Mean Surface Temperature on the dark side of the Moon

120 K

The Road to RTS - Lessons from today's Hi-Tc Compounds

T.M.Rice ETHZ & HKU

Directions:

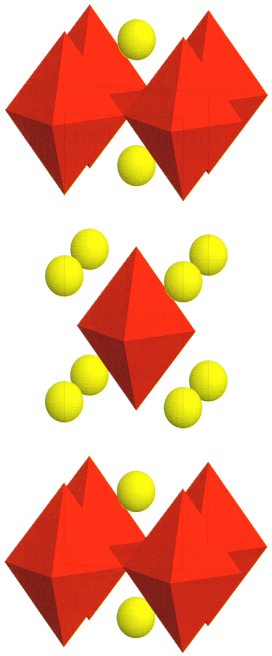
- MgB_2 — Related Compounds ?
- $Ba_{1-x}K_xBiO_3$ — Lattice Analogs of Cuprates ?
- Cuprates — Nickelates as alternatives ?
  — Structured Layers ?

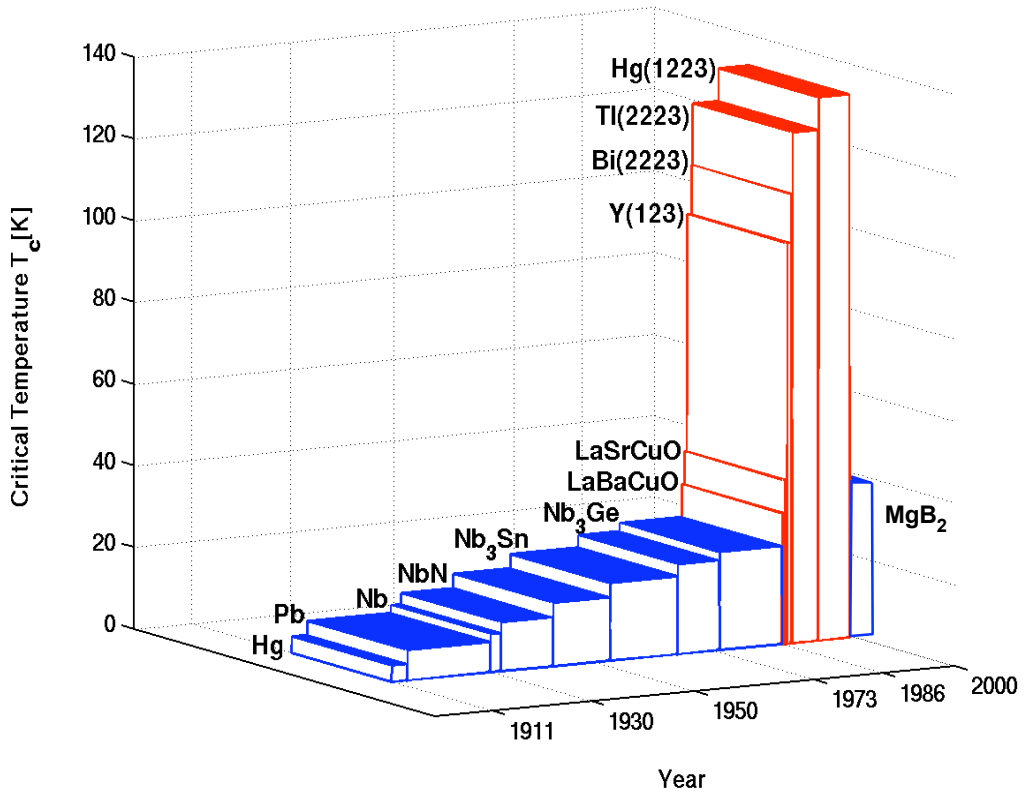
$(La/Ba)_2CuO_4$

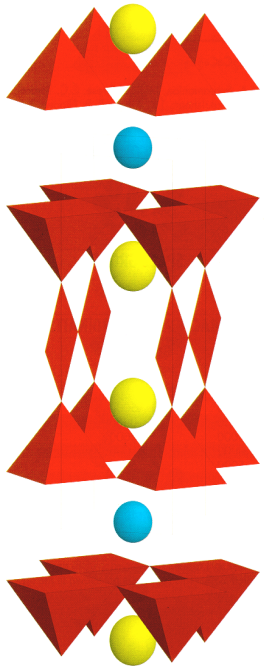
Superconductivity

T_c over time

$YBa_2Cu_3O_7$







G. Bednorz
&
K.A. Müller

C.W. Chu
&
M.K. Wu

MgB_2 — Related Compounds ?

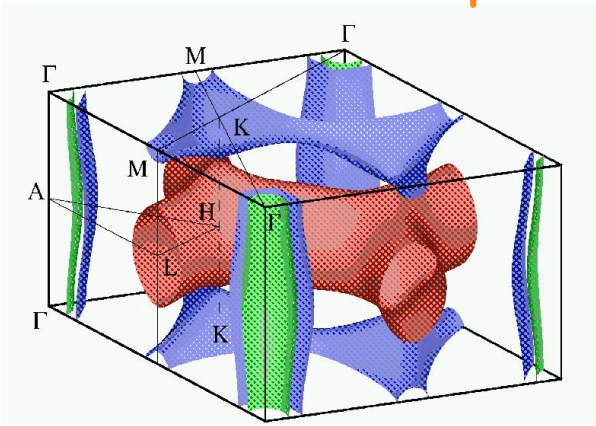
MgB_2 - a high-temperature BCS superconductor

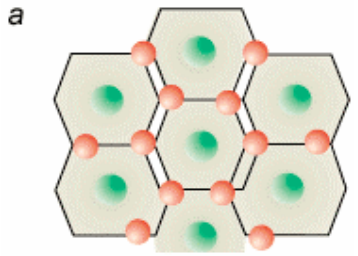
2D σ-band dominant

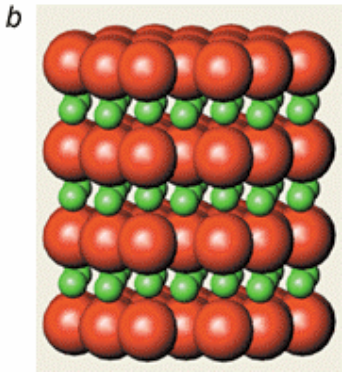
3D π-band passive

T_c = 39 K

(Akimitsu et al. 2001)







<- B

<- Mg

Isoelectronic to Graphite

Strong el.-ph. coupling only to the high energy stretching B-B mode on σ– Fermi Surface sheets (green). Weak on π-sheets ....

Mazin,Andersen,Pickett & - -

Question :

Can we find other compounds where Fermi level lies in σ- band ?

Not easy - e.g. σ- band lies 2 eV below E_F in graphite

Proposal by Rosner,Pickett et al : $Li_{1+x}BC$ should have T_c of 10^2K

No luck so far in realizing this proposal alas !

Design for a Room Temperature Superconductor

W. E. Pickett
Department of Physics, University of California, Davis, California, 95616
(Dated: May 29, 2006)

The vision of "room temperature superconductivity" has appeared intermittently but promine in the literature since 1964, when W. A. Little and V. L. Ginzburg began working on the *proble high temperature superconductivity* around the same time. Since that time the prospects for r temperature superconductivity have varied from gloom (around 1980) to glee (the years imm ately after the discovery of HTS), to wait-and-see (the current feeling). Recent discoveries l clarified old issues, making it possible to construct the blueprint for a viable room tempera superconductor.

Pickett`s Idea condmat 0603482

Generalize MgB_2 to many Fermi surface sheets each couplied strongly to specific phonons leading to enhanced λ without any phonon being driven soft. 2D cylindrical Fermi sheets are optimal for this scenario (no nesting !)

How to go from `design' to a chemical formula ?

Fermi Surface not unlike FS of Na_xCoO_2
But Coulomb interactions dominate !

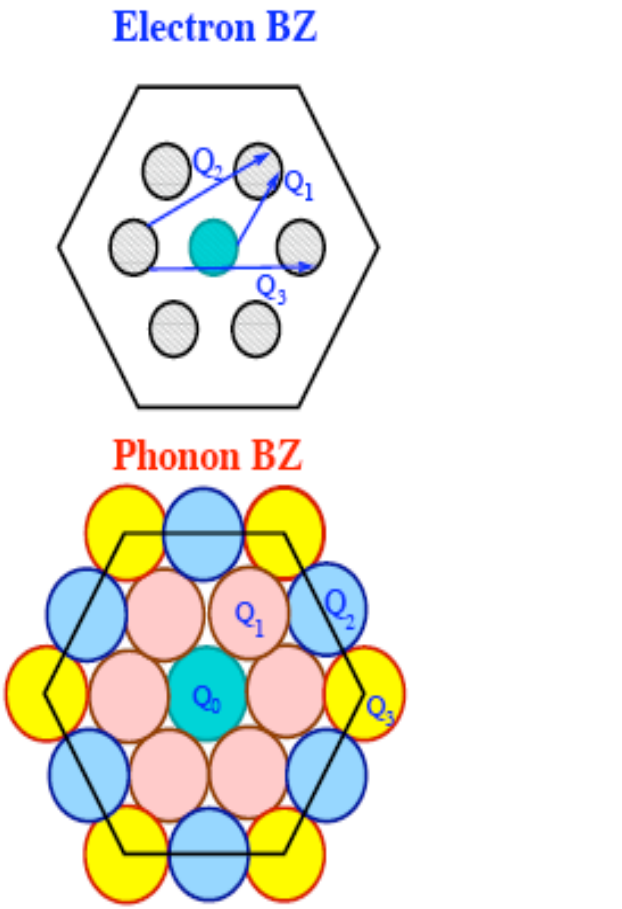


FIG. 4: Top: hexagonal electron Brillouin zone with central Fermi surface circle (an idealization of that of MgB_2) and with six additional circular Fermi surfaces placed at the midpoint of the Γ-K line. Bottom: the phonon Brillouin zone, mapping the circular regions $|Q-Q_j| < 2k_F$, j=0, 1, 2, 3. The figures are drawn for k_F equal to one-eighth of the Γ-K line length, which results in 2D close packing of the circles of diameter $4k_F$. The Kohn circles at the edge have been pictured extending into the neighboring zones to facilitate comparison with the top panel.

B - Doped Diamond :a metallized covalent bond Superconductor

Expt. Tc = 7K with 1% B { Efimov et al `04,Takano et al `04}

New Study proposes a way to greatly enhance Tc !

JPSJ `07

Theoretical Study on Superconductivity in Boron-Doped Diamond

Tomonori SHIRAKAWA[1] *, Satoshi HORIUCHI[1], Yukinori OHTA[1,2] and Hidetoshi FUKUYAMA[3]

[1] *Graduate School of Science and Technology, Chiba University, Chiba 263-8522*
[2] *Department of Physics, Chiba University, Chiba 263-8522*
[3] *Department of Applied Physics, Tokyo University of Science, Kagurazaka, Tokyo 162-8601*

We consider superconductivity in boron (B) doped diamond using a simplified model for the valence band of diamond. We treat the effects of substitutional disorder of B ions by the coherent potential approximation (CPA) and those of the attractive force between holes by the ladder approximation under the assumption of instantaneous interaction with the Debye cutoff. We thereby calculate the quasiparticle life time, the evolution of the single-particle spectra due to doping, and the effect of disorder on the superconducting critical temperature T_c. We in particular compare our results with those for supercell calculations to see the role of disorder, which turns out to be of crucial importance to T_c.

Key difference to previous LDA studies {Boeri et al `04;Lee et al `04}

Fermi level lies in a B - impurity band separate
from valence band of diamond

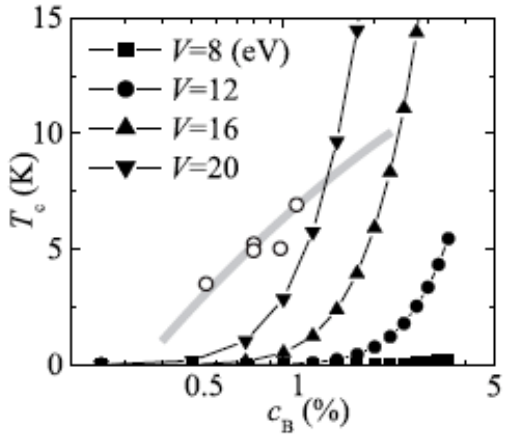
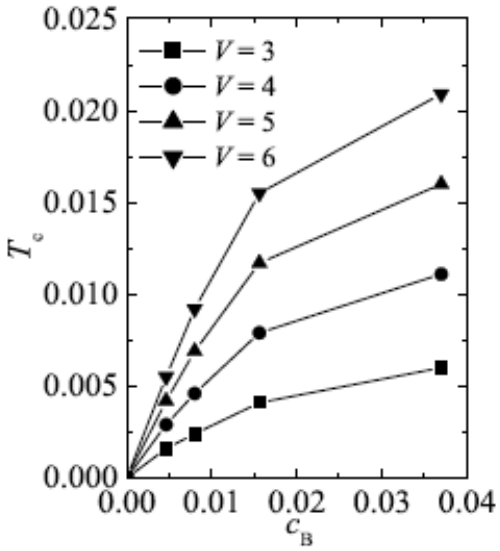


Fig. 11. Comparison between the calculated critical temperature T_c as a function of c_B and the experimental data (open circles and broad curve) estimated by Mukuda *et al.*[6] from the analysis of the NMR spectra. T_c is given in units of K for comparison with experiment. The values of V used for calculations are given in units of eV here.

Tc (eV)



c_B

Fig. 13. Superconducting critical temperature T_c obtained under the assumption of the periodic arrangement of B ions.

Fix net attraction (-V) by fitting to Tc of a random B distribution

e. g. Tc =7K at 1%B

⇒use same V for periodic arrangement of B dopants

⇒ leads to a Tc ≈ 100 K !

DOS of B-impurity band greatly enhanced by periodic B-superlattice

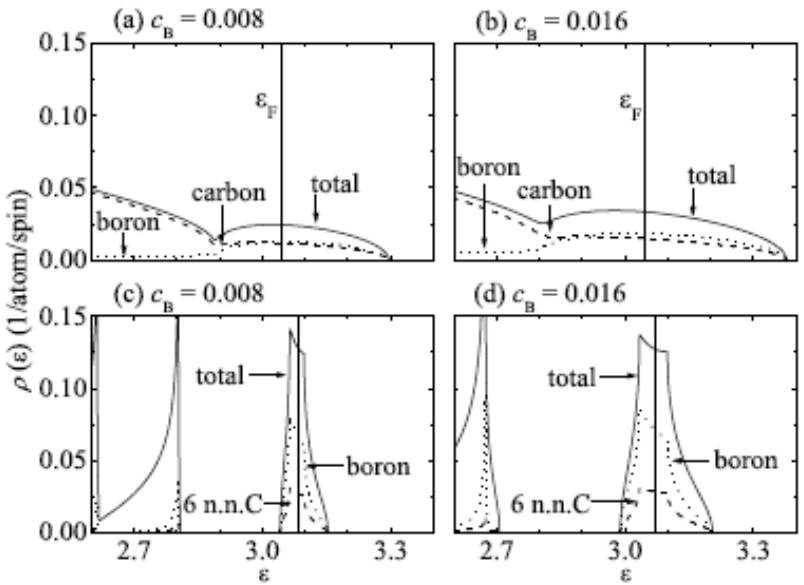


Fig. 12. Densities of states near the Fermi energy obtained by CPA (upper panels) and those calculated under the assumption of the periodic arrangement of B ions (lower panels). The $5\times5\times5$ and $4 \times 4 \times 4$ supercells are assumed in (c) and (d), respectively. Partial densities of states are also shown where '6 n.n.C' means the partial density of states summed over the six nearest-neighbor carbon sites around a boron ion. Vertical lines indicate the Fermi energy ε_F.

<– Random

<— Periodic

$Ba_{1-x}K_xBiO_3$ — Lattice Analogs of Cuprates ?

" High- T_c " Superconductivity in an oxide near a Metal-Insulator Transition Sleight et al `75, Uchida . . .

T_c = 10K at x=0.3

$BaBiO_3$ is a CDW Insulator with Bi^{+3} & Bi^{+5} sites

Substitution of Pb leads to melting of el. Pairs leads and to Superconductivity

- Rice&Sneddon `81
- Yoshioka-Fukuyama `85

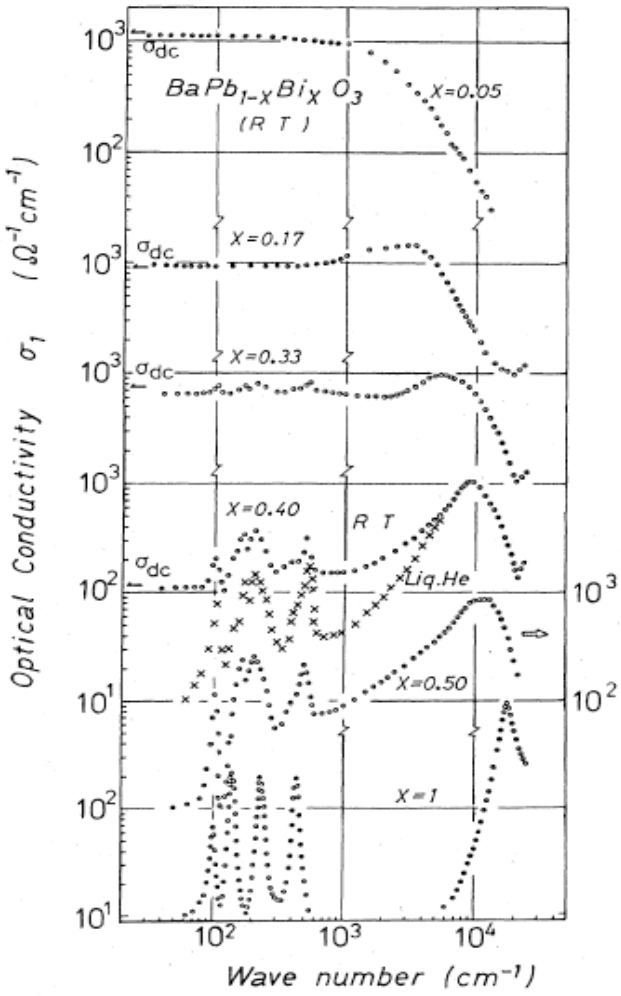


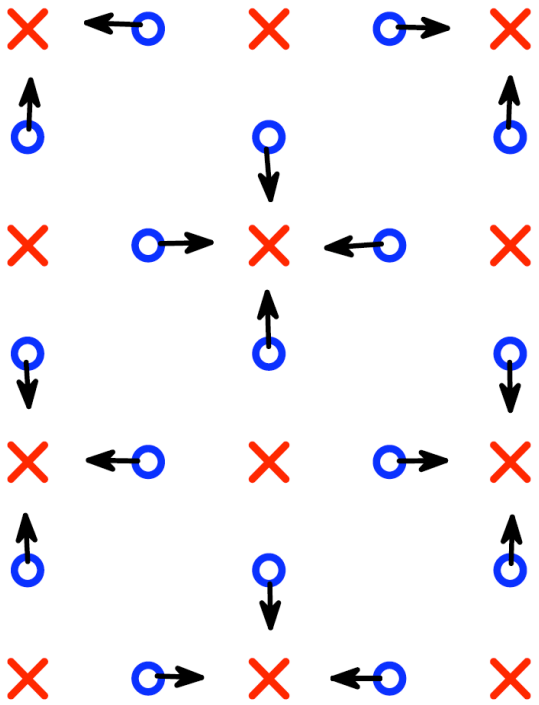
FIG. 5. Real part of the optical conductivity σ_1 for various

Interpenetrating s.c. lattice of X and O ions

XO (1D) , XO_2 (2D) & XO_3 (3D)

O^{2-} - Ion Displacement Pattern
in sc lattice is unfrustrated !

—> A Charge Density Wave in $BaBiO_3$ (X=Bi)
i.e. 2 Sublattices with Bi^{3+} & Bi^{5+} ions
leading to an energy gap in the Bi-6s band



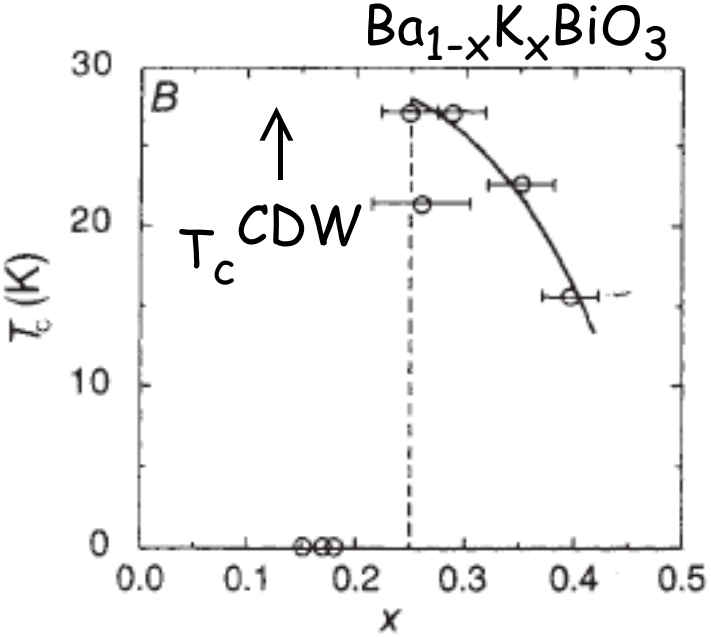
N.B. Careful LDA calculations do not give observed CDW
(Meregalli & Savrasov PRB `99 ,,,,,,,)

A Sign that standard LDA underestimates correlation effects here
Question: Does charge disproportionation require the lattice of
O^{2-}- ions or is it valence skipping(Varma) ?

Hole Doping a CDW Insulator leads to a Superconductor

Phase Diagram has analogies to Cuprates
but T_c is high for BCS but low compared to Cuprates.

Tc is much higher than theoretical
estimates based on standard methods
e.g. LDA (Meregalli&Savrasov `98).
Gives λ =0.34 too small for Tc $\approx$ 30K!



Mattheiss et al,Cava et al, Hinks et al `88

Why is Tc low compared to the cuprates ?

- CDW state is much more stable than AF state !

$T_c^{CDW} = E_f e^{-1/(\lambda-\mu)}$ is much larger than T_N=const. J

Cuprates — Nickelates as alternatives ?

Path to high-temperature superconductivity :

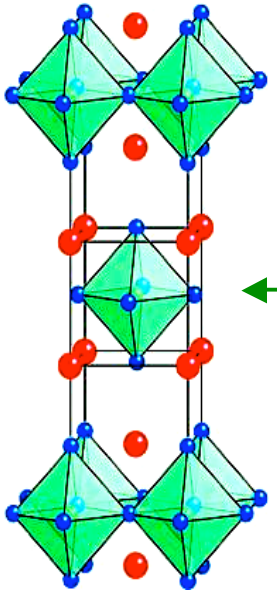
Bernd Matthias: "Avoid magnetism!" Wrong!

1986: J.G. Bednorz & K.A. Müller

Doped antiferromagnetic Mott-insulator

Copper-oxide compounds

$La_{2-x}Sr_xCuO_4$ ...

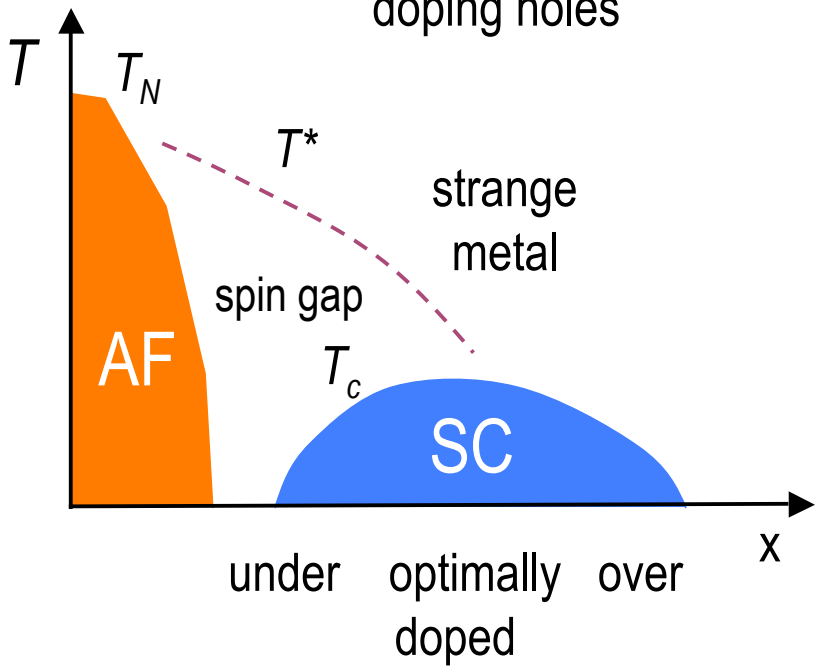


T_c =45 K

← CuO_2 plane

La_2CuO_4 ⟶ $La_{2-x}Sr_xCuO_4$

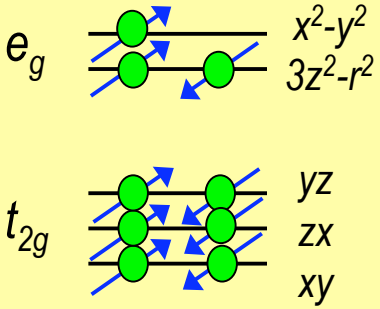
doping holes



CuO_2 plane electronically relevant

Parent compound: La_2CuO_4

Cu^{2+} $3d^9$



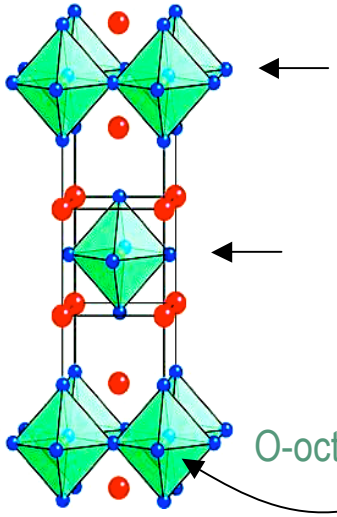
1 hole in 3d-e_g

spin S = 1/2

Strong Coulomb interaction

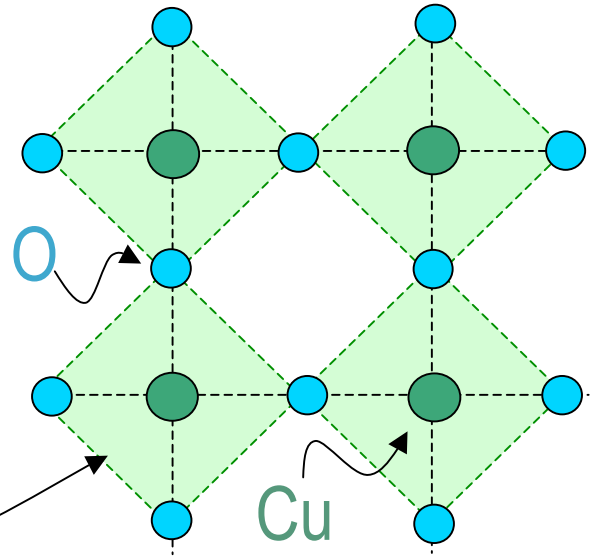
⇓

Mott insulator, Antiferromagnet

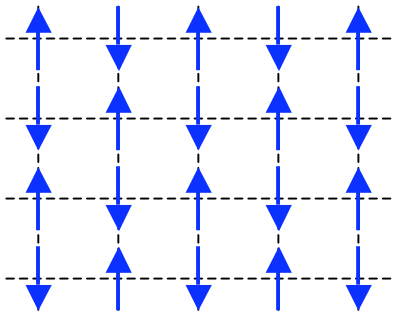


O-octahedra

CuO_2-plane



square lattice of Cu-ions

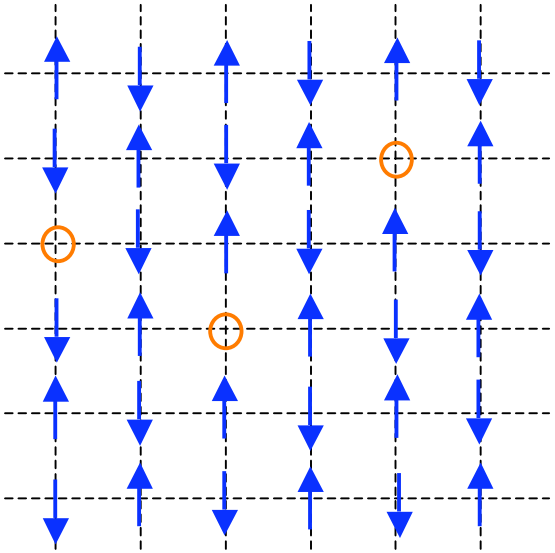


Basic model for doped cuprates

lightly doped AF Mott Insulators: *t-J-model* Anderson (1987), ...

$$H = -t \sum_{\langle i,j\rangle,s} \left\{ c_{is}^{+} \left(1 - n_{i,-s}\right)\left(1 - n_{j,-s}\right) c_{js} + hc. \right\} + J \sum_{\langle i,j\rangle} \vec{S}_i \cdot \vec{S}_j$$

Projection: at most 1 electron per site
("infinite" Coulomb repulsion)



Assumption: doubly occupied configs are energetically extremely expensive

Hole-doping => mobile missing spins

New physics !

Basic models of doped cuprates

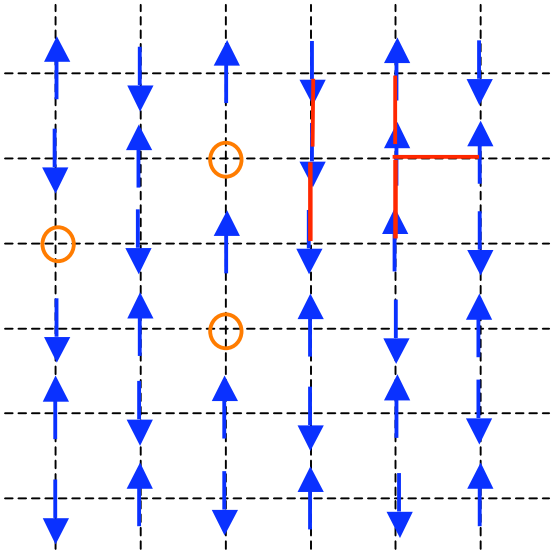
Resonating valence bond (RVB): Anderson (1987), ...

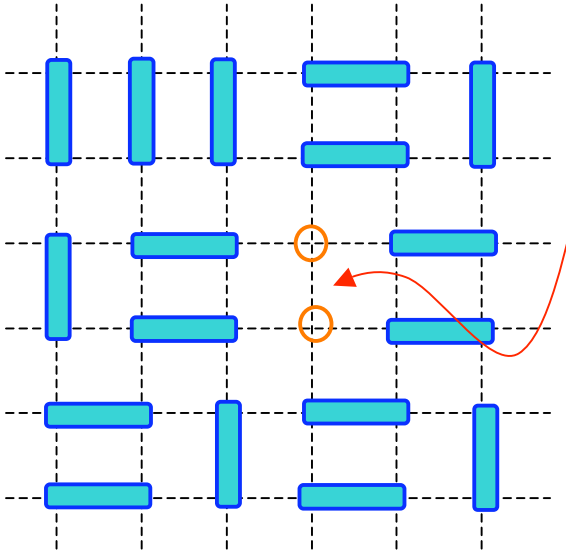
basic model of lightly doped system: *t-J-model*

$$H = -t \sum_{\langle i,j\rangle,s} \left\{ c^{+}_{is} \left(1 - n_{i,-s}\right)\left(1 - n_{j,-s}\right) c_{js} + hc. \right\} + J \sum_{\langle i,j\rangle} \vec{S}_i \cdot \vec{S}_j$$

Projection: at most 1 electron per site
("infinite" Coulomb repulsion)

RVB state





pairing of holes favored

singlet

as preformed Cooper pairs

Are there other planar S = 1/2 AF systems
with larger values of (t,J) and so larger Tc ?

Nickelates ?

Favored valence is Ni^{2+} with S =1 [2 holes,octa. coord.
& Hund`s Rule]

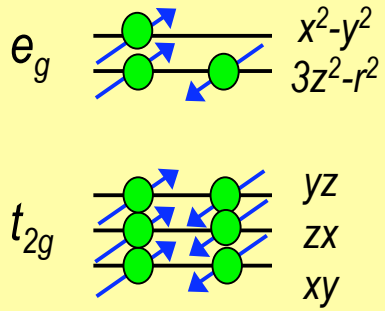
Can we force a different valence with S= 1/2 ?

- Ni^{3+}: No Good! 3 holes favor a $3d^8 2p^5$ config.
=> metallic behavior e.g. $LaSrNiO_4$

- Ni^{+} : Rare! Needs planar coordination
as in $LaNiO_2$

NiO_2 planar compounds : e.g. compound: $LaNiO_2$

Ni^+ $3d^9$



1 hole in 3d-e_g

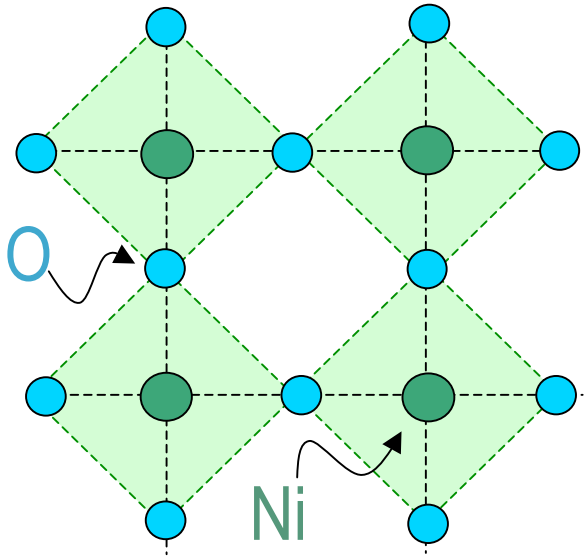
spin S = 1/2

Strong Coulomb Interaction

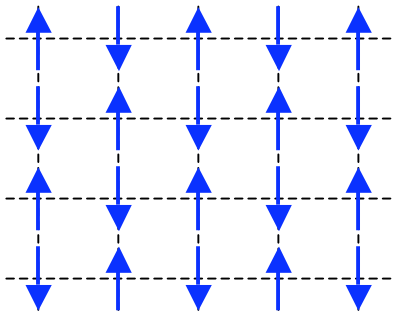
⇓

Mott insulator, Antiferromagnet ?

NiO_2-plane



square lattice of Ni^+-ions



$LaNiO_2$

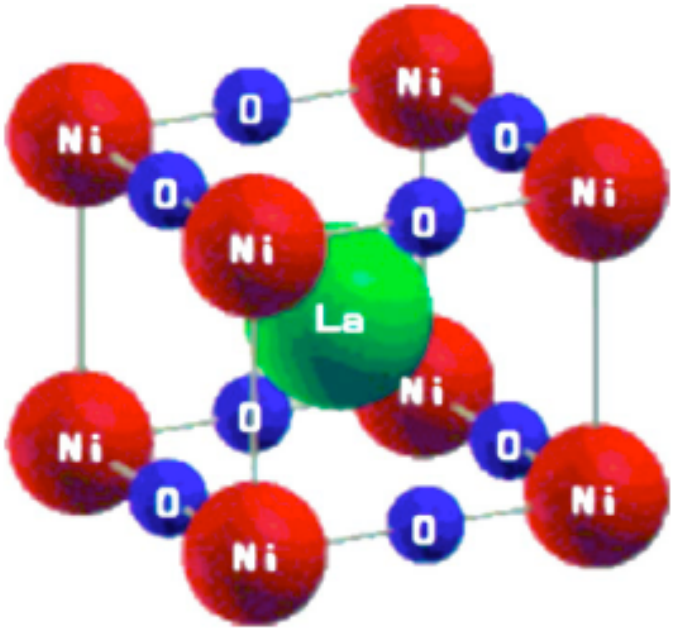


FIG. 1. (Color online) Crystal structure of $LaNiO_2$, isostructural to $CaCuO_2$. Ni ions are in the origin and La ions in the center of the unit cell. It has no axial oxygens.

Differing Results in LDA + U

Anisimov,Bukvalov & Rice PRB `99
get AFI similar to $CaCuO_2$

Lee & Pickett PRB `04
get weakly AFM unlike $CaCuO_2$

Expt. Hayward et al J.Am.Chem.

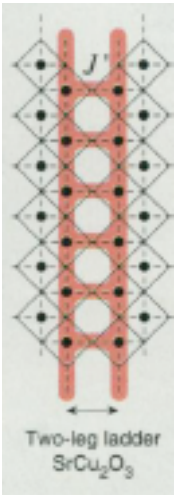
⇒ insulator with Curie -Weiss $\chi(T)$
⇒ S=1/2 & Θ= - 257K; no AF order
⇒ Nonstoichiometric Mott Insulator?

Conclusion
Nickelates are not promising !

Cuprates — Structured Layers ?

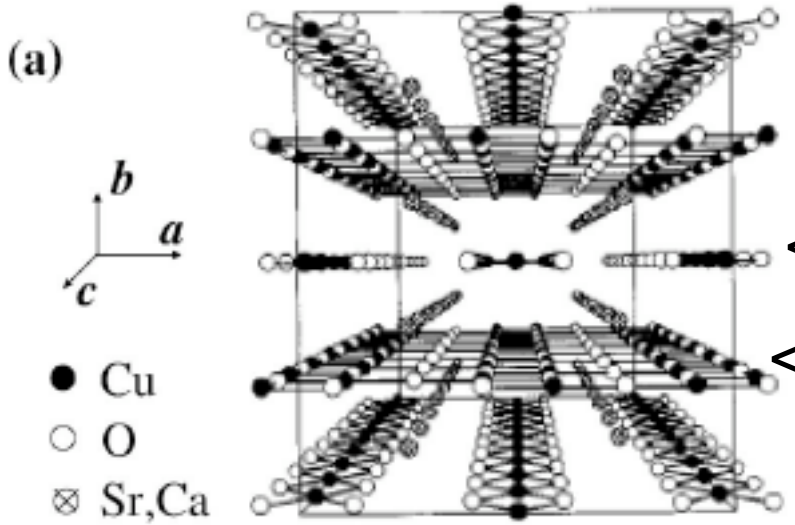
2-Leg Ladder Compounds with Cu_2O_3 - planes

$SrCu_2O_3$



180° O-Cu-O Bonds form 2-leg ladders

$Sr_{14}Cu_{24}O_{41}$ — Tel. No. Compound



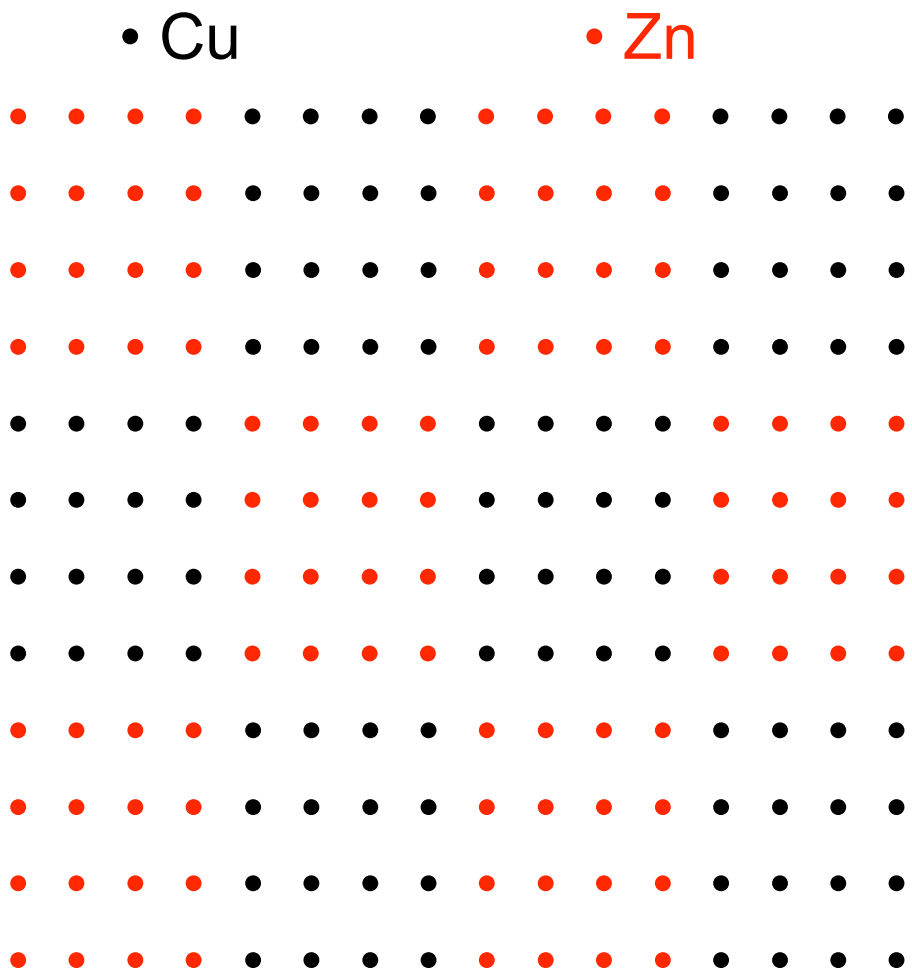
<— CuO_2 chains

<— Cu_2O_3 planes

- 2-leg AF S=1/2 Ladders form short range RVB spin liquids
- Holes form more stable pairs but 1D nature of ladders leads to competition between SC and CDW (hole pair xtals)
- Only doped example is $Sr_{14}Cu_{24}O_{41}$ which forms a hole pair xtal.
- Are there compounds with doped Cu_2O_3 - planes similar to the many cuprates with doped CuO_2 planes and would this enhance T_c ?

Pattern CuO_2 with ZnO_2 —> weakly coupled CuO_2 islands

Can it lead to a U<0 Hubbard model when hole doped ?



Interisland Hopping
$\approx t'/4$

$U \approx -J$ + Coulomb
+ el. ph

Energy gain from singlet
Groundstate of island ?

- Simple extensions of the current set of high Tc superconductors are not promising.

- New directions needed !

Basic model for doped cuprates

Resonating valence bond (RVB): Anderson (1987), ...

basic model of lightly doped system: *t-J-model*

$$H = -t \sum_{\langle i,j\rangle,s} \left\{ c_{is}^{+} \left(1 - n_{i,-s}\right)\left(1 - n_{j,-s}\right) c_{js} + hc. \right\} + J \sum_{\langle i,j\rangle} \vec{S}_i \cdot \vec{S}_j$$

Gutzwiller variational wave function:

projected "uncorrelated" state → no double occupancy

$$\left|\Psi_g\right\rangle = \hat{P}\left|\Psi_0\right\rangle = \prod_i \left(1 - n_{i\uparrow} n_{i\downarrow}\right)\left|\Psi_0\right\rangle$$

best $\left|\Psi_0\right\rangle$ is a BCS state with $d_{x^2-y^2}$ symmetry:

$$\left|\Psi_0\right\rangle = \prod_{k<k_F} \left(u_{\vec{k}} + v_{\vec{k}} c_{\vec{k}\uparrow}^{+} c_{-\vec{k}\downarrow}^{+}\right)\left|0\right\rangle$$

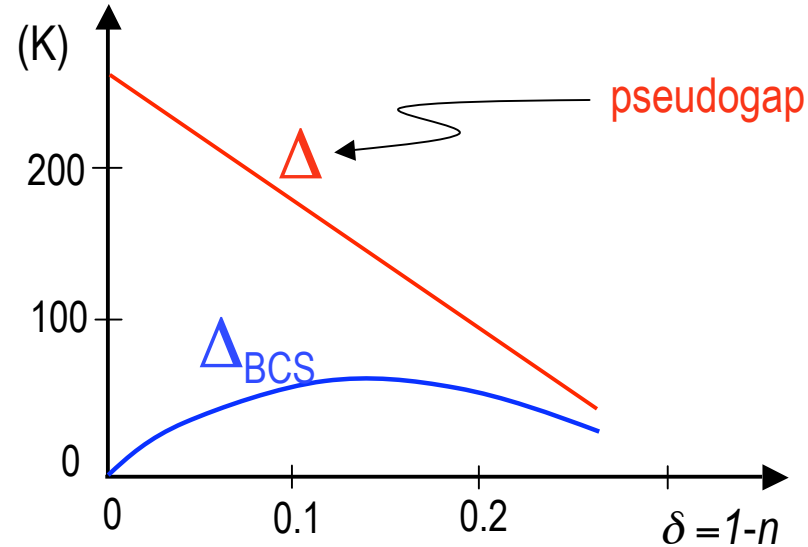
Gros (1987),Zhang et al (1988) ...

recent review: Anderson - Zhang: J. Phys. Cond. Matter (2004)

→ RVB-phase with a spin gap

superconducting phase with $d_{x^2-y^2}$ symmetry when doped with holes

Renormalized Mean Field Approximation & Variational Wavefn.

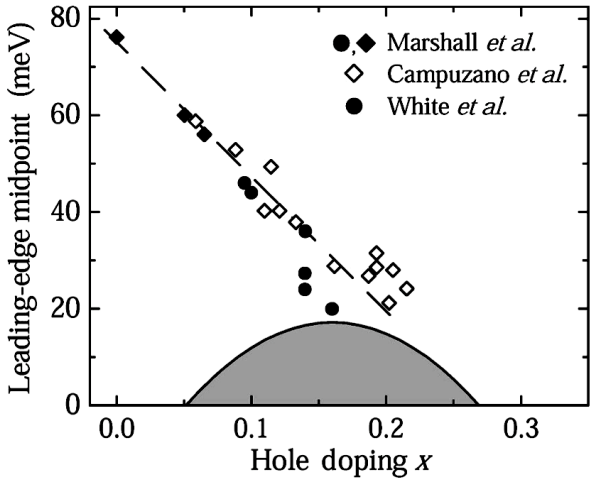


F.C. Zhang et al. , Supercond. Sci. Technol. 1, 36 (1988)

BCS-order parameter:

$$\Delta_{\mathrm{BCS}} = g_{\Delta}\Delta = \frac{2(1-n)}{2-n}\Delta$$

diminishing charge fluctuations
decreases the BCS-order parameter



ARPES
Angle-resolved
Photoemission
spectroscopy

A.Damascelli et al.,
Rev. Mod. Phys. 75,
473 (2003).

Shape of gap:

$$\Delta_{\vec{k}} = \Delta_0\left(\cos k_x - \cos k_y\right)$$

B_{1g} $d_{x^2-y^2}$-wave