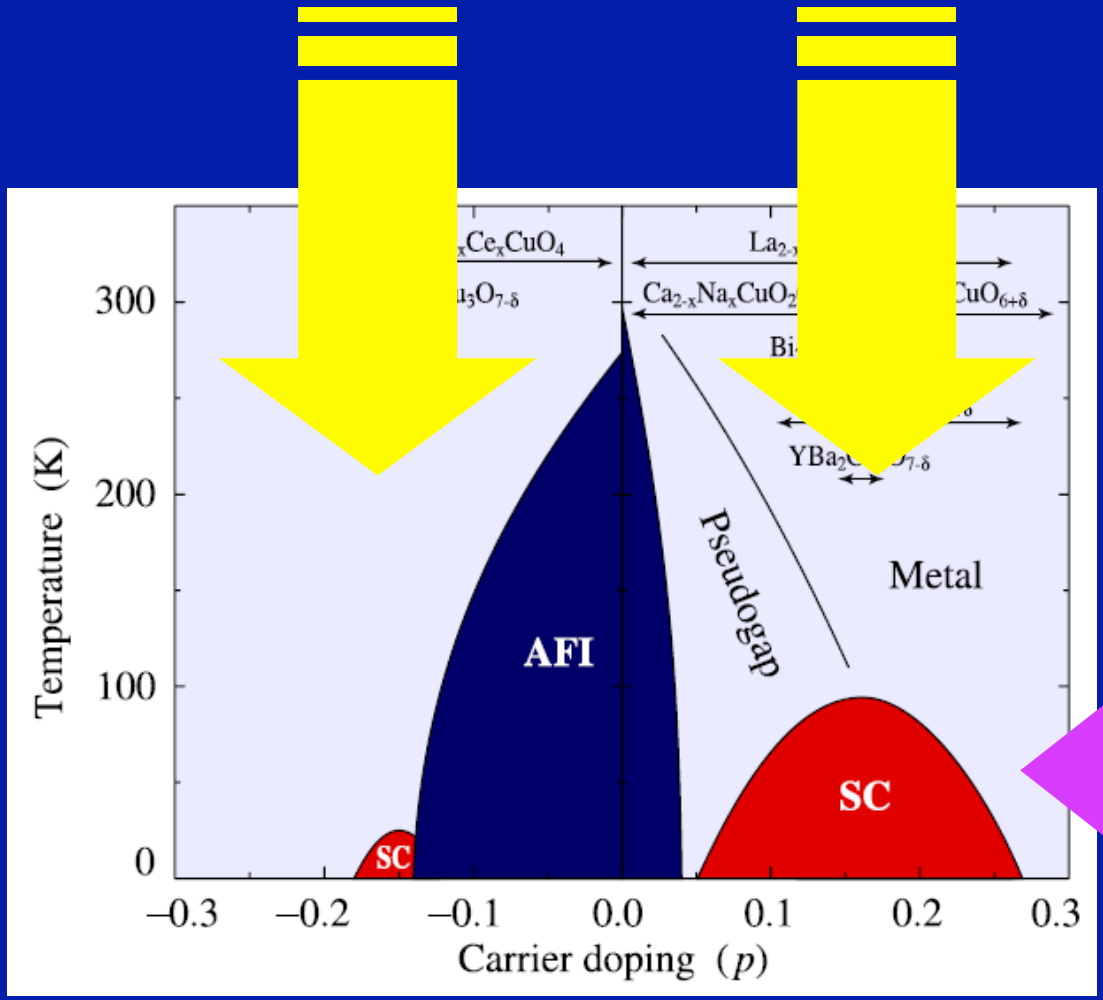
Obvious difficulties with these lectures :

- Huge number of publications (> 100 000 in 25 years !)
- A rich diversity of phenomena and materials
- → *Impossible to be even close to exhaustive !*
- Several issues still controversial
- No consensus on some key issues, including the very mechanism of superconductivity…

Choices made in these lectures:

- Focus on a selected set of issues only
- Present best established facts
- Emphasize some key questions – mention some answers among open possibilities
- *Leave a lot of work –in particular about recent developments- to the colleagues (mostly experimentalists) who generously accepted to present seminars !*
- Start at high energy and zoom down to lower energies

From high to low energy…



From high to low doping…

Programme : 5 séances
Articulation cours/séminaire

9 novembre

Cours	Introduction. Matériaux. Structure électronique. Modèles.
Cours	Les grands régimes du diagramme de phases.
Séminaire	**Henri ALLOUL** *(LPS, Orsay)* - RMN dans les cuprates: pseudogap, dynamique de spins et corrélations électroniques : passé et ...futur ?

16 novembre

Cours	Origine physique du « pseudogap », dichotomie nœuds/antinoeuds (I).
Séminaires	**Kamran BEHNIA** *(ESPCI)* - Transport d'entropie dans les cuprates supraconducteurs.
	Christophe BERTHOD *(Université de Genève)* - Spectroscopie STM dans les cuprates.

23 novembre

Cours	Origine physique du « pseudogap », dichotomie nœuds/antinoeuds (II).
Séminaires	**Yvan SIDIS** *(LLB, CEA-Saclay)* - Dynamique de spins dans les oxydes de cuivre supraconducteurs à haute température critique : apport de la spectroscopie neutronique.
	Philippe BOURGES *(LLB, CEA-Saclay)* **-** Ordre et excitations magnétiques dans la phase pseudogap des cuprates supraconducteurs : existence de boucles de courants ?

30 novembre

Cours — La phase supraconductrice des cuprates : principales propriétés.

Séminaires — **Alain SACUTO** *(Université Denis Diderot, Paris)* - Température critique et appariement dans les oxydes de cuivre supraconducteurs.

Jérome LESUEUR *(ESPCI)* **-** Une mesure directe des fluctuations supraconductrices dans la phase sous-dopée des cuprates.

7 décembre Pas de séance [GDR MICO meeting]

14 décembre

Cours — Titre annoncé ultérieurement.

Séminaire — Orateur encore indeterminé, et:

Cyril PROUST *(Toulouse)* **-** Oscillations quantiques et magnétotransport dans les cuprates supraconducteurs.

Lecture 1

Introduction. Materials. Electronic Structure. Models.

1. Historical perspective

The long quest for better superconductors…

(Very brief account only)

2011: the 100th anniversary of the discovery of superconductivity

The Nobel Prize in Physics 1913

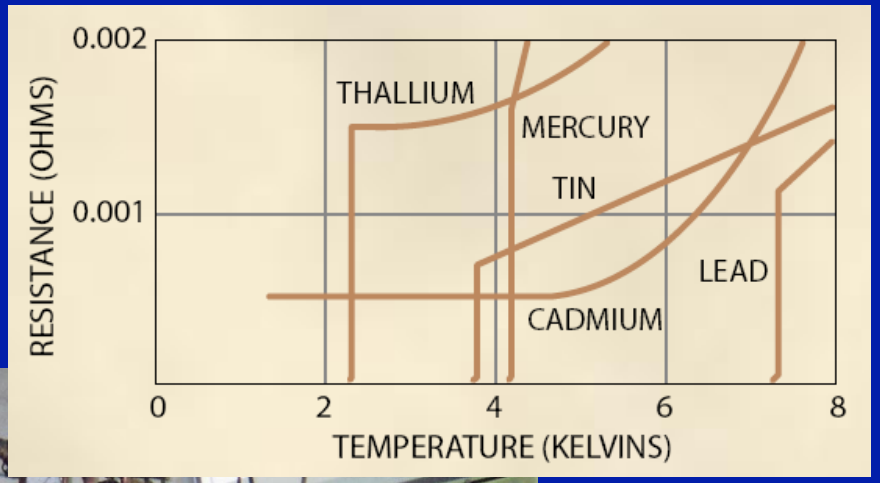
"for his investigations on the properties of matter at low temperatures which led, inter alia, to the production of liquid helium"

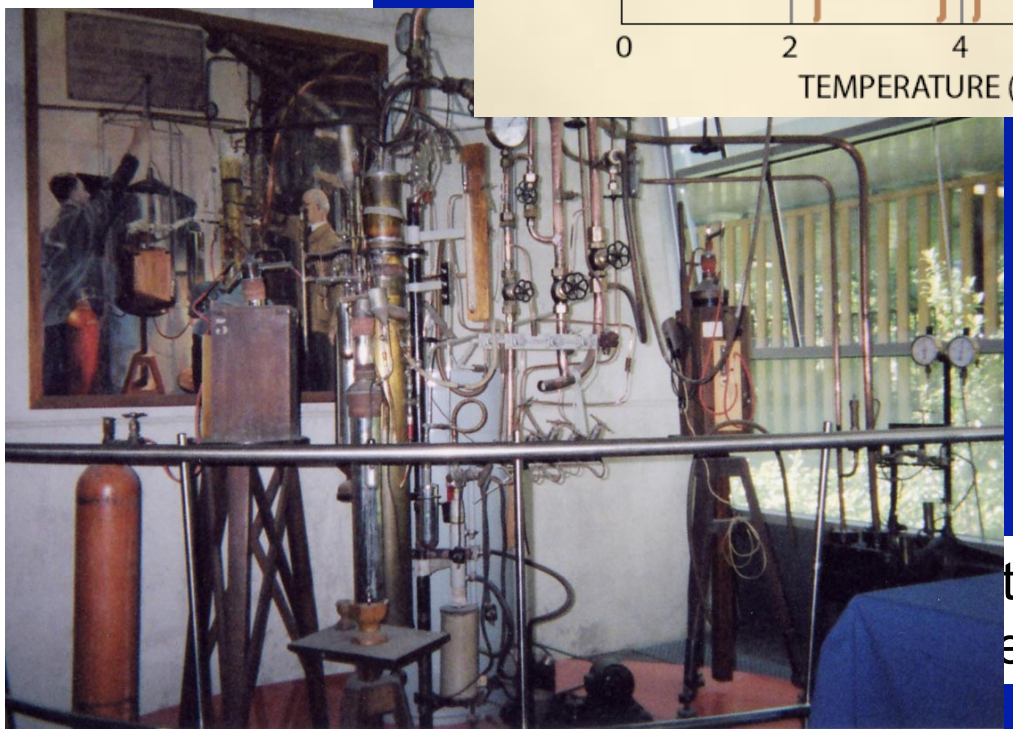
Heike Kamerlingh Onnes

the Netherlands

Leiden University
Leiden, the Netherlands

b. 1853
d. 1926

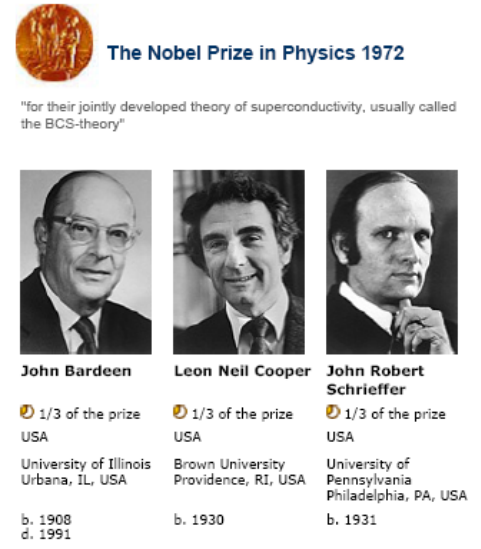




teur d'Hélium
eiden:

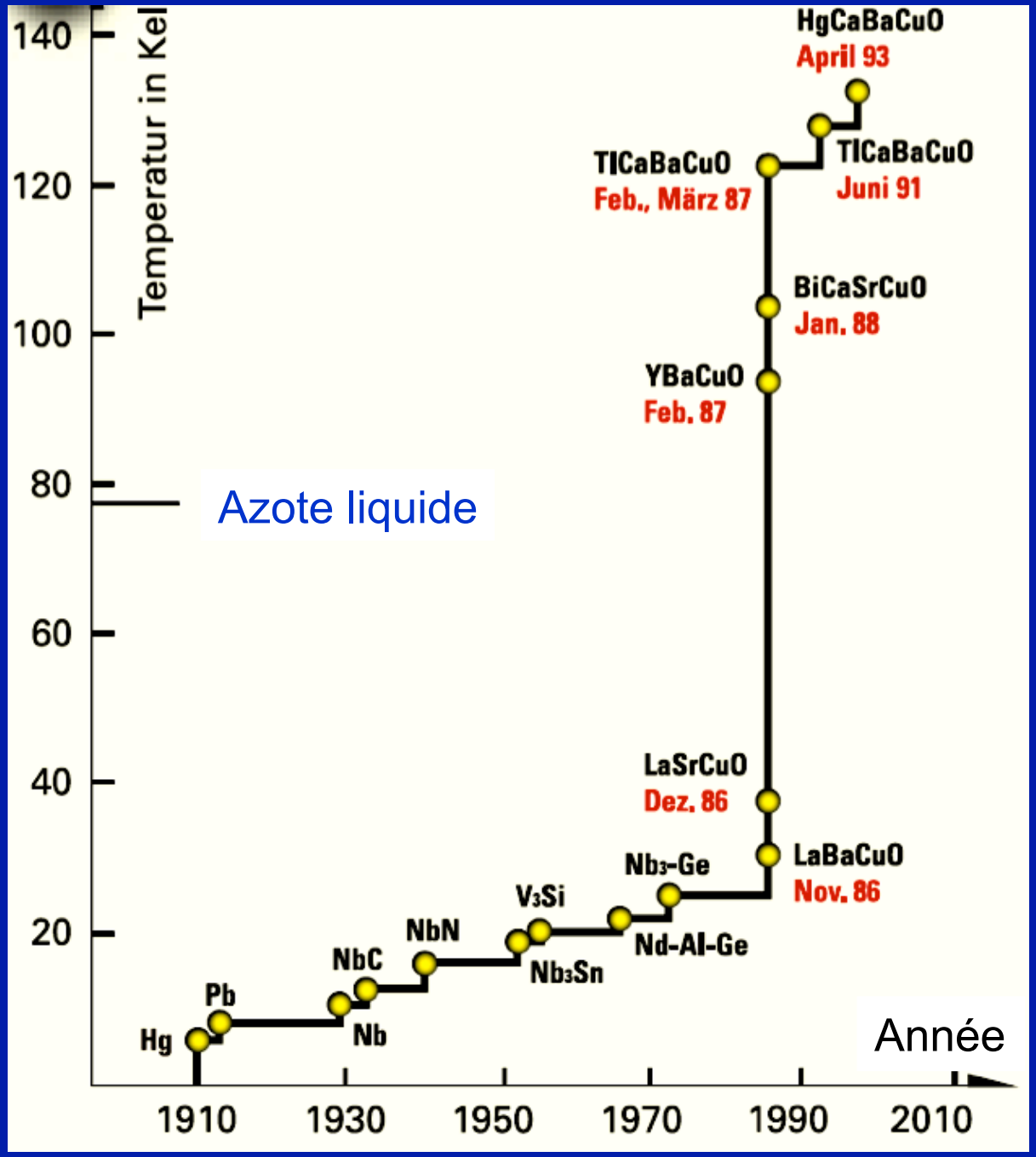
The quest for better superconductors has been, for many years, guided by ideas from the BCS theory

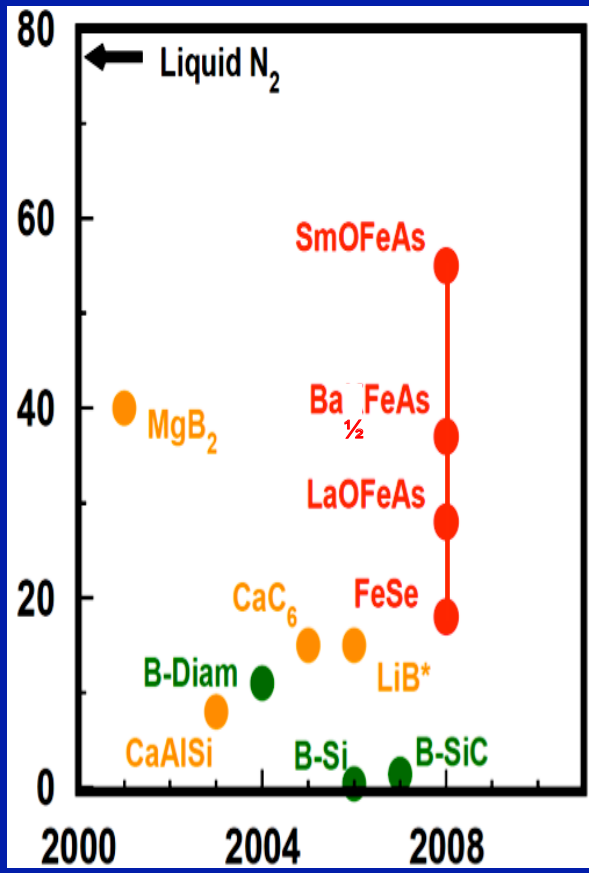
$$kT_c = 1.13\,\hbar\omega_D\, e^{-1/VN(\epsilon_F)}$$



- **Increase Debye frequency** → explore compounds with light elements (MgB_2 !)
- **Increase electron-phonon coupling V** (close but avoiding structural/CDW transitions e.g. YNi_2B_2C)
- **Increase density of states** → explore transition metals (A15 compounds Nb_3Ge)

(One of Bernd Matthias's "rules": d-elements are good)


Temperatur in Kel
140
120
100
80
60
40
20
HgCaBaCuO
April 93
TlCaBaCuO
Juni 91
TlCaBaCuO
Feb., März 87
BiCaSrCuO
Jan. 88
YBaCuO
Feb. 87
Azote liquide
LaSrCuO
Dez. 86
LaBaCuO
Nov. 86
Nb3-Ge
V3Si
Nd-Al-Ge
NbN
Nb3Sn
NbC
Pb
Nb
Hg
Année
1910
1930
1950
1970
1990
2010


80
60
40
20
0
Liquid N2
SmOFeAs
Ba½FeAs
LaOFeAs
FeSe
LiB*
MgB2
CaC6
B-Diam
CaAlSi
B-Si
B-SiC
2000
2004
2008

A truly unexpected discovery…

- The undoped ("parent") compounds are magnetic and insulating !
- Guiding principle for Bednorz and Muller research inspired from their experience with ferroelectric oxides:

local (Jahn-Teller) distortions of MO_6 octahedra could provide strong coupling to phonons ?

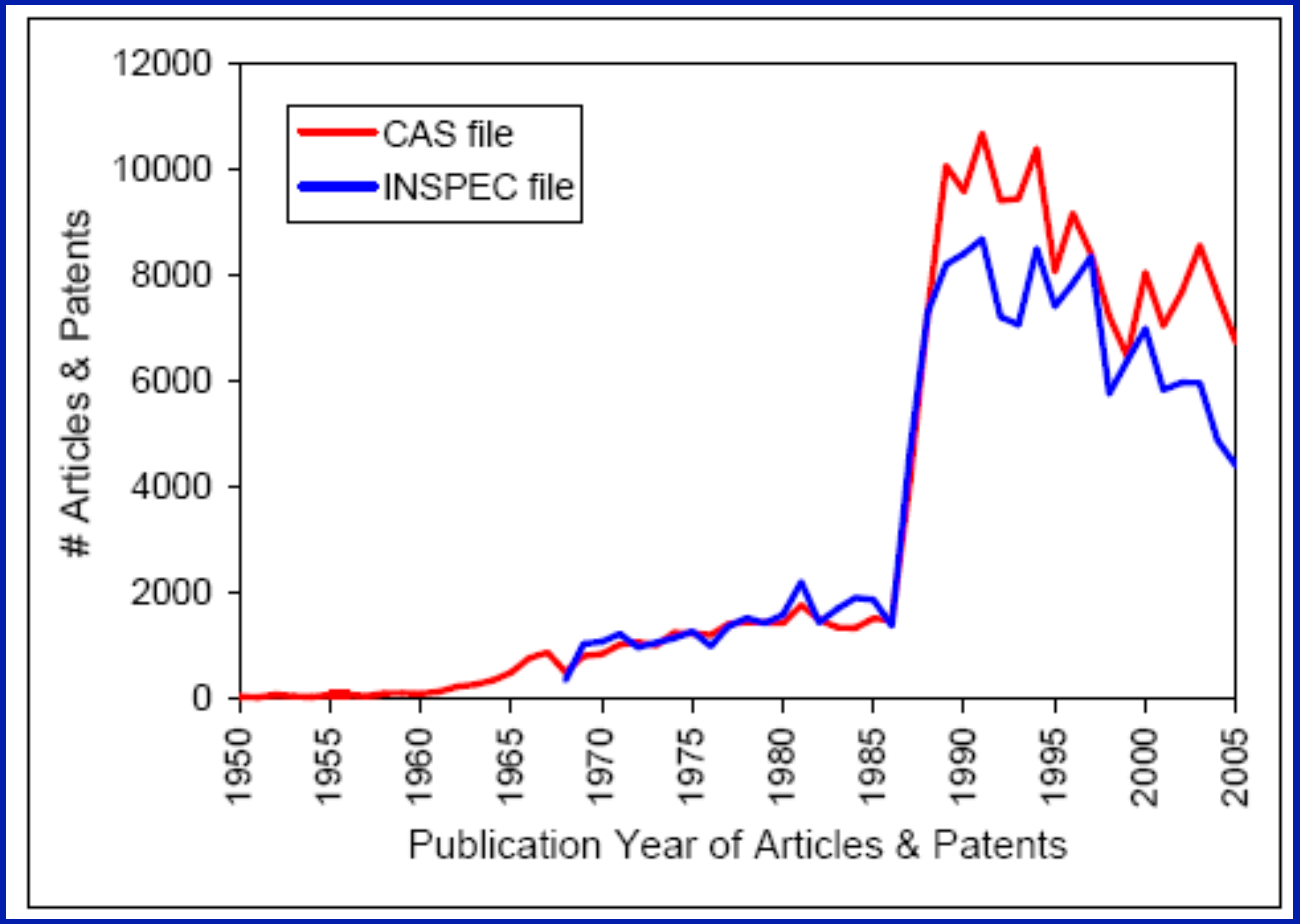


Figure 1: Time dependent number of publications related to superconductivity, i.e. with "supercond?" (truncated search term) appearing in the titles and/or index terms (keywords). Sources: CAPLUS on STN [3] and INSPEC on STN [6].

[Bath and Marx, 2005]

2. The copper oxide high-Tc superconductors: *materials*

2.1 The structure of La_2CuO_4

- La_2CuO_4 is an antiferromagnetic insulator
- La^{3+} and O^{2-} → Cu in Cu^{2+} state ($3d^9$)
- "Hole doping": substitution of La^{3+} by $A=Ba^{2+}$ or Sr^{2+} → $La_{2-x}A_xCuO_4$
- Yields a superconductor with T_c ~ 35K for x~0.15 ("optimal doping")

→ Bednorz and Muller, 1986: LaBaCuO

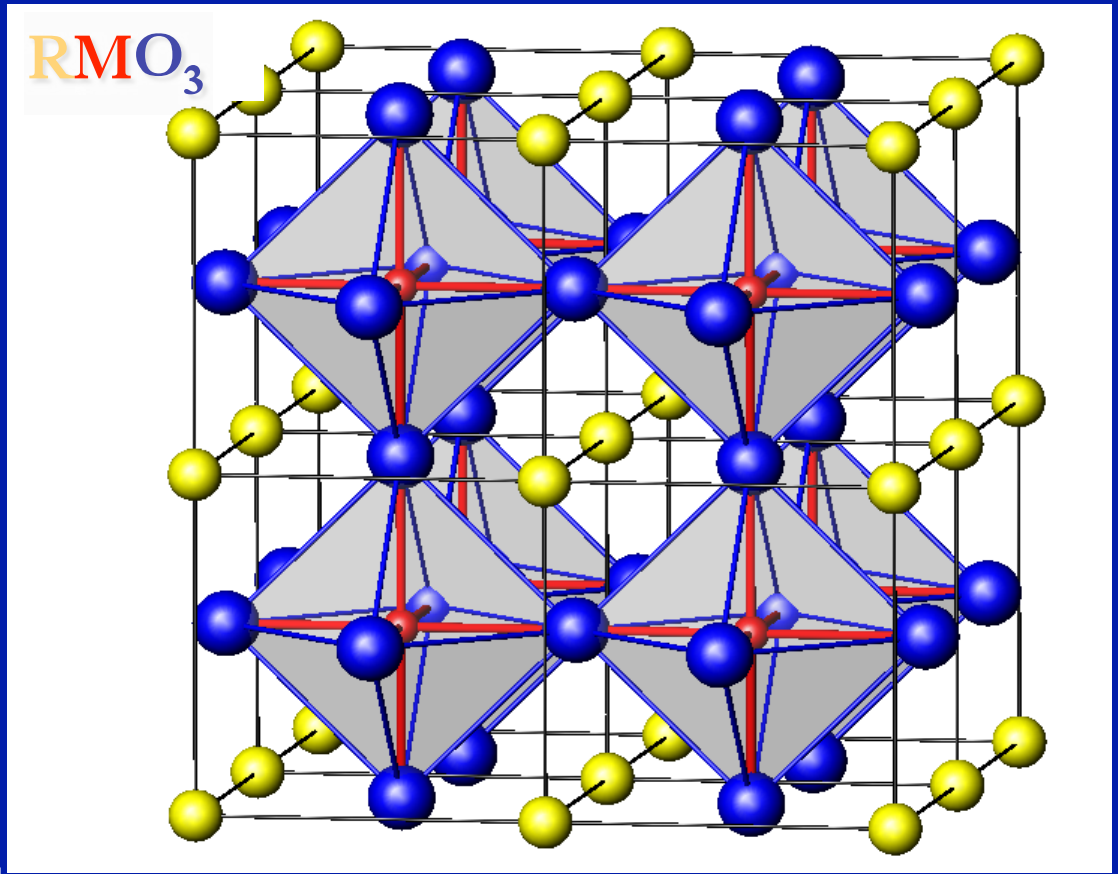
Recall 2009-2010 lectures: the perovskite structure (here, perfectly cubic)

For example: $SrVO_3$

Perfectly cubic perovskite RMO_3 :

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

- Cations R (e.g. rare-earth) form simple cubic lattice



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

Layered perovskites: the Ruddlesden-Popper series $R_{n+1}M_nO_{3n+1}$ with tetragonal symmetry

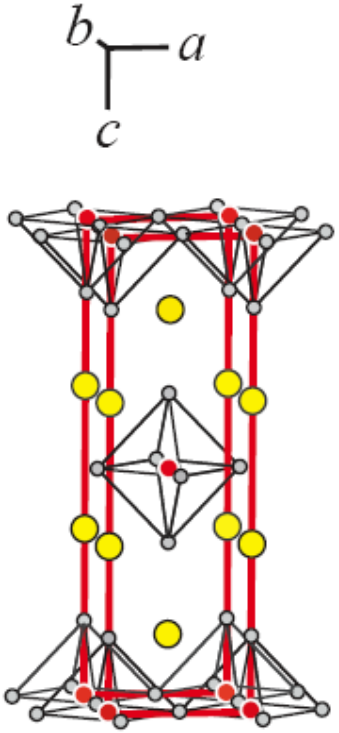
Unit-cell

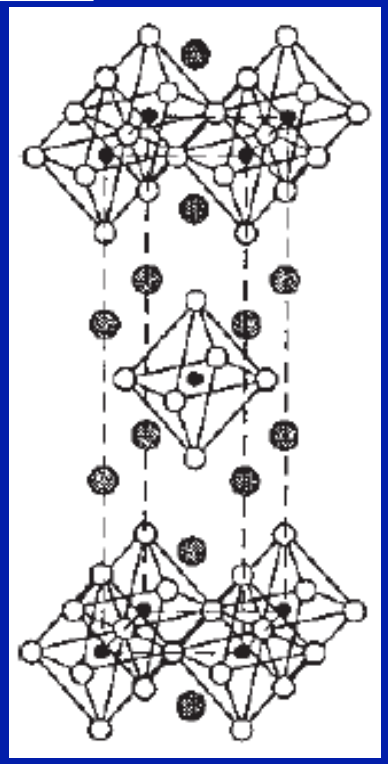
n=2

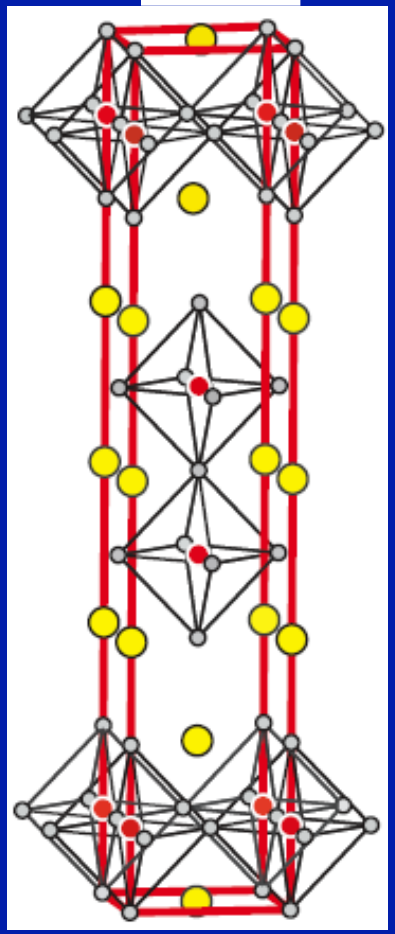
n=3

$Sr_3Ru_2O_7$

I4/mmm







MO_2 layer →

RO layer →

MO_2 layer →

RO layer →

MO_2 layer →

La_2CuO_4

= CuO2 + (LaO)2

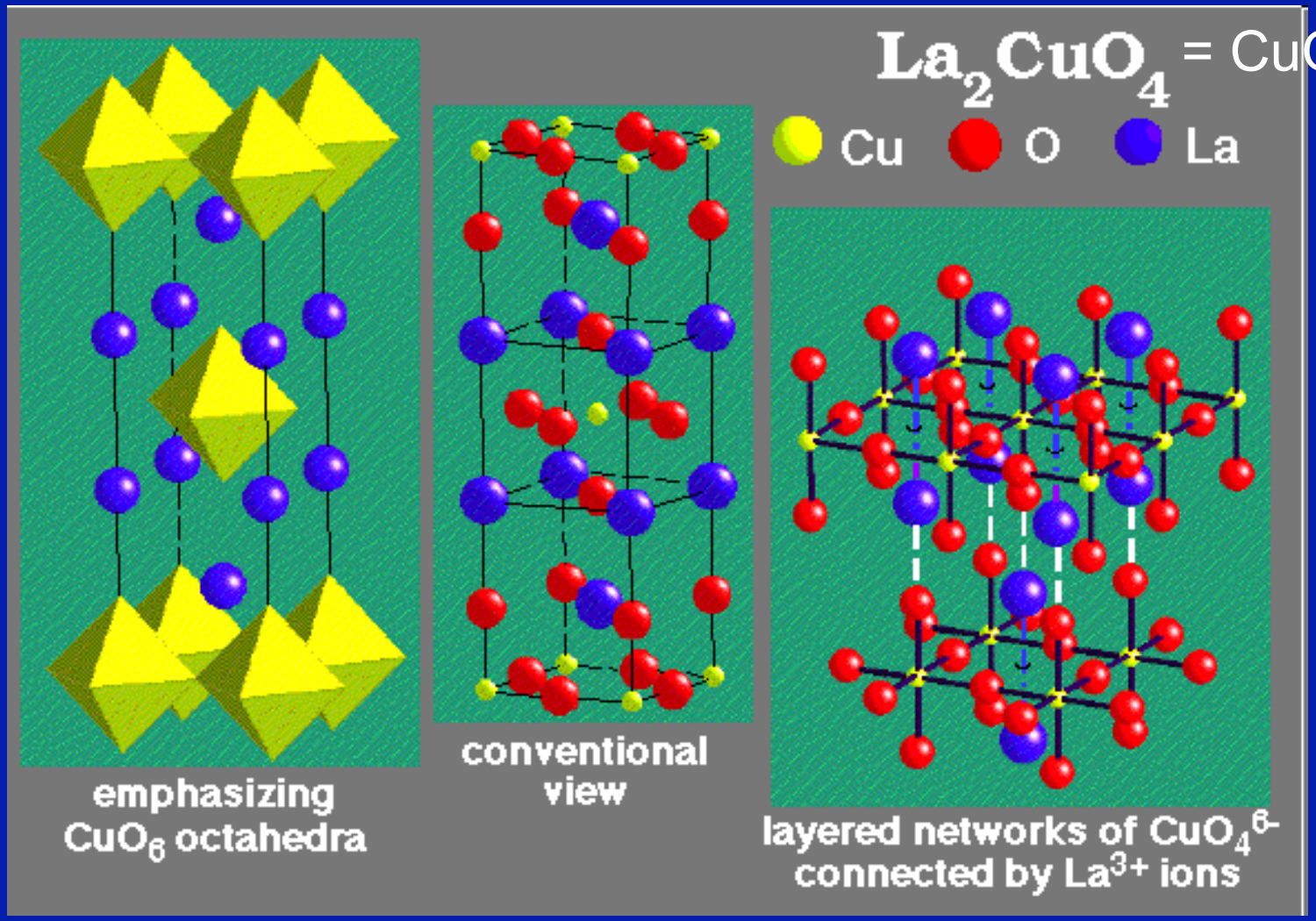
I4/mmm

Sr_2RuO_4

Increasing n : ``from d=2 to d=3”

Usual perovskite RMO_3 corresponds to n→infinity

Different views of the La_2CuO_4 structure

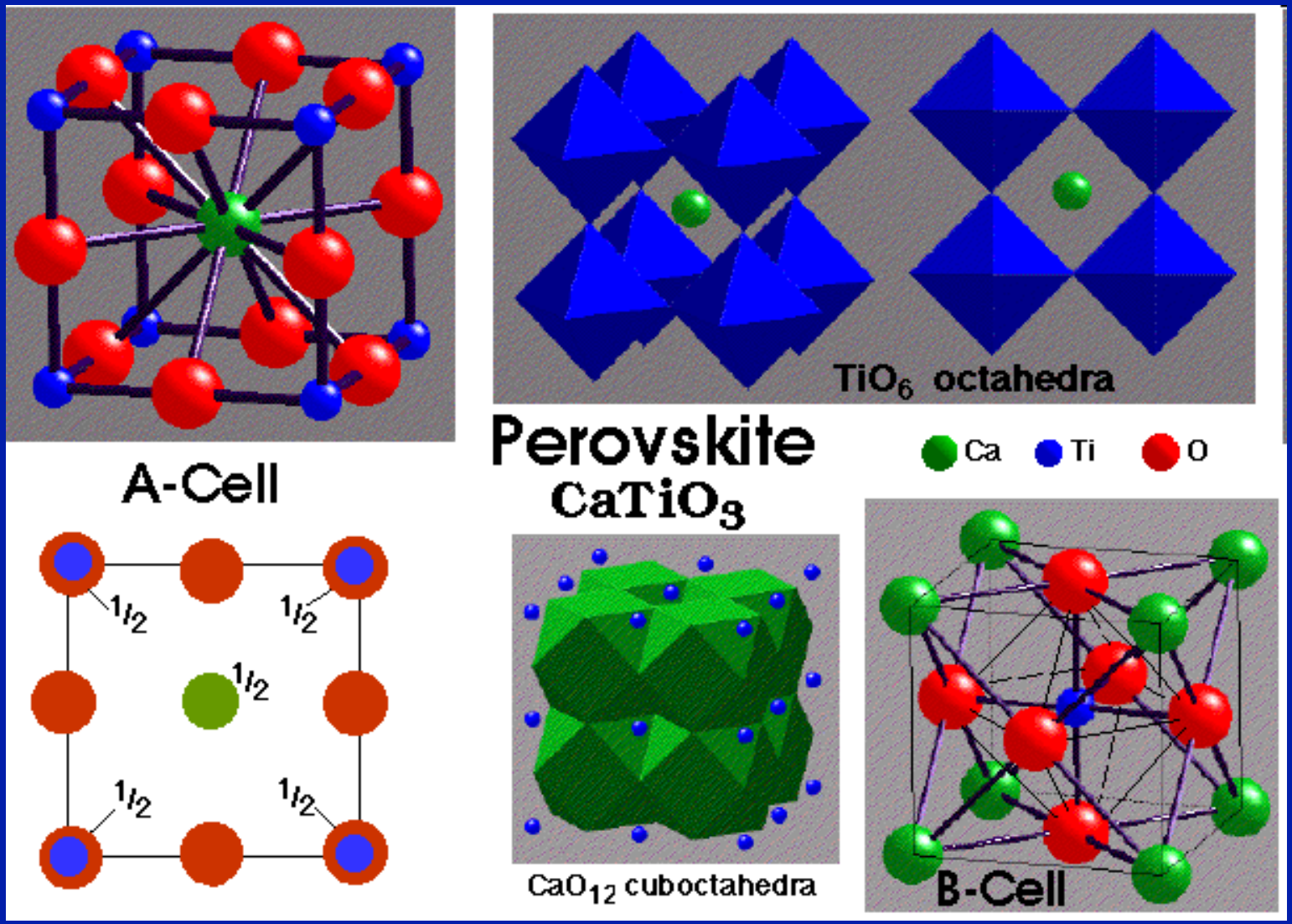


From S.J.Heyes,

Inorganic Chemistry, Oxford

http://www.chem.ox.ac.uk/icl/heyes/structure_of_solids/Lecture4/Lec4.html

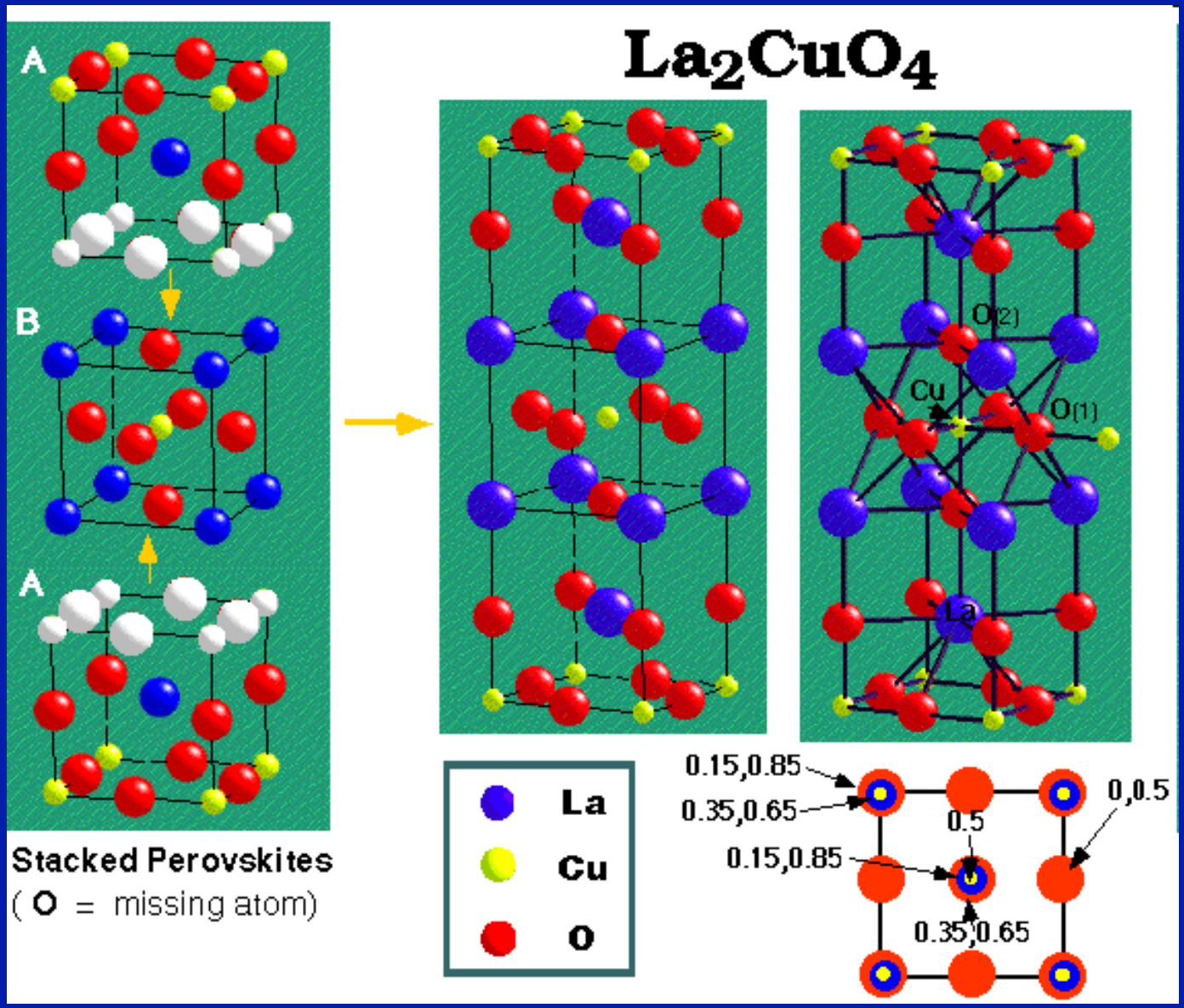
ABO_3 perovskite: A(R)-centered and B(M)-centered units



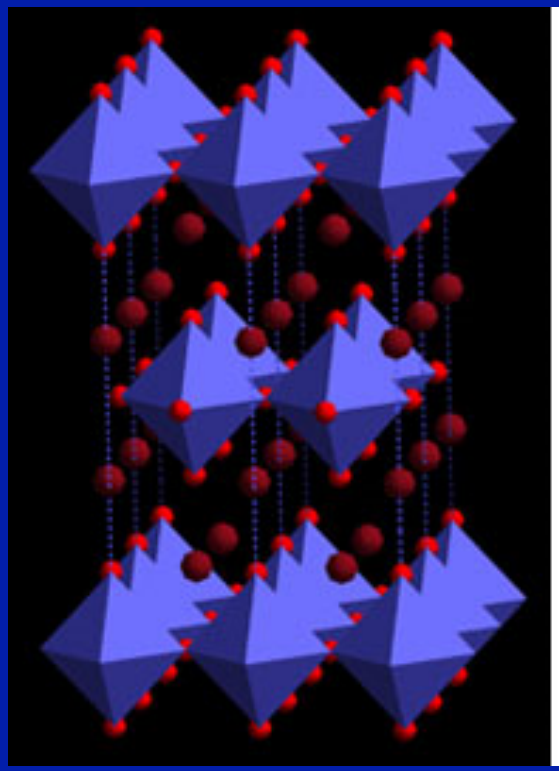
From S.J.Heyes, Inorganic Chemistry, Oxford

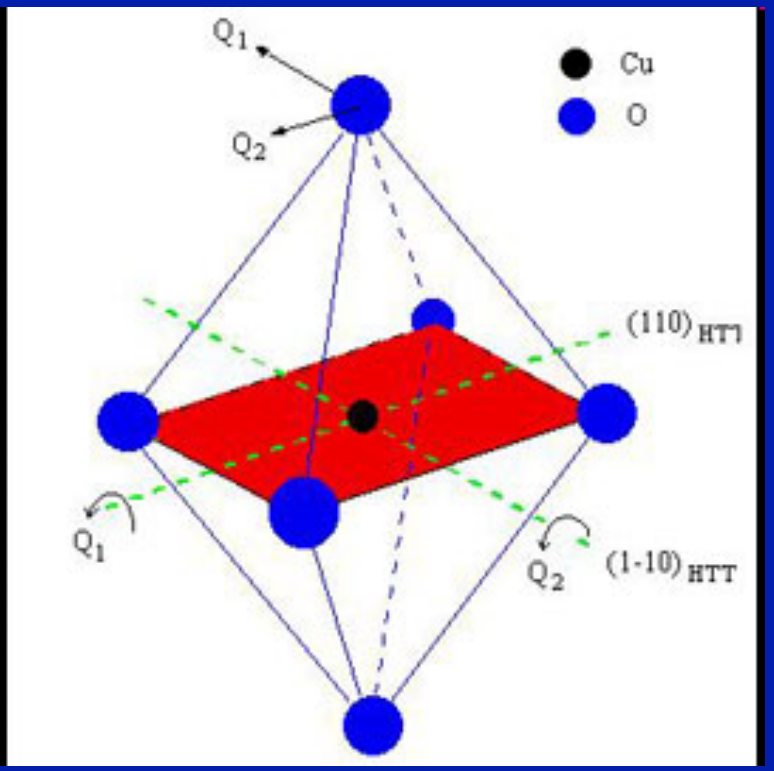
http://www.chem.ox.ac.uk/icl/heyes/structure_of_solids/Lecture4/Lec4.html

La_2CuO_4: can be viewed as stacking of A(La)- and B(Cu)-units



-Quasi two-dimensionality
- Elongation of the CuO_6 octahedron
(Jahn-Teller distortion)
- Several structural distortions are observed





In tetragonal (HTT) phase: a = 3.78 Å, c = 13.2 Å

Co-O(1) distance (in-plane) = a/2=1.89 Å, Cu-O(2) « apical » = 2.42 Å

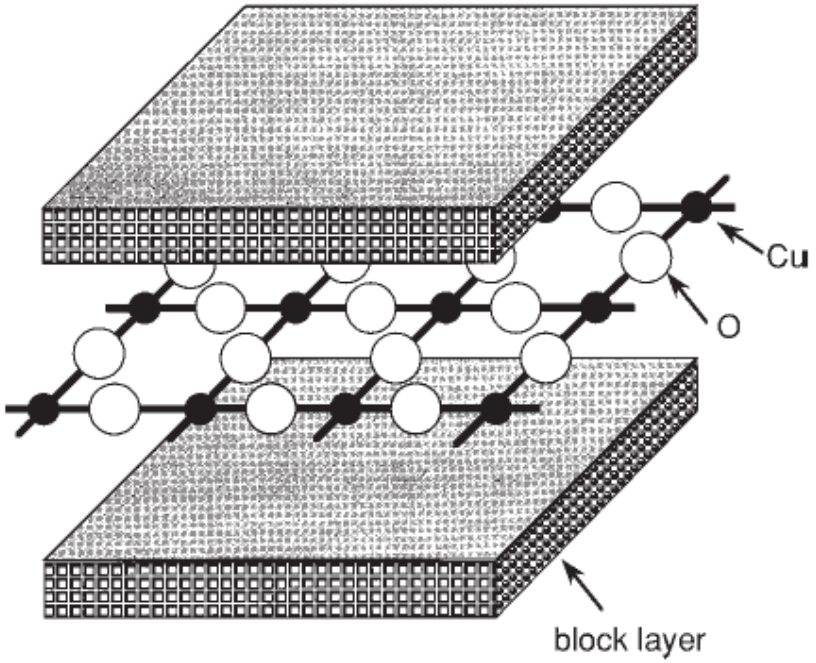
At ~ 530K orthorombic distortion sets in (rotation along Q1 or Q2) = LTO1

Also, LTO2 and LTT phases, depending on Sr-doping and temperature

Summary: key structural building blocks

- CuO_2 planes
- « Charge reservoir » in between (e.g. $[LaO]_2$ rock-salt)
- In La_2CuO_4: Elongated CuO_6 octahedra as structural units

→ Other cuprates are obtained by keeping the CuO_2 layer units and modifying the rest of the structure

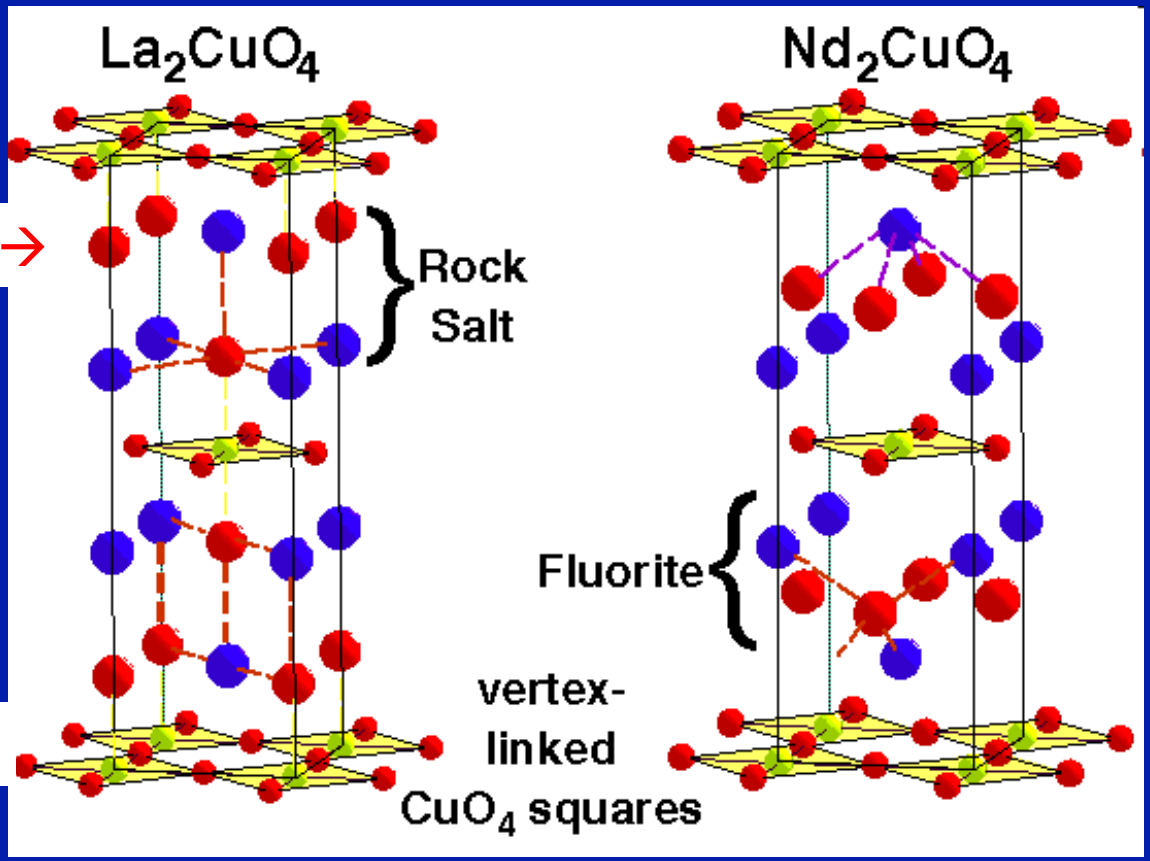


Imada et al. Rev. Mod. Phys 70, 1039 (1998)

2.2 Nd_2CuO_4 vs. La_2CuO_4 electron vs. hole- doping

[Tokura, Takagi and Uchida, Nature 337, 245 (1989), see Emery same vol.]

$Nd_{2-x}Ce_xCuO_4$ (« NCCO ») vs. $La_{2-x}Sr_xCuO_4$ (« LSCO »)



No apical oxygens !

Makes electron doping possible (less repulsion)

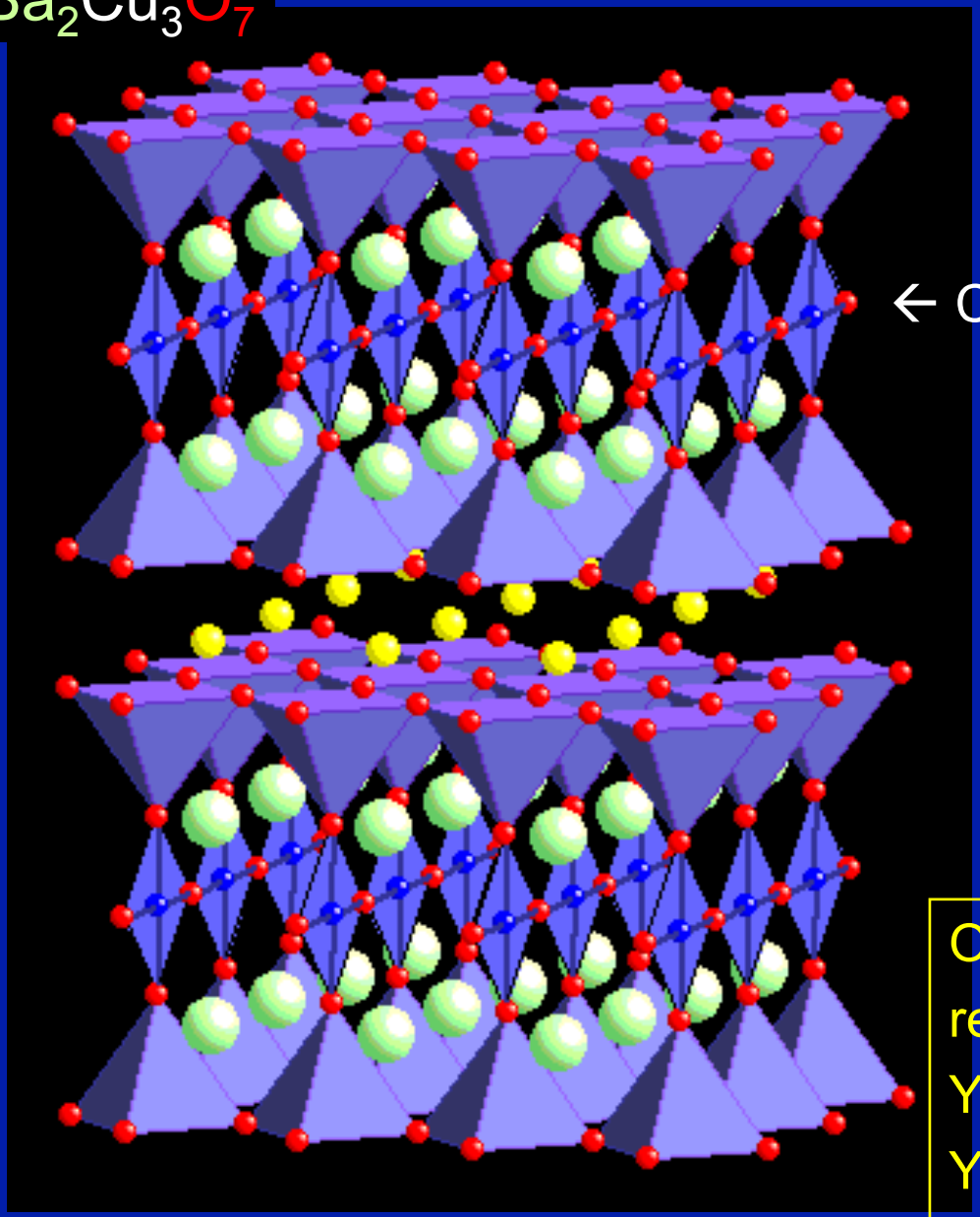
Sr^{2+} substitution on La^{3+} sites: « hole doping »

Ce^{4+} substitution on Nd^{3+} sites: Cu^{2+} → Cu^{+} « electron doping »

2.3 From CuO_6 to CuO_5 units: $YBa_2Cu_3O_7$

- T_c~90K The first superconductor above liquid Nitrogen temperature = huge step !
- Discovered by Paul Chu et al. [Houston]
- *Historical account: R.M. Hazen « The breakthrough - The race for the superconductor » [La course aux supraconducteurs, Plon 1989]*

$YBa_2Cu_3O_7$



CuO_5 square-base pyramids

← CuO CHAIN

← CuO_2 layer

← CuO_2 layer

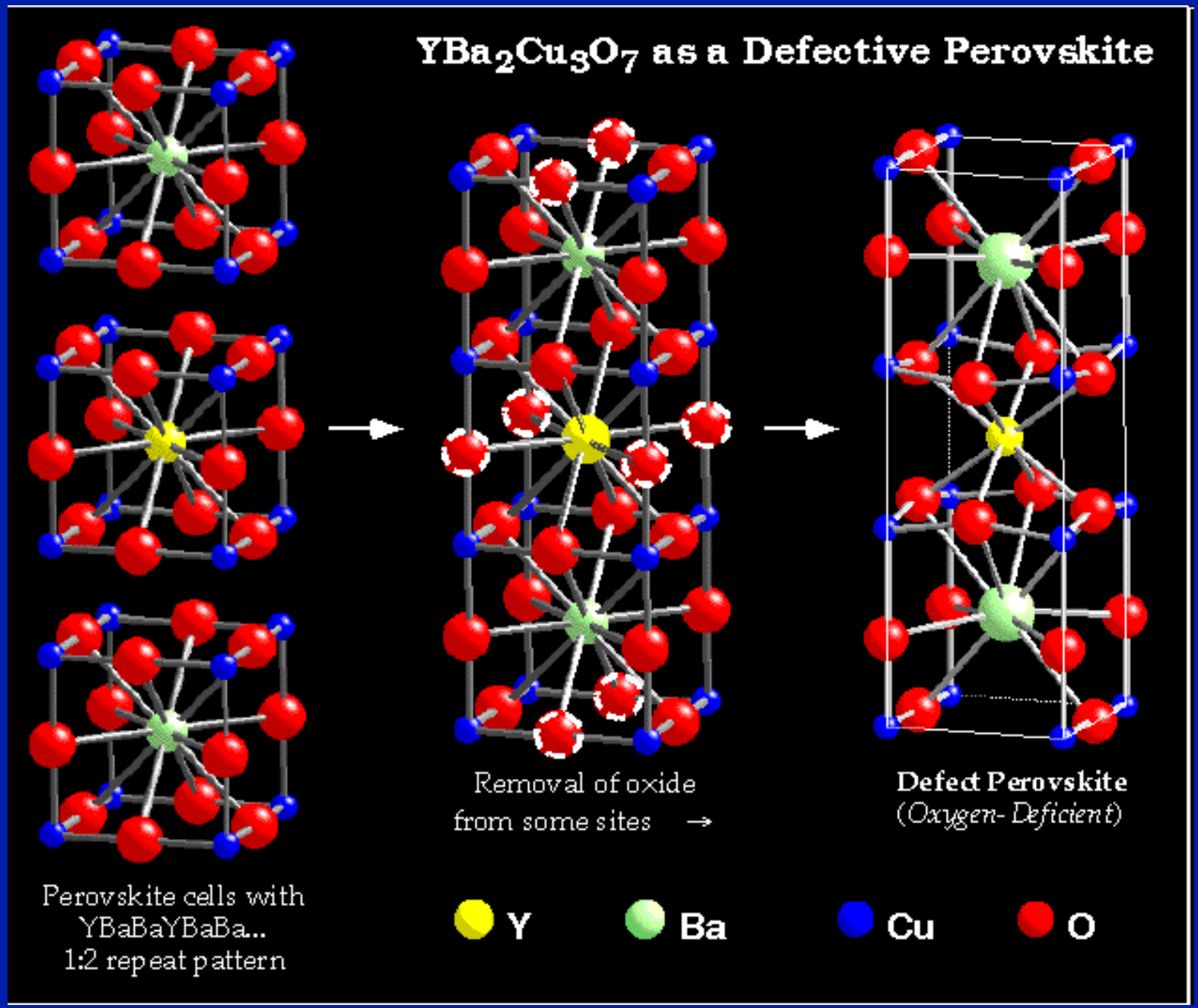
} bilayer

Oxygens in the chains can be removed rather easily:

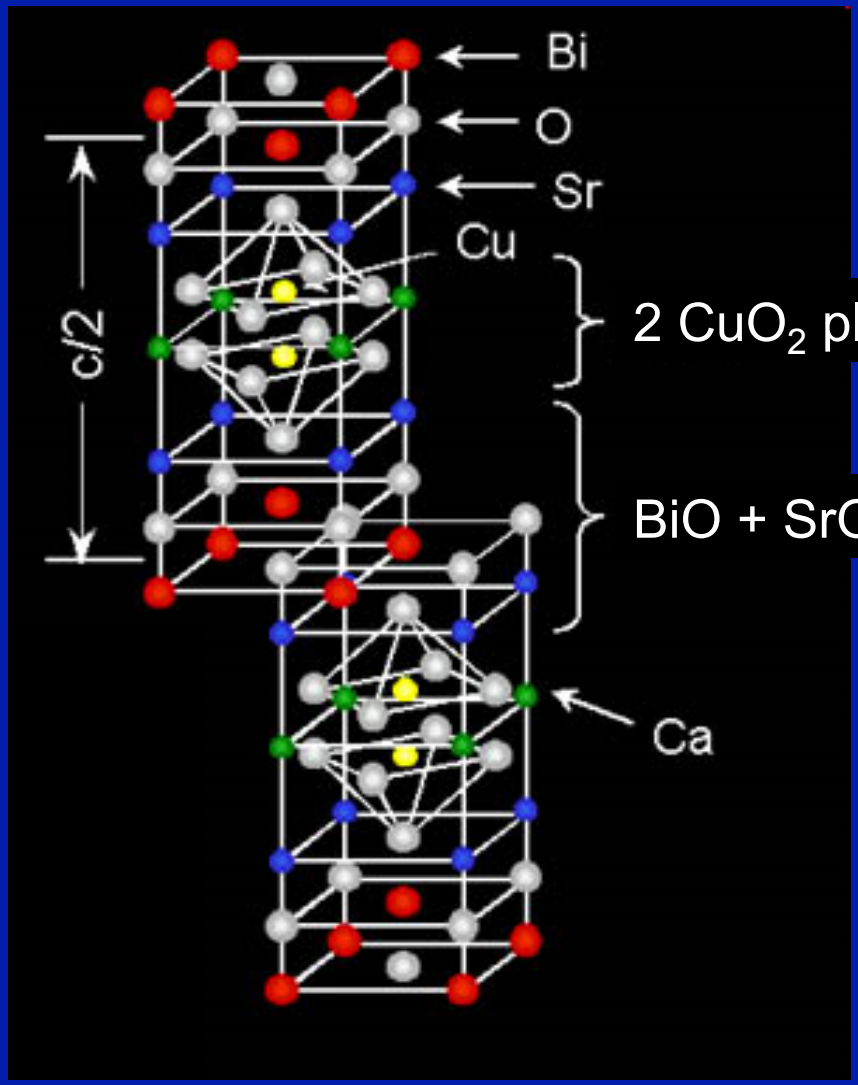
$YBa_2Cu_3O_7$: all in-chain oxygens

$YBa_2Cu_3O_6$: no in-chain oxygens

$YBa_2Cu_3O_{7-y}$


YBa2Cu3O7 as a Defective Perovskite
Perovskite cells with
YBaBaYBaBa...
1:2 repeat pattern
Removal of oxide
from some sites →
Defect Perovskite
(Oxygen- Deficient)
Y
Ba
Cu
O

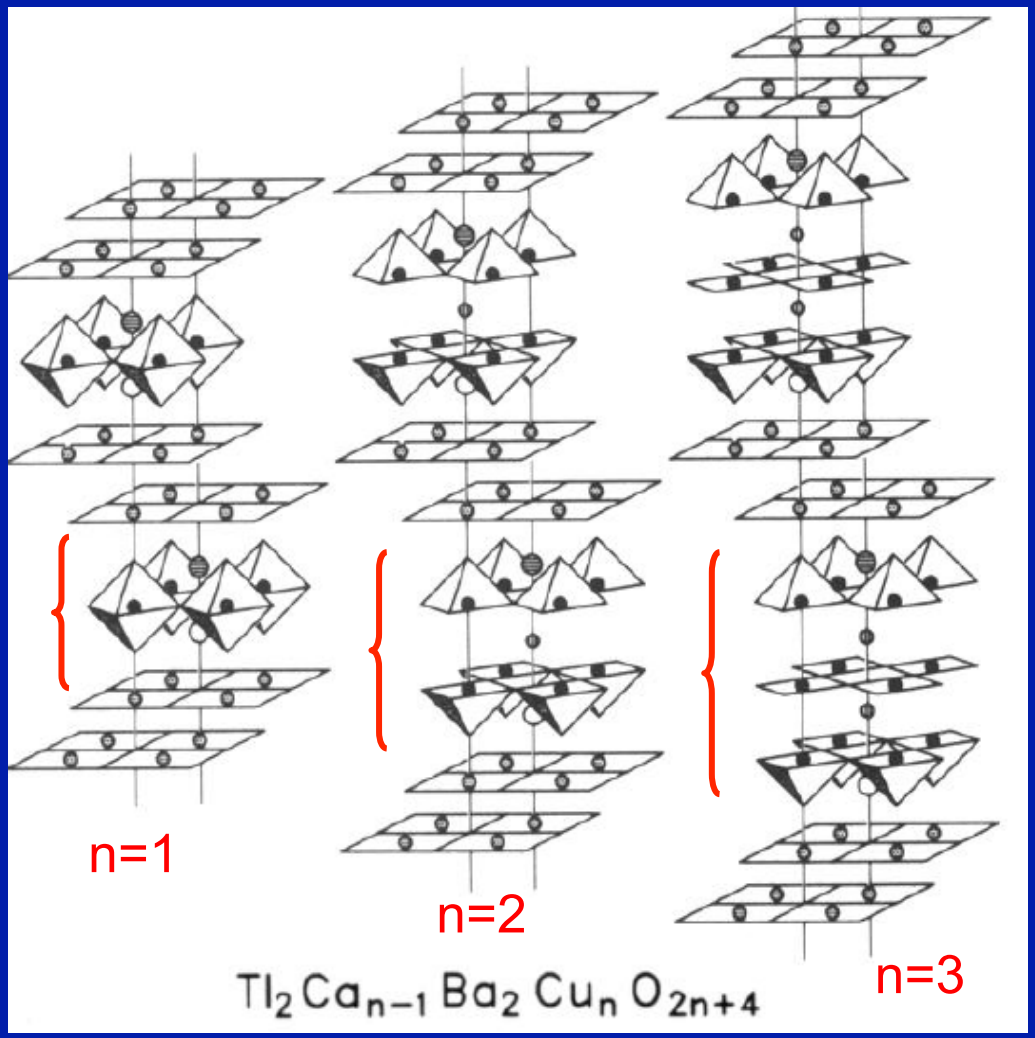
2.4 $Bi_2Sr_2CaCu_2O_8$ and $Tl_2CaBa_2Cu_2O_8$

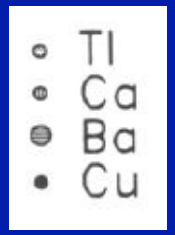


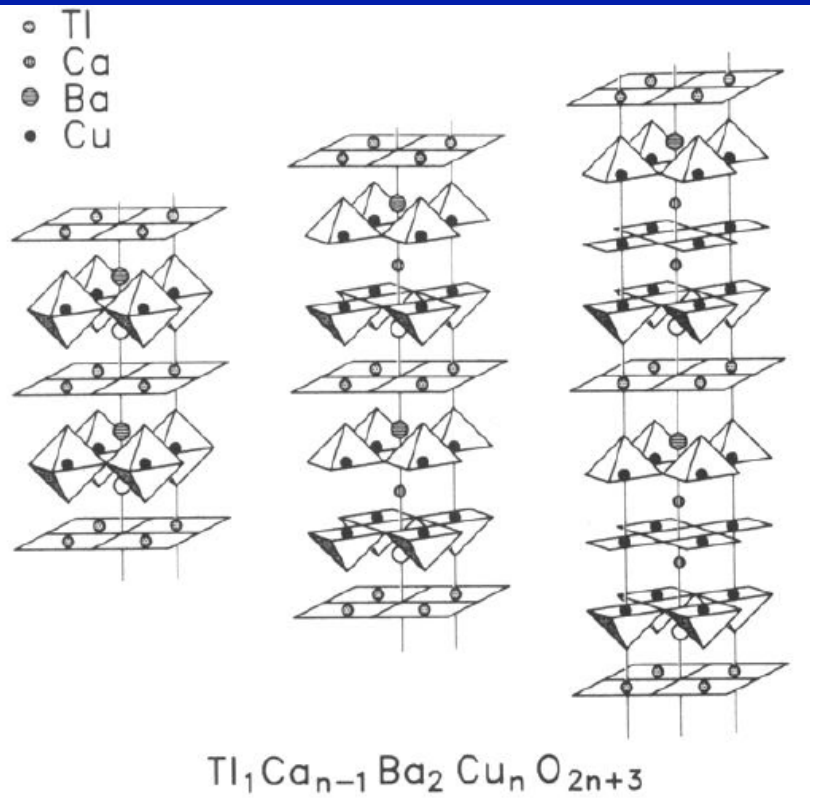
(Bi2212 and Tl2212: **2 CuO_2 layers)**

CuO_5 units as in YBCO

Varying the number of CuO_2 layers:





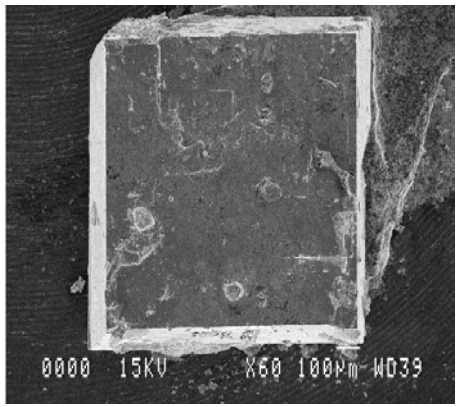


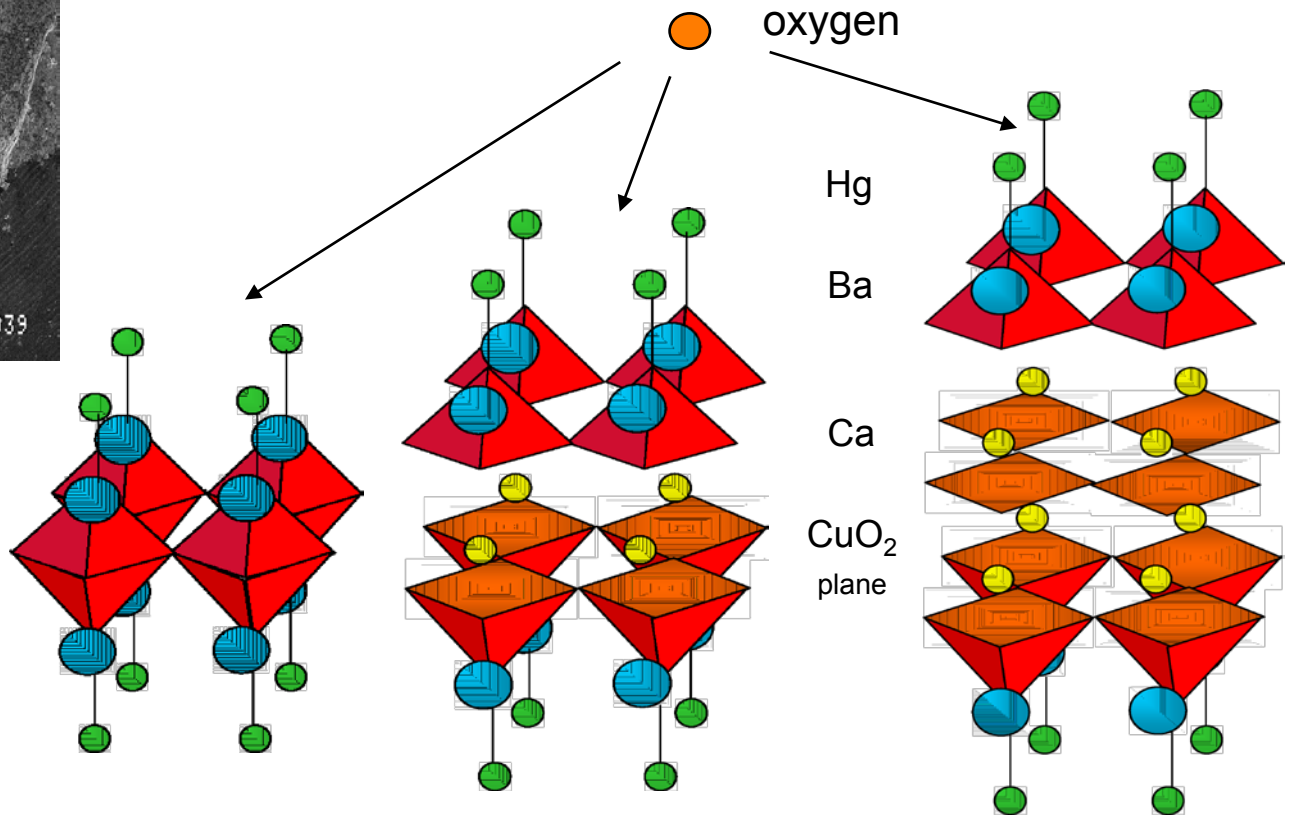
"2201" "2212" "2223"

Mercurate single crystals

D. Colson, CEA-SPEC

purely tetragonal





Hg-1201
Tc=95 K

Hg-1212
Tc=120 K

Hg-1223
Tc=135 K

Tc=165 K (30 GPa)

3. Basics of electronic structure

Local chemistry: ionic picture

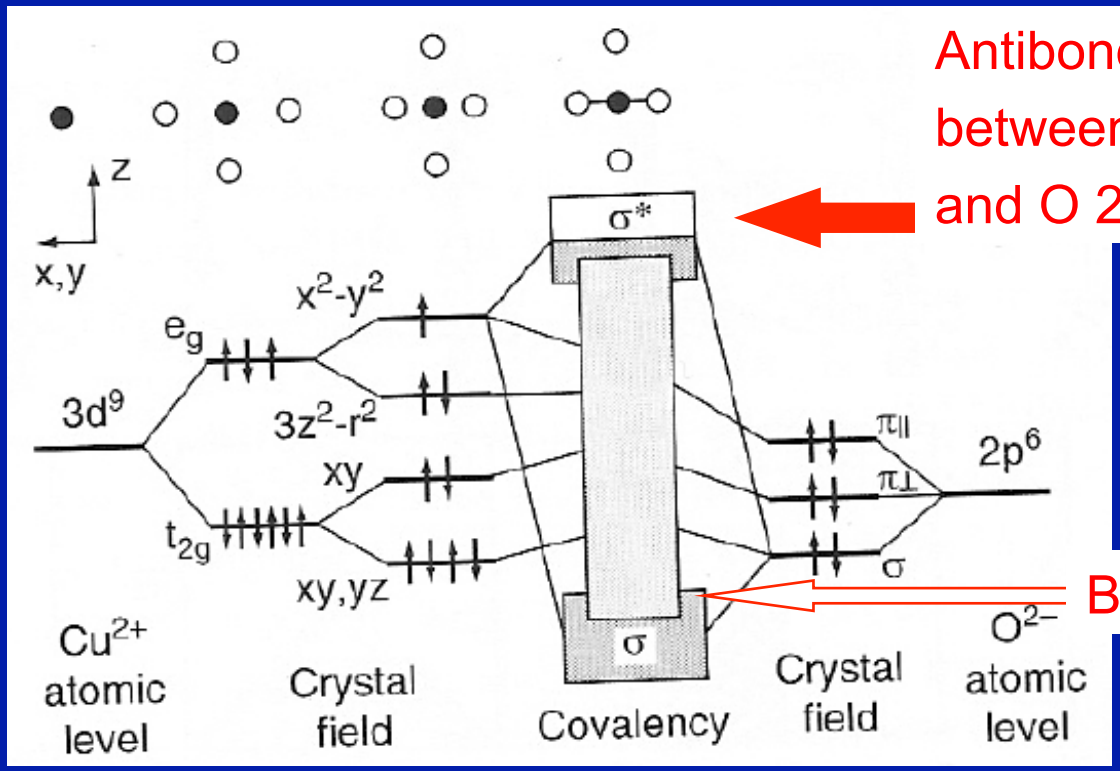
- La_2CuO_4:
- La: $[Xe]6s^25d^1 \rightarrow La^{3+}$
- O: $[He]2s^22p^4 \rightarrow O^{2-}$
- Charge neutrality Cu: $[Ar]4s^13d^{10} \rightarrow Cu^{2+}$ $[Ar]3d^9$
- → 1 hole in an otherwise filled 3d shell
- Similarly: $YBa_2Cu_3O_6$ (parent compound)

  Y^{2+}, $Ba^{2+} \rightarrow Cu^{2+}$

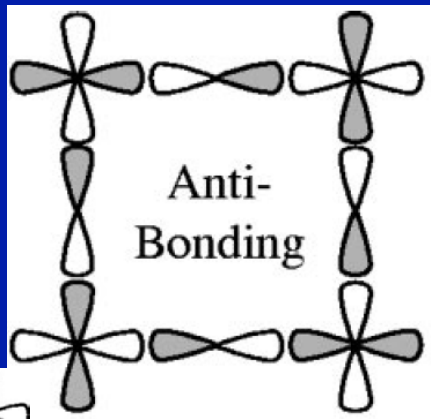
Doping: $La_{2-x}Sr_xCuO_4$ Sr^{2+} → removes 1 electron per copper atom

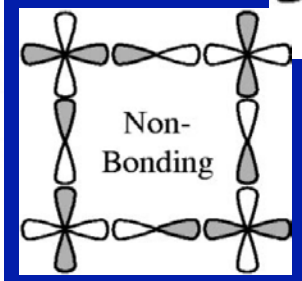
Electronic structure within a CuO_2 plane: schematic description

- Strong covalency between Cu-3d and O-2p orbitals
- Crystal-field splitting

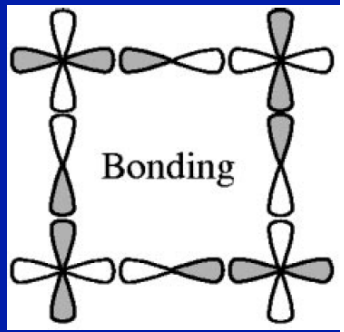


Antibonding band between Cu d_{x2-y2} and O $2p_x$,$2p_y$



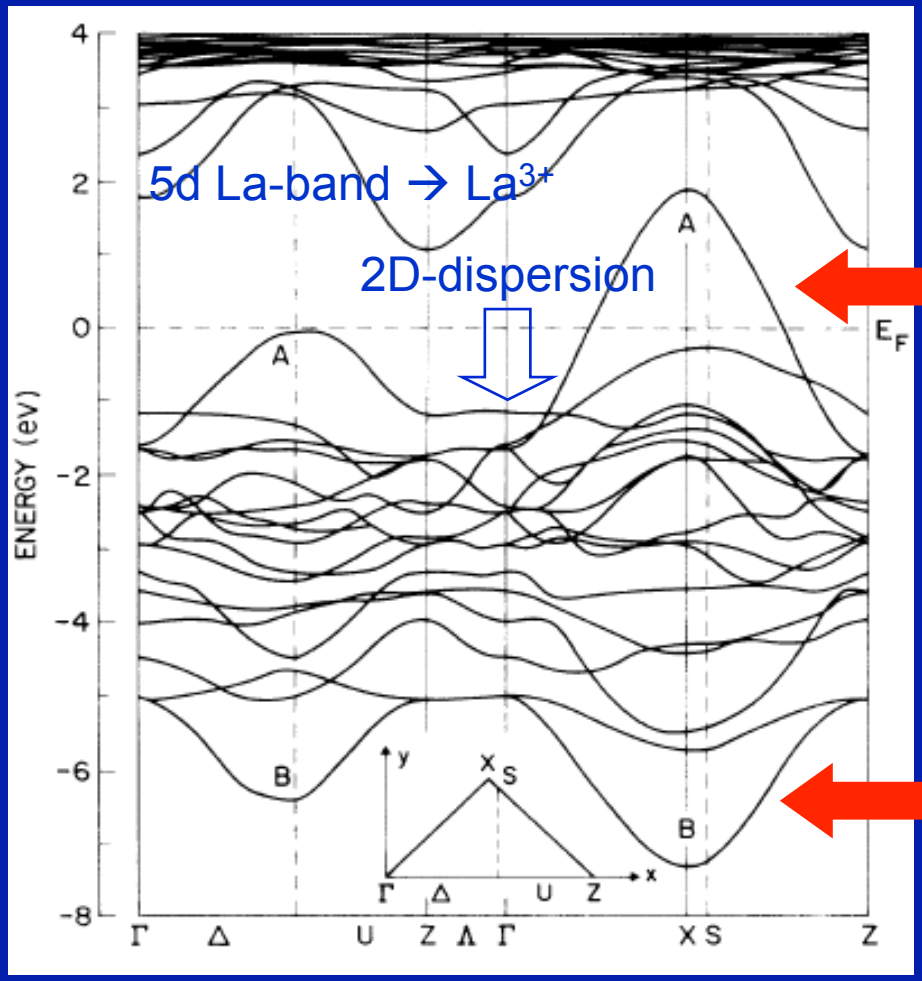


Bonding band



cf. Fink et al. IBM J.Res.Dev 33 (1989) 372
Damascelli et al. Rev Mod Phys 2003

The LDA band-structure: a metal !



17 bands (4*3 O + 5 Cu)

Most narrow, except:

Antibonding

½ - filled antibonding band

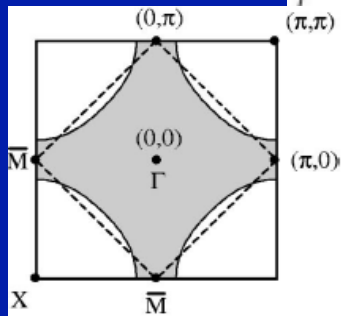
→ A metal within (non-magnetic) LDA

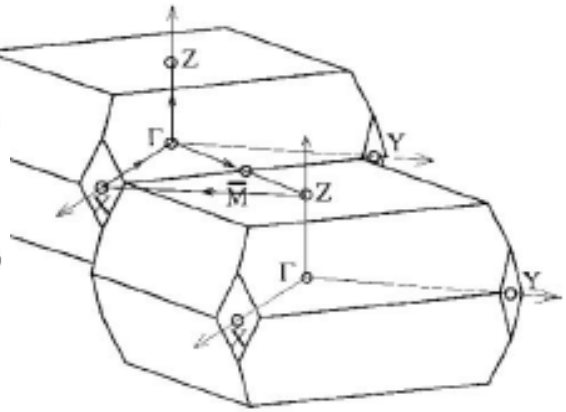
Bandwidth ~ 4 eV

Note: total DOS at E_F not very large:

1-2 states/eV depending on doping

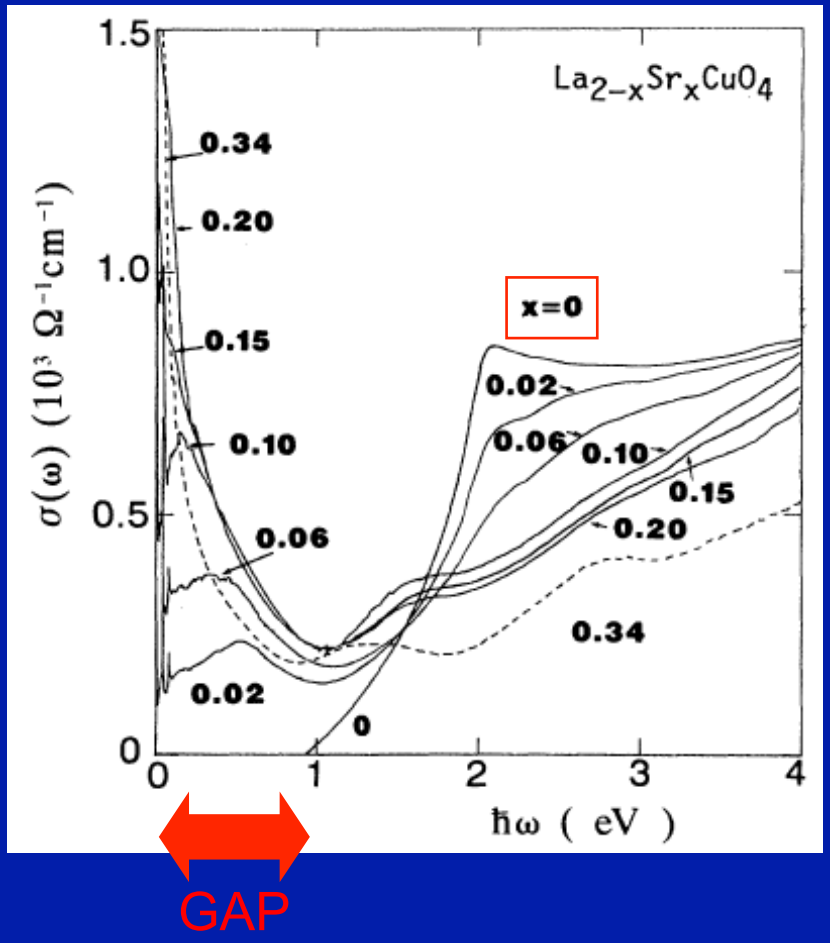
Bonding





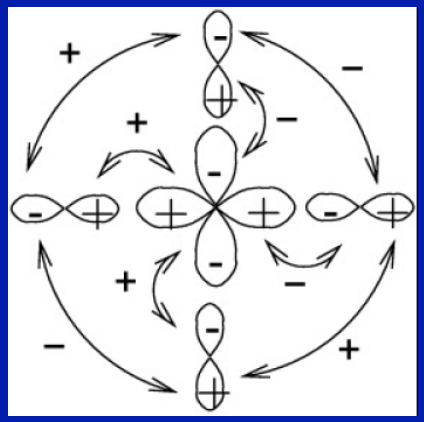
La_2CuO_4 L. Mattheiss, PRL 58, 1028 (1987)

La_2CuO_4: an insulator, metallized by hole-doping La→Sr



Optical conductivity of $La_{2-x}Sr_xCuO_4$ (Uchida et al. PRB 43, 7942 (1991))

Three-band model description of CuO_2 planes



Emery, PRL (1987)
Varma et al. Sol State Comm

"Hole" representation

Vacuum state: filled Cu-$3d^{10}$ shell, filled O-$2p^6$ shell

d^+,p^+ create holes in filled shell

$$H_{3B} = \varepsilon_p \sum_{i\sigma} p^+_{i\sigma} p_{i\sigma} + \varepsilon_d \sum_{i\sigma} d^+_{i\sigma} d_{i\sigma} - t_{pd} \sum_{ij\sigma} s^{pd}_{ij}\, d^+_{i\sigma} p_{j\sigma} - t_{pp} \sum_{ij\sigma} s^{pp}_{ij}\, p^+_{i\sigma} p_{j\sigma} + \text{h.c.} +$$
$$+ U_{dd} \sum_i \hat{n}^d_{i\uparrow} \hat{n}^d_{i\downarrow} + U^{\sigma\sigma'}_{pd} \sum_{\langle ij \rangle} \hat{n}^d_{i\sigma} \hat{n}^p_{j\sigma'} + U_{pp} \sum_i \hat{n}^p_{i\uparrow} \hat{n}^p_{i\downarrow}$$

Typical values of key parameters (La_2CuO_4) - some variations depending on authors and method (constrained LDA, cluster calculations – not fully settled):

- Charge transfer energy
- Hopping parameters
- Interactions

$$\Delta \equiv \varepsilon_p - \varepsilon_d \simeq 2.7 - 3.5 \text{ eV}$$

$$t_{pd} \simeq 1.3 - 1.6 \text{ eV} \quad , \quad t_{pp} \simeq 0.7 \text{ eV}$$

$$U_{dd} \simeq 8 - 10 \text{ eV} \quad U_{pp} \simeq 4 - 6 \text{ eV} \quad U_{dd} \simeq 0.6 - 1.3 \text{ eV}$$

1-electron band-structure of 3-band model (t_{pd} only) – for illustrative purposes-

$$\begin{vmatrix} \omega-\varepsilon_d & t_{pd}(e^{-ik_x a}-1) & t_{pd}(1-e^{ik_y a}) \\ t_{pd}(e^{ik_x a}-1) & \omega-\varepsilon_p & 0 \\ t_{pd}(1-e^{-ik_y a}) & 0 & \omega-\varepsilon_p \end{vmatrix}$$

$$(\omega-\varepsilon_d)(\omega-\varepsilon_p)^2 - t_{pd}\left(e^{-ik_x a}-1\right)(\omega-\varepsilon_p)t_{pd}\left(e^{ik_x a}-1\right) - t_{pd}\left(1-e^{ik_y a}\right)(\omega-\varepsilon_p)t_{pd}\left(1-e^{-ik_y a}\right) = 0$$

$\omega = \varepsilon_p$ Non-bonding band

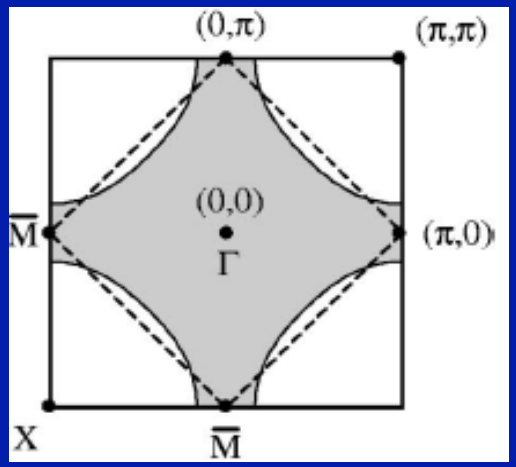
or:

$$\omega^2 - (\varepsilon_p+\varepsilon_d)\omega + \varepsilon_p\varepsilon_d - 4t_{pd}^2\left[\sin^2\frac{k_x a}{2} + \sin^2\frac{k_y a}{2}\right] = 0$$

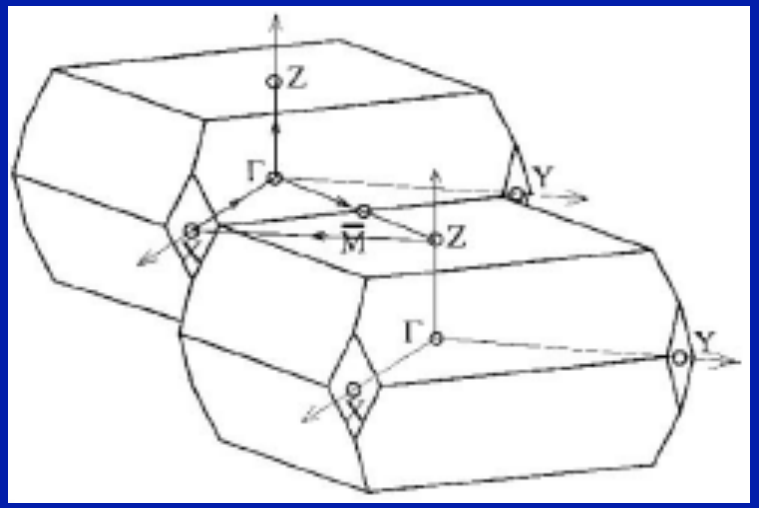
$$\delta \equiv (\varepsilon_p-\varepsilon_d)^2 + 16t_{pd}^2\left[\sin^2\frac{k_x a}{2} + \sin^2\frac{k_y a}{2}\right]$$

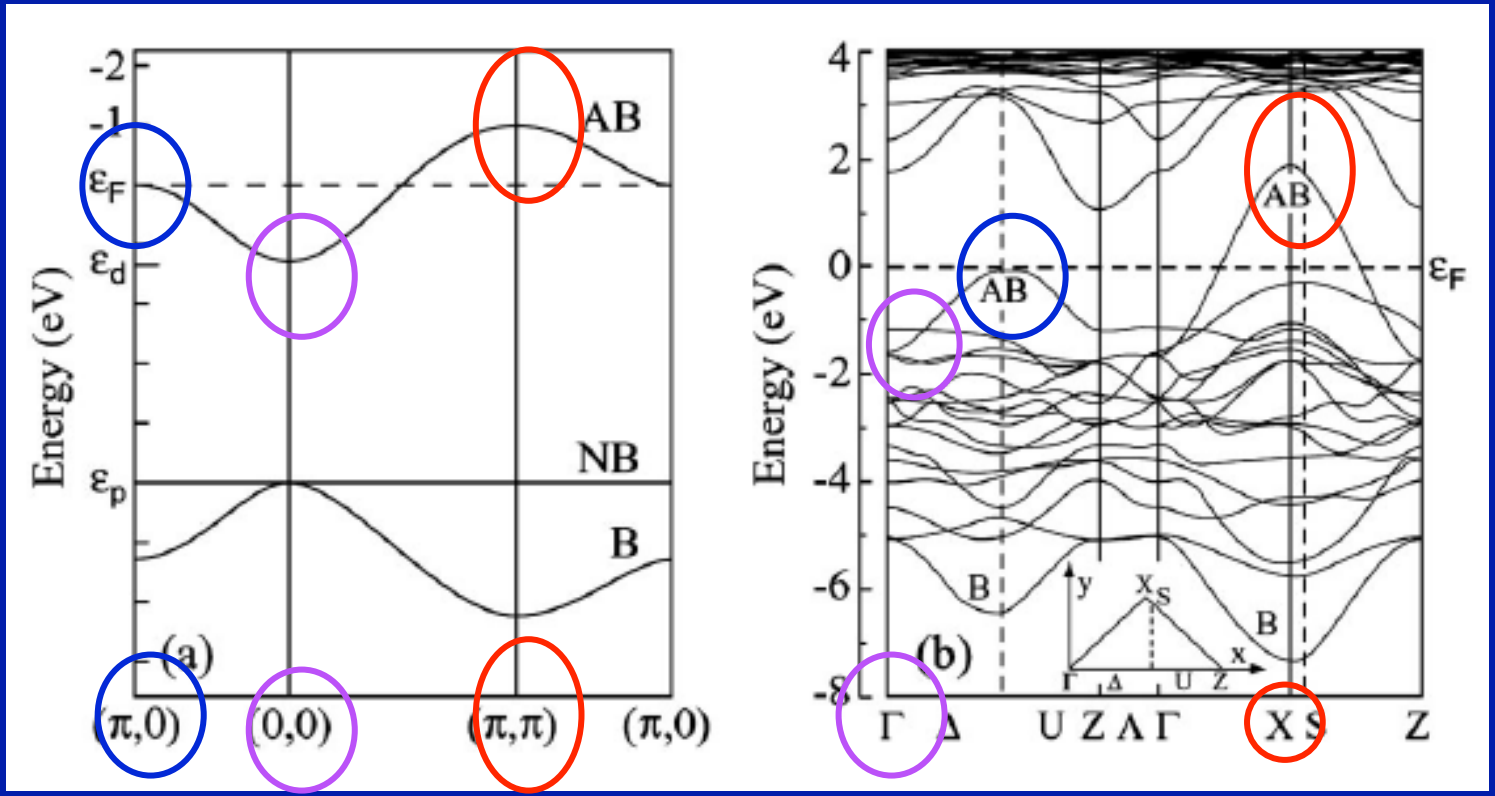
$$\omega_\pm \equiv \frac{1}{2}\left\{\varepsilon_p+\varepsilon_d \pm \sqrt{\delta}\right\}$$

Bonding / Antibonding bands.



Realistic (bct) band-structure vs. simplified 3-band model



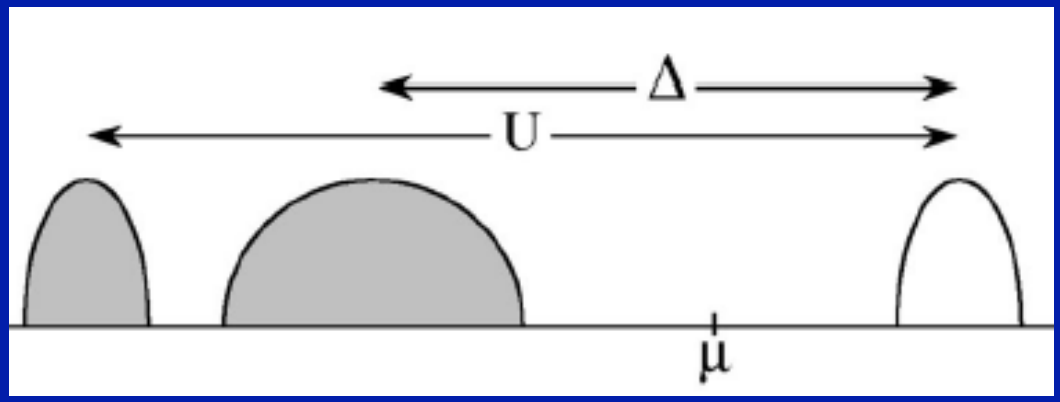


La_2CuO_4: a `charge-transfer' insulator

(cf. 2009-2010 lectures)

One-electron excitations in the insulating state: schematic view

(as probed e.g. in optical spectroscopy)



|GS>→ |$3d^8$>

O-states

|GS>→ |$3d^{10}$> (Upper Hubbard band)

|GS>→ |$3d^9$ hole in O2p>

→ The lowest-energy hole-excitation is NOT Cu $3d^9$→Cu$3d^8$ as in a Mott insulator, but rather creating a hole on the oxygen site because $\Delta << U_{dd}$

Doping:
- With holes on oxygen sites
- With electrons on copper site

Confirmed by several high-energy spectroscopic techniques:
EELS, XAS, etc…

(see e.g book by Plakida, Springer 2010, pp. 202 sqq)

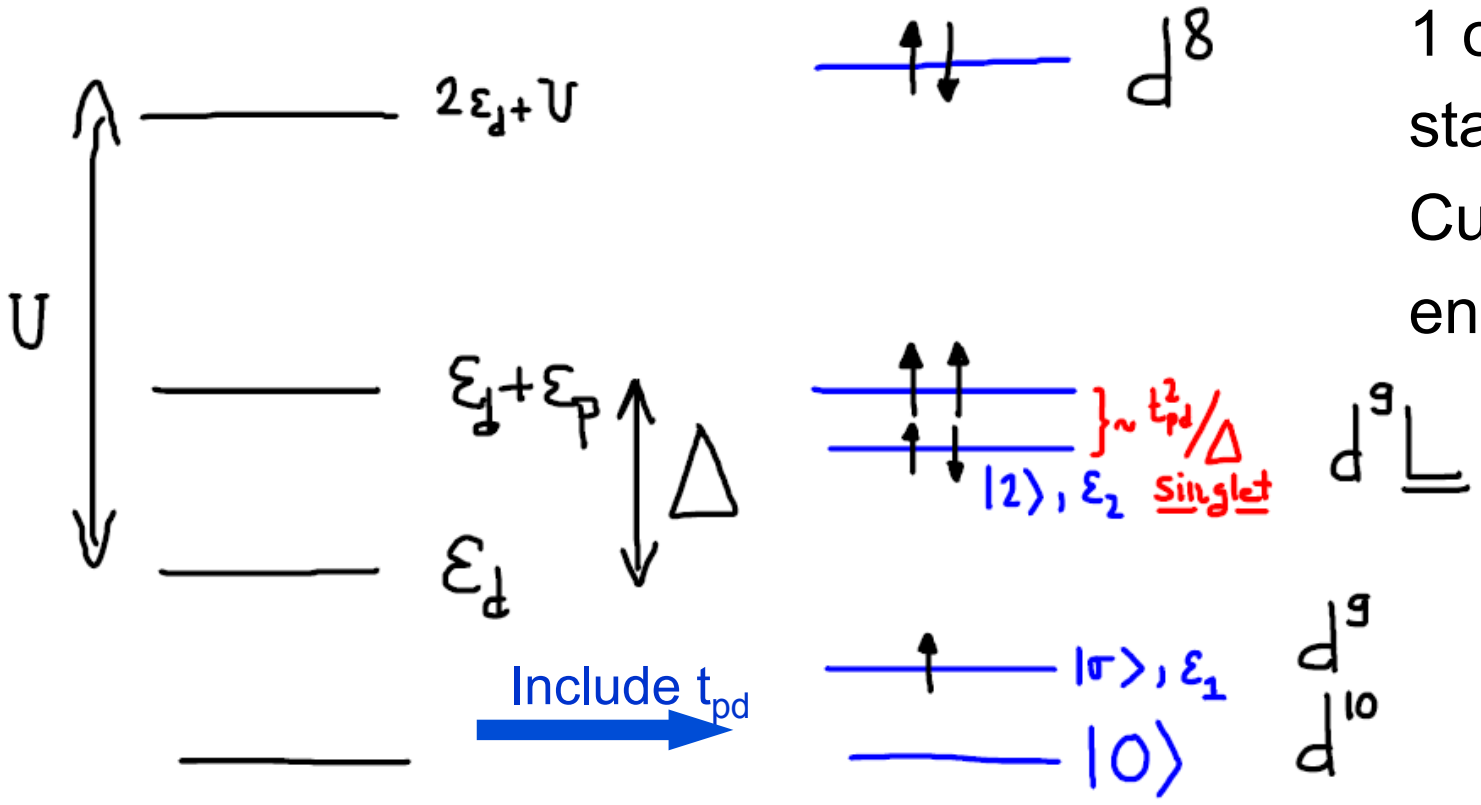
The Zhang-Rice singlet

- a more precise description of hole excitations -

Qualitative idea:

States of CuO_4 cluster, hole-representation:

Singlet state of two holes (1 in Cu-shell, 1 on oxygens) stabilised by Cu-O exchange energy



* Eliminate d^8 state, and also d^9L^h triplet

→Effective Hubbard-like model with

$U_{eff} \sim \Delta$

- Further eliminate d^{10} state

→Effective t-J model for hole-doped cuprates (Zhang-Rice, cf. Anderson)

States: $d^9 = |\sigma\rangle$ and $|ZR;d^9L^h\rangle = |0\rangle$ (3 states)

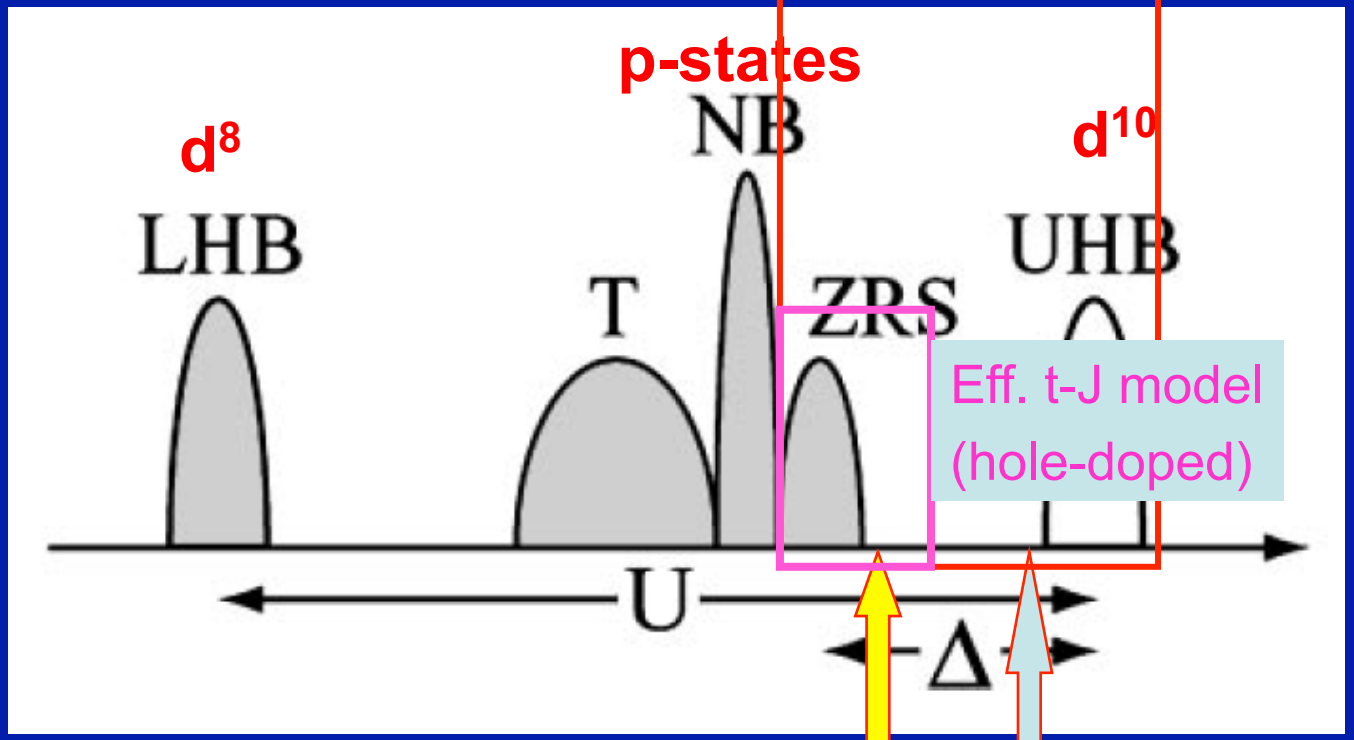
- Electron-doped: keep d^9 and d^{10} instead

The ZR singlet plays the role of the ``lower Hubbard Band'' for the low-energy effective Hubbard model.

Warning: There are limitations to these low-energy reductions, depending on parameters …

1-electron excitations from
~ d^9 ground-state

Eff. Hubbard model



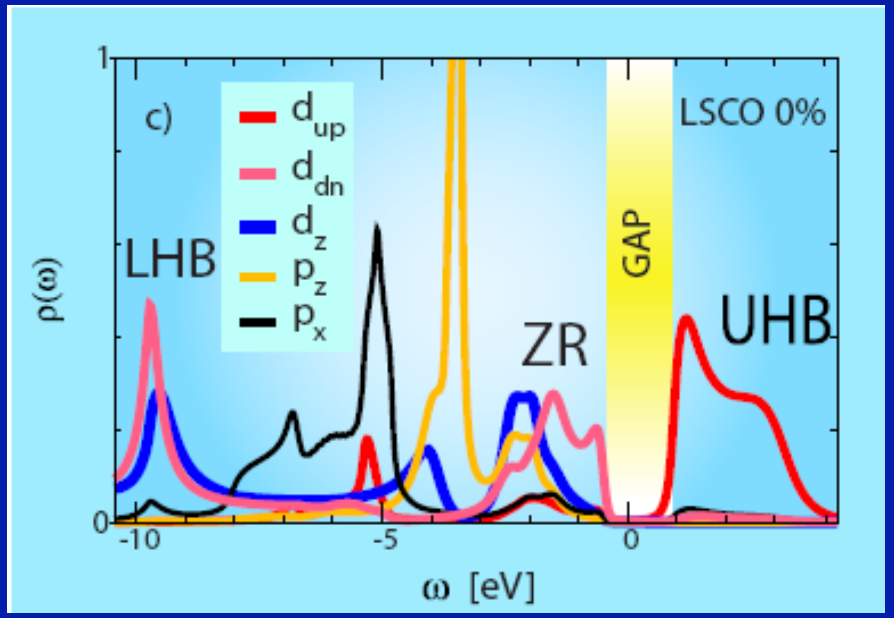
Eff. t-J model
(hole-doped)

~ position of chemical potential
for hole-doped

~ position of chemical potential
for electron-doped

Sketch inspired from
Damascelli et al.
Rev Mod Phys 2003

Recent DMFT calculations for undoped LSCO using a realistic bandstructure confirm this qualitative description



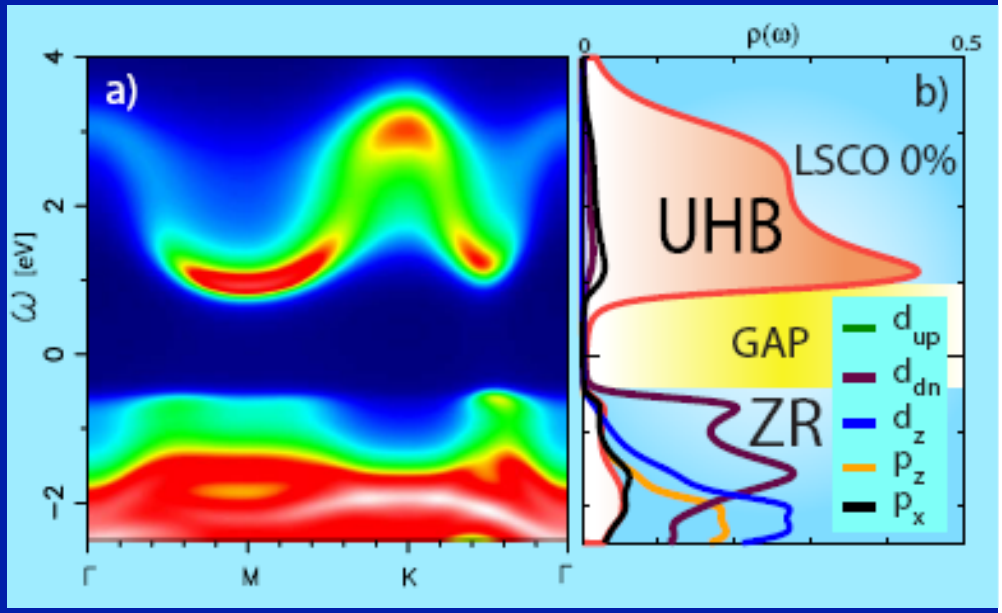


FIG. 7. (Color online) (a) Frequency-dependent spectral weight $A(k,w)$ obtained by LDA+DMFT of a six-band model description of the parent compound of LSCO. (b) Partial density of states of the d_{x2-y2}, d_{3z2-r2}, $p_{(x,y)}$, and $p_{\pm z}$ orbitals. We observe a direct gap of 1.8 eV in LSCO. Notice that the spectral weight is very incoherent close to the Fermi energy in the lower band. (c) Partial density of states on a larger energy scales. The LHB is located at a very low energy −10 eV, and the UHB is also shown. The d_{3z2-r2} and $p_{\pm z}$ orbitals have a strong weight between −4 and −1 eV.

Weber et al.
PRB 82, 125107
(2010)

Theoretical method for effective hamiltonian construction

- The original ZR paper uses a perturbation theory in t_{pd}/Δ which is not really justified given the relevant parameter range
- "Cell-cluster" perturbation theories have been constructed which have wider degree of generality and can handle U_{dd}, U_{pd} etc…
- See e.g several articles by (mid-1990's)

- Feiner, Raimondi, Jefferson et al.
- Hayn, Yushankai, Plakida et al.

- Pave the CuO_2 planes by overlapping CuO_4 clusters
- Construct oxygen Wannier functions, orthonormalized between clusters, … beware of appropriate phase relations

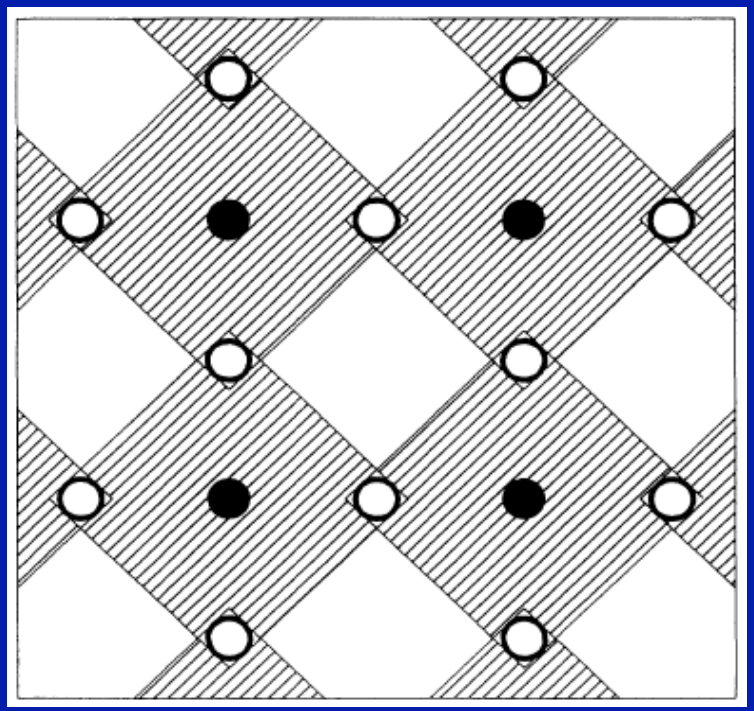
$$w_{\mathbf{k},\sigma} \doteq 2\mathrm{i}\left(\sin\frac{k_x}{2}\,p_{x,\mathbf{k},\sigma} + \sin\frac{k_y}{2}\,p_{y,\mathbf{k},\sigma}\right)/f(\mathbf{k})$$

→ This combination bonds with Cu-d

$$v_{\mathbf{k},\sigma} \doteq 2\mathrm{i}\left(\sin\frac{k_y}{2}\,p_{x,\mathbf{k},\sigma} - \sin\frac{k_x}{2}\,p_{y,\mathbf{k},\sigma}\right)/f(\mathbf{k})$$

→ This one does not

$$f(\mathbf{k}) \doteq 2\sqrt{\sin^2\frac{k_x}{2} + \sin^2\frac{k_y}{2}}$$



Overlapping CuO_4 cells. ● Cu; ○ oxygen.

$$H_{pd} = t_{pd}\sum_{\mathbf{l},\mathbf{m},\sigma}\left[T_{\mathbf{l}-\mathbf{m}}\,d^{\dagger}_{\mathbf{l},\sigma}w_{\mathbf{m},\sigma} + \mathrm{h.c.}\right]$$

$$T_{\mathbf{R}} \doteq \frac{1}{L}\sum_{\mathbf{k}} f(\mathbf{k})\,\mathrm{e}^{\mathrm{i}\mathbf{k}\mathbf{R}} = \int_{BZ}\frac{\mathrm{d}^2\mathbf{k}}{(2\pi)^2} f(\mathbf{k})\,\mathrm{e}^{\mathrm{i}\mathbf{k}\mathbf{R}}$$

Table 1. Numerical values for $T_{\mathbf{R}}$.

$\mathbf{R}$	$T_{\mathbf{R}}$
$(0,0)$	1.916183
$(\pm1,0),(0,\pm1)$	−0.280186
$(\pm1,\pm1)$	−0.047013
$(\pm2,0),(0,\pm2)$	−0.027450
$(\pm2,\pm1),(\pm1,\pm2)$	−0.013703

→Fast decay with distance !

Intra-cluster many-body hamiltonian (here with U_{dd} only):

$$H_0^w = \sum_{\mathbf{l}} h_{\mathbf{l}}$$

$$h_{\mathbf{l}} = \sum_{\sigma} \left[\epsilon_d d^\dagger_{\mathbf{l},\sigma} d_{\mathbf{l},\sigma} + \epsilon_p w^\dagger_{\mathbf{l},\sigma} w_{\mathbf{l},\sigma} + t_0 (d^\dagger_{\mathbf{l},\sigma} w_{\mathbf{l},\sigma} + w^\dagger_{\mathbf{l},\sigma} d_{\mathbf{l},\sigma}) \right] + U d^\dagger_{\mathbf{l},\uparrow} d_{\mathbf{l},\uparrow} d^\dagger_{\mathbf{l},\downarrow} d_{\mathbf{l},\downarrow}.$$

$$t_0 \doteq T_{(0,0)} t_{pd} \approx 1.916\, t_{pd}$$

In the infinite-U limit, the cluster eigenstates are:

$$|0\rangle \equiv |d^{10}\rangle$$

$$|\sigma\rangle \ , \ \varepsilon_1 = \frac{\varepsilon_p + \varepsilon_d}{2} \frac{1}{2} \sqrt{\Delta^2 + 4t_0^2} \simeq \varepsilon_d - O\left(t_{pd}^2/\Delta\right)$$

$$|2\rangle \equiv |\mathrm{ZR}\rangle \ , \ \varepsilon_2 = \frac{3\varepsilon_p + \varepsilon_d}{2} \frac{1}{2} \sqrt{\Delta^2 + 8t_0^2} \simeq \varepsilon_p + \varepsilon_d - O\left(t_{pd}^2/\Delta\right)$$

Inter-cluster coupling (only kinetic here):

$$V^w = t_{pd} \sum_{\mathbf{l},\mathbf{m},\sigma}^{\mathbf{l}\neq\mathbf{m}} T_{\mathbf{l}-\mathbf{m}} \left[d^\dagger_{\mathbf{l},\sigma} w_{\mathbf{m},\sigma} + w^\dagger_{\mathbf{l},\sigma} d_{\mathbf{m},\sigma} \right]$$

Construct effective hamiltonian perturbatively in V :

$$H_{\text{eff}} = H_0 + P_0 V P_0 + P_0 V \frac{1 - P_0}{E - H_0} V P_0 + \cdots$$

Yields Hubbard-like model (see e.g Plakida et al, PRB 51, 16599 (1995)

$$H = (\varepsilon_1 - \mu) \sum_{i\sigma} X_i^{\sigma\sigma} + (\varepsilon_2 - 2\mu) \sum_i X_i^{22} +$$
$$+ \sum_{\langle ij \rangle} \left[t_{ij}^{11} X_i^{\sigma 0} X_j^{0\sigma} + t_{ij}^{22} X_i^{2\sigma} X_j^{\sigma 2} + \sigma t_{ij}^{12} (X_i^{2\overline{\sigma}} X_j^{0\sigma} + \text{h.c.}) \right]$$

$X_{\alpha\beta} \equiv |\alpha\rangle\langle\beta|$ Hubbard operator : transforms |β> → |α>

Hoppings are of order t_{pd}^2/Δ in the $t_{pd} << \Delta$ limit

Reduction to t-J model : eliminate state d^{10}

$$H = \sum_{\langle ij \rangle} t_{ij} \, (1 - \hat{n}_{i\bar{\sigma}}) d^{+}_{i\sigma} d_{j\sigma} (1 - \hat{n}_{j\bar{\sigma}}) + \text{h.c.} \; + \; J \sum_{\langle ij \rangle} \left(\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} \hat{n}_i \hat{n}_j \right)$$

Written here with:

|0> = ZR singlet (previously |2>)

|σ> = spin-σ hole in Cu d^{10} shell (spin –σ on Cu site)

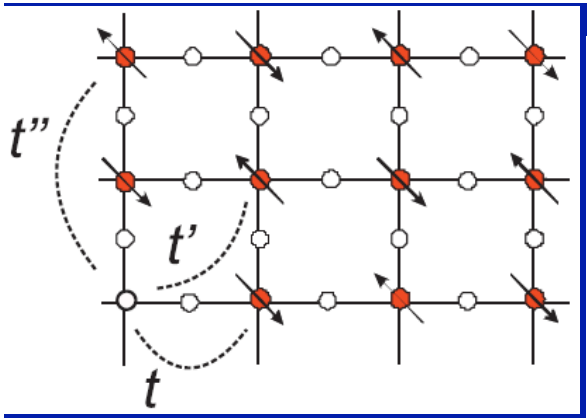
Each site (=CuO_4 cluster) is either in the ZR state (``empty'') or has one hole in Cu d10 shell (occupied by a spin). Motion of ZR singlets and of Cu spins are tight one to the other.

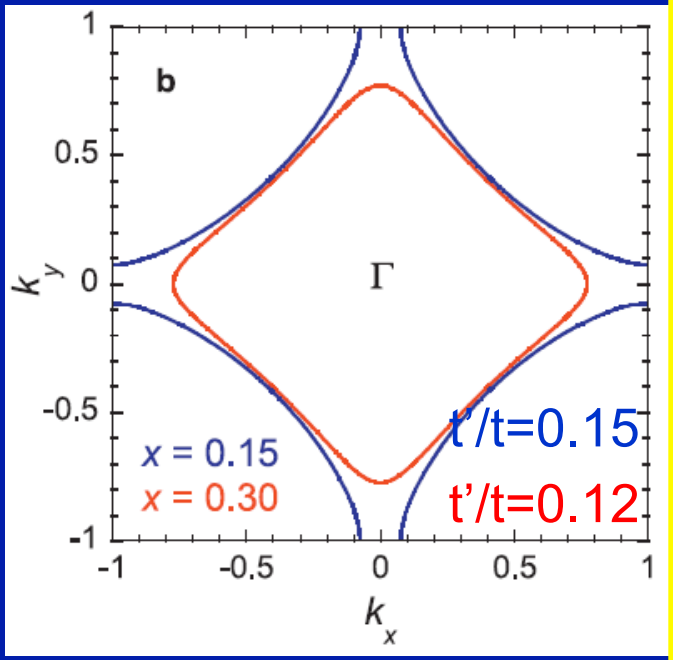
Superexchange interaction between spins on Cu sites, in the strong-coupling limit $t_{pd} << \Delta$:

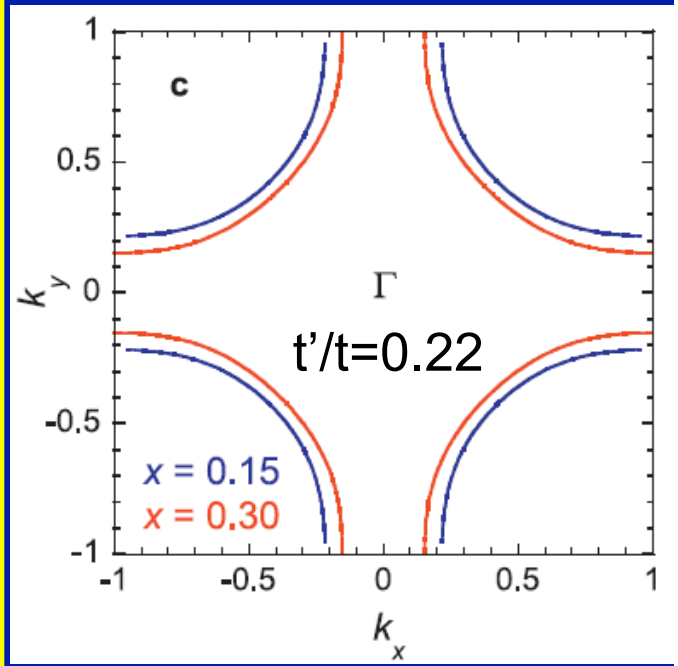
$$J = \left(\frac{2t_{pd}^2}{\Delta} \right)^2 \left[\frac{1}{\Delta} + \frac{1}{U_{dd}} \right]$$

Reduction to 1-band model (if valid at all…) requires longer-range hopping

$$\epsilon(\mathbf{k}) = \epsilon_0 - 2t(\cos k_x + \cos k_y) + 4t'(\cos k_x \cdot \cos k_y) - 2t''(\cos 2k_x + \cos 2k_y).$$







Cf. lecture 4 material dependence of Tc, Role of axial orbital

Lower-Tc cuprates have a Smaller t’/t. Here, schematic FS for LSCO at two doping levels

Higher-Tc cuprates have a larger t’/t. Here, schematic FS for $Tl_2Ba_2CuO_{6+\delta}$

Validity of effective low-energy models ?

- Low-energy effective models are only valid at… low energy → don't ask too much of them !
- Hubbard model reduction seems OK, although admittedly the role of U_{pd} is not fully understood
- t-J model is probably valid at a qualitative level (although not quantitatively justified) on the hole-doped side. On electron-doped side Δ may be too small indeed…

A distinctive aspect of cuprates:

- ***Only 1 band crosses the Fermi level***
- Stems from a single linear combination of `active' orbitals
- 1 hole (1 electron) in a single band:

  ½ - filled system

Lowest possible degeneracy

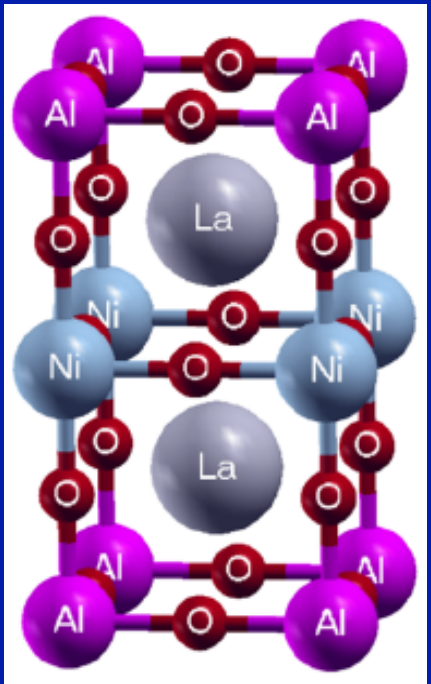
→Strongest correlations and quantum effects

Single-band systems are RARE:

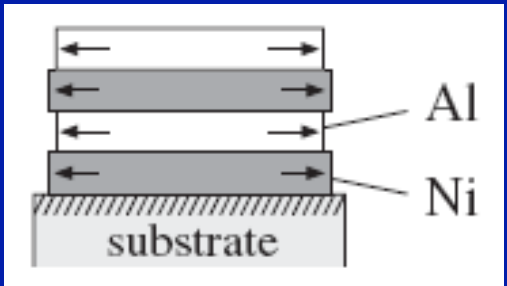
Other known example: 2D k-BEDT organics

(also hi-Tc superconductors: large kT_c/E_F !)

Recent suggestions to turn nickelates into 1-band materials in oxide multilayers



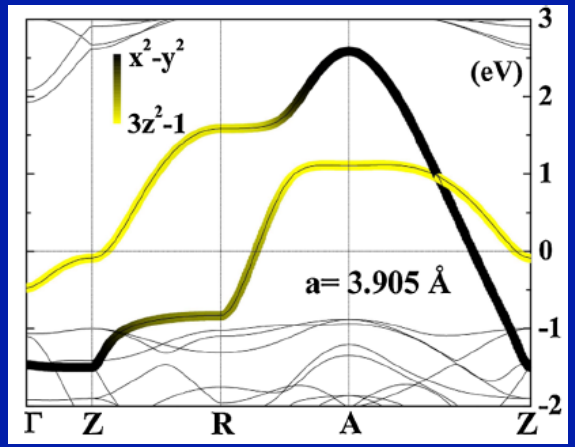
1/1 $LaNiO_3/LaAlO_3$ heterostructure



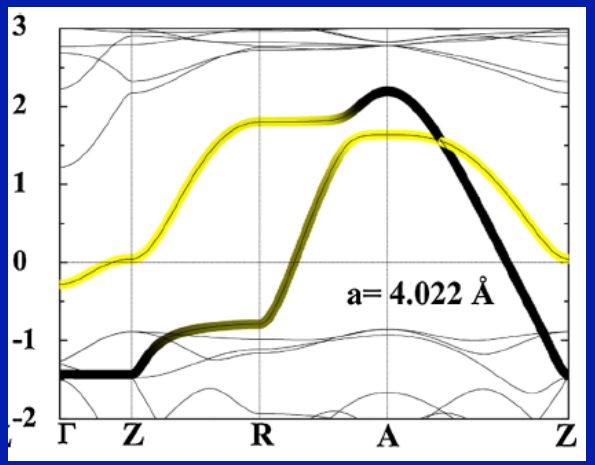
Strain alone does not do the job

→ Correlation-induced renormalization of splitting between the two e_g states ?

Cf. Poteryaev et al. PRB 78, 045115 (2008)



Without strain (LDA)



With strain (LDA)

Chaloupka and Khaliullin, PRL 100, 016404 (2008)
Hansmann et al., PRL 103, 016401 (2009)