How to identify the mechanism of superconductivity in the cuprates (and in other high Tc's)?

Gabriel Kotliar

Rutgers University

C H Yee

Work with Chuck Yee and Turan Birol (Rutgers)

T. Birol

…….

Is there a chance to reach a concensus about the origin of the PG phase ?

……..

- Make predictions that are then tested experimentally.
- When they work, one gains more confidence in the methodology.
- Even when these are not completely born out experimentally they lead to further progress and better methodologies.

Search for universal features (and simplified pictures!) but also understand material dependence.
Compromise between speed and accuracy. Simple pictures vs full accuracy.

Goal: material design. "Understanding mechanism " use insights to suggest concrete materials which would have interesting properties AND which can be made in the lab.
Tools towards that goal are not yet there, but we are much closer than when the field of correlated materials began. Lots of progress in understanding in strongly correlated materials and more powerful theoretical tools translate into more predictive capabilities in the materials arena.

.

- MFT divides the problem into two separate parts: a) obtaining different mean field solutions and b) evaluating their energies.
- MFT allows to follow a “state” as you vary parameters.
- MFT Compares different “states” of the system for the same valu of parameters. → Understand “Mechanism”
- Long wavelegth spatial fluctuations and defects are left out.
- Bridge between atomic information and physical and spectroscopical properties. [Structure-property relation] . Help fin the right “coordinate system” in the “space of materials”
- Limitations Correlated Materials at T=0 have a Landscape of Ordered. Needs some guesswork.

- For large clusters understand effects of boundary conditions.

VERY IMPORTANT: understand the limitations and the nature of the errors of the approximation method, is what makes the method useful. Example DFT, DMFT,…..

Outline of the discussion

- Exhibit 1: some comments on what early mean field theories of cuprates predicted and connections to CDMFT [small addition to AM Tremblay and Andy Millis' talk](pre 1990 work)
- Exhibit 2: A theoretical prediction, 112 , NEW family of iron pnictide superconductors. (very recent)
- Exhibit 3: Understanding Tcmax, and a NEW prediction of a superconducting material. Hg(CaS)2 (CuO)2 (very recent)

P. W. Anderson, *Science* **235**, 1196 (1987) Mott insulator→ high Tc

$$H = -\sum_{\langle ij\rangle,\sigma} t_{ij} c^{+}_{i\sigma} c_{j\sigma} + J \sum_{\langle ij\rangle} (S_i S_j - \frac{1}{4} n_i n_j)$$

Slave Boson Formulation: Baskaran Zhou Anderson (1987)
Extended s superconductivity

$$c_{i\sigma} = f_{i\sigma} b^{\dagger}_{i}$$

$$\kappa_{ij} = \langle f^{\dagger}_{i\uparrow} f_{j\uparrow} \rangle + \langle f^{\dagger}_{i\downarrow} f_{j\downarrow} \rangle$$

$b^{+}i\ bi + f^{+}si\ fsi = 1$

$$\Delta_{ij} = \langle f_{i\uparrow} f_{j\downarrow} \rangle - \langle f_{i\downarrow} f_{j\uparrow} \rangle$$

.

Bond variables have a life of their own. Mean Field Theory focuses on the impact on the short range physics.

$$\Delta_{ij} = < f^{+}_{i\sigma} f^{+}_{j\bar{\sigma}} > \qquad \kappa_{ij} = < f^{+}_{i\sigma} f_{j\sigma} >$$

PHYSICAL REVIEW B VOLUME 37, NUMBER 7 1 MARCH 1988

Resonating valence bonds and *d*-wave superconductivity

G. Kotliar
Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139
(Received 15 May 1987; revised manuscript received 19 November 1987)

Affleck and Marston 1988 flux states
Affleck et. al. SU(2) symmetry

RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 38, NUMBER 7 1 SEPTEMBER 1988

Superexchange mechanism and *d*-wave superconductivity

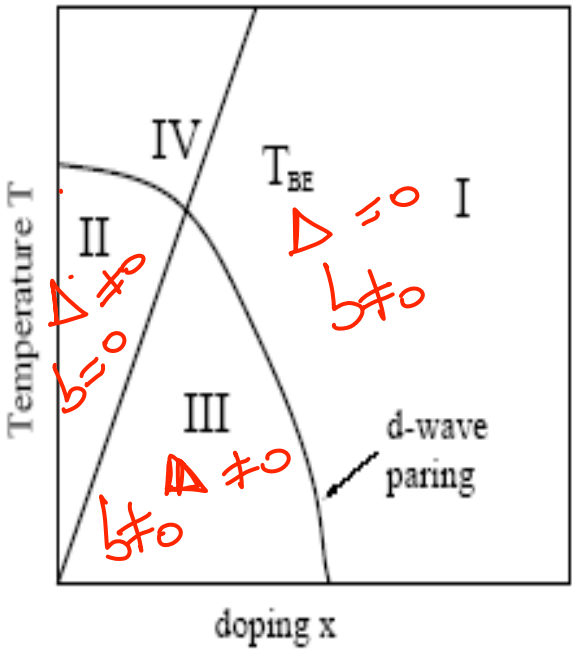
Gabriel Kotliar and Jialin Liu
Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139
(Received 7 March 1988)

Many possible solutions to the mean field equations in the underdoped regime. IMPORTANT CLUE supported by many later developments.
Interpret carefully !!!!
Learning to treat ELECTRONS, very far from Landau FLT assymptote.

RVB phase diagram of the Cuprate Superconductors. Superexchange.

- Tc controlled by J.
- Trvb, onset of spin pairing.
- < b>, T_{BE} , coherence temperature, formation of QF
- Superconducting dome. Pseudogap evolves into SC
- Problems: a) poor description of the incoherent part b) MFT too uniform c) other states i.e. AF.
- Restricted form of the electron self energy.

G. Kotliar and J. Liu Phys.Rev. B 38,5412 (1988)



Related approach using wave functions at T=0 :T. M. Rice group

But there are many more competing states, even in SU(N) for N large.

There are even dimer states which are nematic! Grilli Castellani and Kotliar PRB 45 (1992) but required bigger J's.

And there are also linear instabilities towards inconmensurate states!.

$$\kappa_Q(k) = < f^+_{k+Q/2} f_{k-Q/2} > \qquad \kappa_Q(k) = < f^+_{k+Q/2} f^+_{-k+Q/2} >$$

RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 42, NUMBER 13 1 NOVEMBER 1990

Flux-density wave and superconducting instability of the staggered-flux phase

Ziqiang Wang and Gabriel Kotliar
Department of Physics, Rutgers University, Piscataway, New Jersey 08854

Xiao-Fang Wang
Department of Physics, Columbia University, New York, New York 10027
(Received 22 May 1990)

We study the stability of the staggered-flux phase in the t-J model away from half filling using a systematic large-N slave-boson approach. Found, below a critical doping concentration $\delta_c = a(J/t)^2$, is a flux-density-wave instability with an incommensurability wave number $\sim\delta^{3/4}$. The instability towards a modulated-flux state is due to low-lying phase fluctuations of the valence bonds. When the doping parameter exceeds δ_c, we find a fully gapped d-wave superconducting state due to residual quasiparticle interactions.

And SU(2) symmetries bring to pair density waves of spinons

Cluster DMFT: retains many of the good features of the slave boson MFT while removing MANY important shortcomings. Now lifetimes and the incoherent part of the electron spectral function is included. There is strong anisotropy of the quasiparticle weight, nodal antinodal dichotomy…… NEW LANGUAGE WHEN WE CAN'T USE Fermi Liquid Theory

PHYSICAL REVIEW B **76**, 104509 (2007)

Strongly correlated superconductivity: A plaquette dynamical mean-field theory study

Kristjan Haule and Gabriel Kotliar
Department of Physics, Rutgers University, Piscataway, New Jersey 08854, USA
(Received 31 May 2007; published 13 September 2007)

We use cluster dynamical mean-field theory to study the simplest models of correlated electrons, the Hubbard model and the *t*–*J* model. We use a plaquette embedded in a medium as a reference frame to compute and interpret the physical properties of these models. We study various observables such as electronic lifetimes, one electron spectra, optical conductivities, superconducting stiffness, and the spin response in both the normal and the superconducting state in terms of correlation functions of the embedded cluster. We find that the shortest electron lifetime occurs near optimal doping where the superconducting critical temperature is maximal. A

One prediction, Fermi liquid of the typical scattering rate in the underdoped regime. Beautiful experiments S. I . Mirzaei 110, 5774-5778 (2013)

PHYSICAL REVIEW B **80**, 064501 (2009)

Pseudogap opening and formation of Fermi arcs as an orbital-selective Mott transition in momentum space

Michel Ferrero,[1,2] Pablo S. Cornaglia,[1,3] Lorenzo De Leo,[1] Olivier Parcollet,[2] Gabriel Kotliar,[4] and Antoine Georges[1]

Momentum-sector-selective metal-insulator transition in the eight-site dynamical mean-field approximation to the Hubbard model in two dimensions

Emanuel Gull,[1] Olivier Parcollet,[2] Philipp Werner,[3] and Andrew J. Millis[1]
[1]*Department of Physics, Columbia University, 538 West 120th Street, New York, New York 10027, USA*
[2]*Institut de Physique Théorique, CEA, IPhT, CNRS, URA 2306, F-91191 Gif-sur-Yvette, France*
[3]*Theoretische Physik, ETH Zurich, 8093 Zürich, Switzerland*
(Received 9 September 2009; revised manuscript received 22 October 2009; published 1 December 2009)

Link +Plaquette as reference frame

Real Space Picture

1
0

Ferrero et. al. PRB 80 064501 (2009)

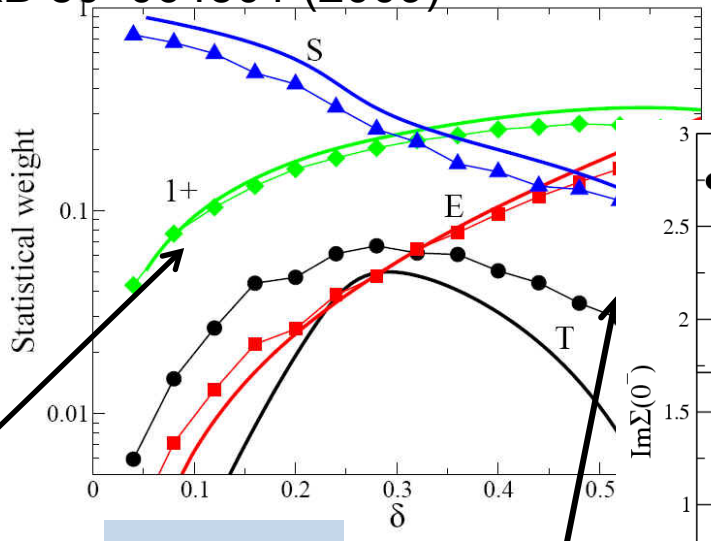
1+= 1/√2(|0, ↑> + | ↑, 0>)

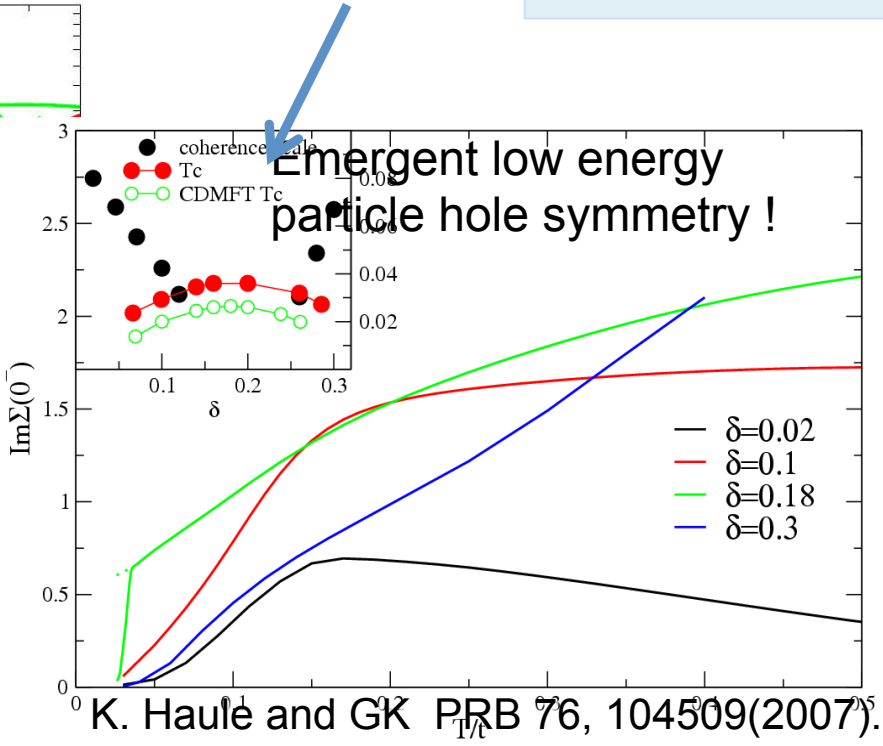
E=|0, 0>

T=| ↑, ↑ >

S=1/√2(| ↑, ↓> -| ↑↓ >)

Holes in a sea of singlets





Emergent low energy particle hole symmetry !

K. Haule and GK PRB 76, 104509(2007).

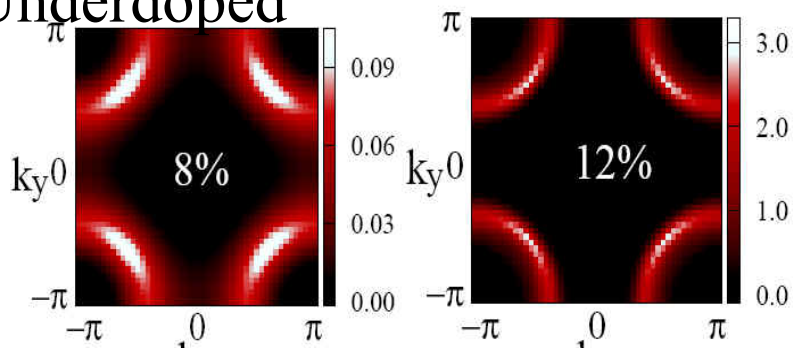
Fermi Liquid

Phys. Rev. B 80, 064501 (2009)

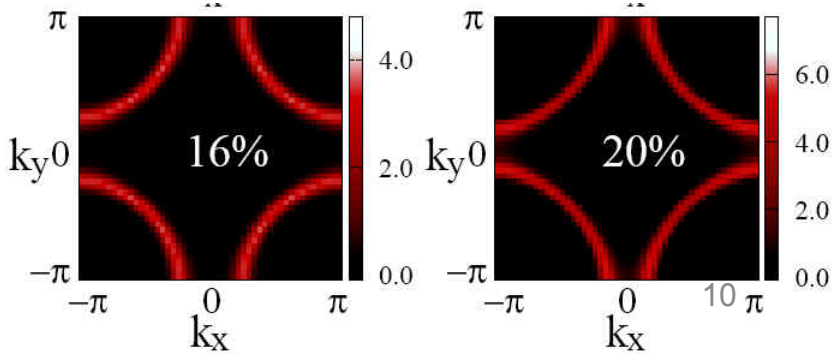
Momentum Space Picture Cumulants

Stanescu and Kotliar (2006) Civelli et.al.

Underdoped



Overdoped



Caveats from LDA+DMFT NCCO vs LSCO besides the obvious electron hole asymmetry…

•Good agreement with many subtle experimental features in NCCO even within single site DMFT.

•No need to use x dependent values of the interaction U (or D CT gap)

•In general, better modeling with DMFT (more cluster sites, more orbitals etc) better results.

- Strength of correlations (as quantified by single site DMFT) the most fundamental difference between NCCO and LSCO compounds.
- NCCO ($D < D_{c2}$)and LSCO ($D > D_{c_2}$)straddle the Zaanen Sawatsky Allen localization delocalization boundary.
- Can be traced to the absence of apical oxygen in NCCO (structure property relation).
- Introduces subtle differences in the metallization process and interplay of magnetism and superconductivity.
- Proximity to the metal to CTI transition, key to dopability, key to high Tc
- Weber et. al. Nature Physics Weber Haule and GKNature Phys. 6, 574 (2010).

Outline of the discussion

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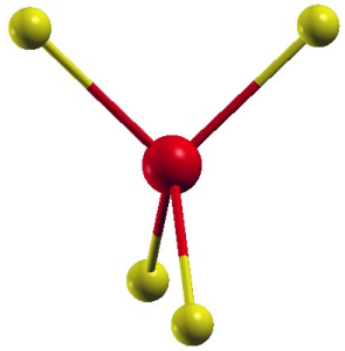
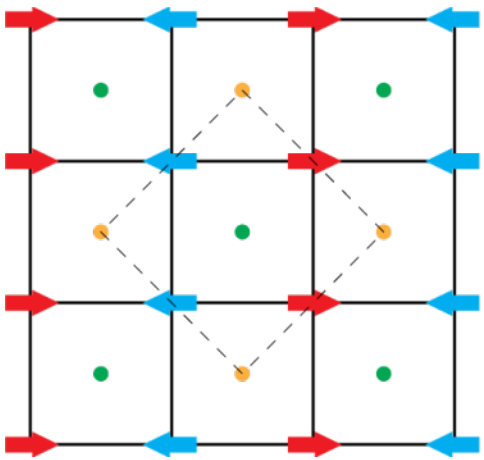
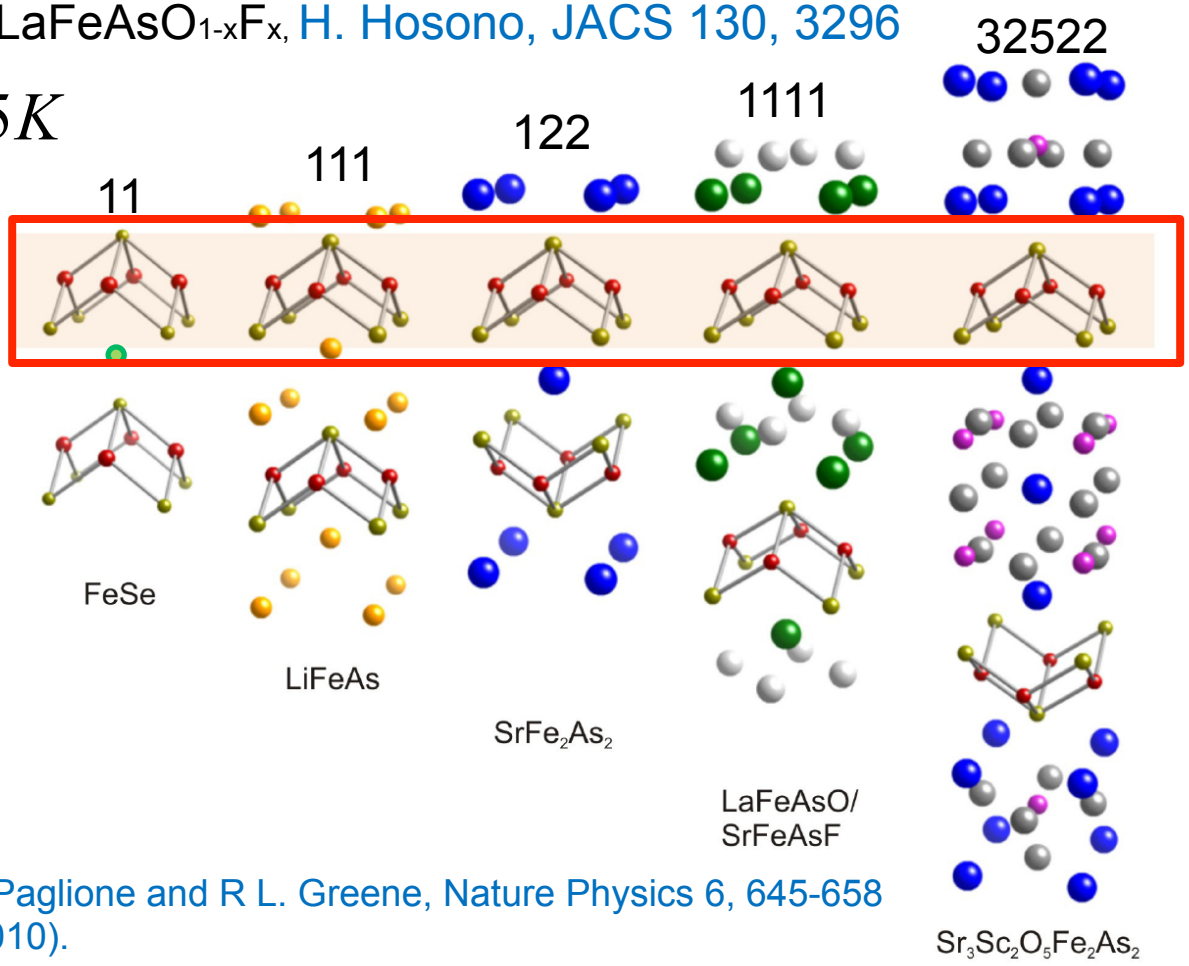
- Exhibit 2: A theoretical prediction, the 112 family of iron pnictide superconductors.
- Exhibit 3: Understanding Tcmax, and a new prediction of a superconducting material. Hg(CaS)2 (CuO)2

Landscape of Fe based SC

First discovery in 2008: $LaFeAsO_{1-x}F_x$, H. Hosono, JACS 130, 3296 (2/13/2008). $T_C^{\max} \sim 65K$







J. Paglione and R L. Greene, Nature Physics 6, 645-658 (2010).

Theoretical understanding: iron pnictides as Hunds metals, various properties were predicted using LDA+DMFT !!! Very interesting qualitatively new features relative to Mott Hubbard systems.

Density-functional calculations of the electronic structures and magnetism of the pnictide superconductors $BaFeAs_2$ and $BaFeSb_2$

J. H. Shim, K. Haule, and G. Kotliar

Phys. Rev. B **79**, 060501(R) – Published 1 February 2009

We investigate the structural, electronic, and magnetic properties of the hypothetical compound $BaFePn_2$ (Pn = As and Sb), which is isostructural to the parent compound of the high-temperature superconductor $LaFeAsO_{1-x}F_x$. Using density-functional theory, we show that the Fermi surface, electronic structure, and spin-density wave instability of $BaFePn_2$ are very similar to the Fe-based superconductors. Additionally, there are very dispersive metallic bands of a spacer Pn layer, which are almost decoupled from $FePn$ layer. Our results show that experimental study of $BaFePn_2$ can test the role of charge

internal coordinates of Ba (0.25, 0.25, z_{Pn}), Fe (0.75, 0.25, z_{Pn}).
O is ex-

Journal of the Physical Society of Japan **83**, 025001 (2014)
http://dx.doi.org/10.7566/JPSJ.83.025001

AsO
35
41
42
51
12
67
55

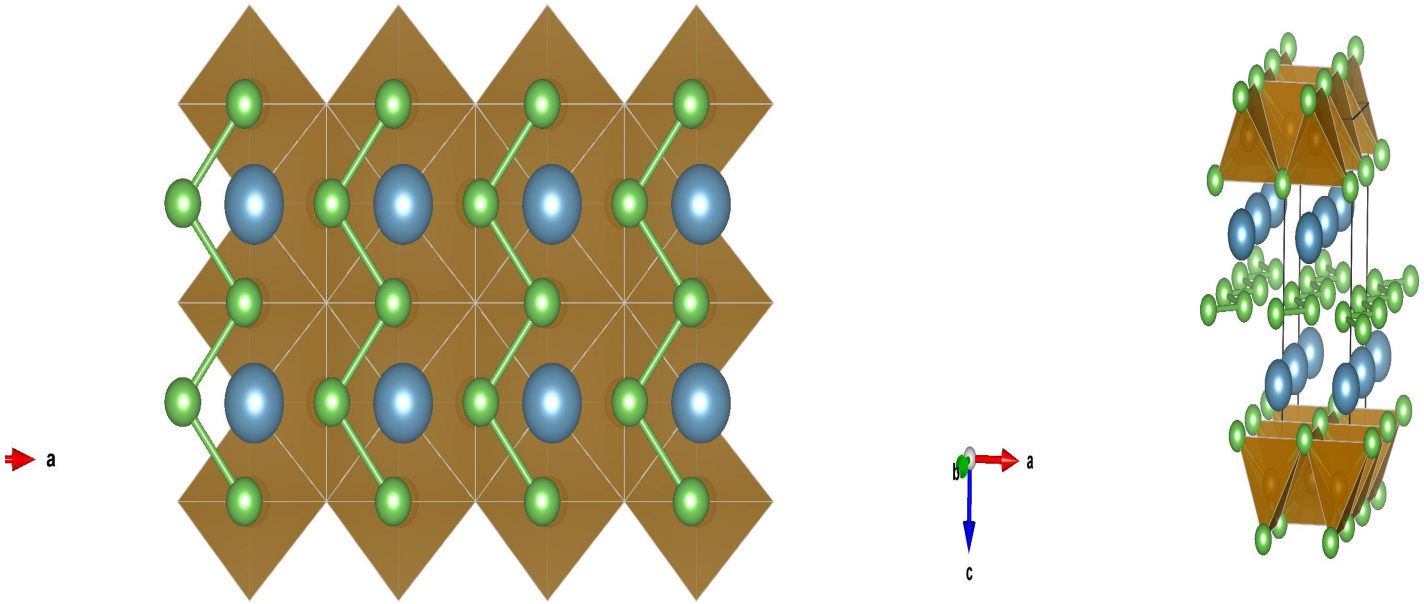
Enhanced Superconductivity up to 43 K by P/Sb Doping of $Ca_{1-x}La_xFeAs_2$

Kazutaka Kudo[1,2*], Tasuku Mizukami[1], Yutaka Kitahama[1], Daisuke Mitsuoka[1], Keita Iba[1], Kazunori Fujimura[1], Naoki Nishimoto[1], Yuji Hiraoka[1,2], and Minoru Nohara[1,2]

Intrinsically structurally detwinned Fe pnictide superconducting family with metallic spacer layers

Shan Jiang[1,*], Chang Liu[2,*], Huibo Cao[3], Turan Birol[4], Jared A. Allred[5], Wei Tian[3], Lian Liu[6], Kyuil Cho[7], Matthew Krogstad[5], Jie Ma[3], Keith Taddei[5], Makariy. A. Tanatar[7], Ruslan prozorov[7], Rafael. M. Fernandes[8], Stephen Rosenkranz[5], Yasutomo J. Uemura[6], G. Kotliar[4], Ni Ni[1]

It turns out that the prediction of a metallic CaAs layer was correct but that in turn lead to the formation of zig-zag chains. Acts like a uniaxial pressure field to detwin domains



112 family with metallic spacer layer was predicted and observed.

- The original motivation for proposing this family of compounds was to differentiate excitonic mechanisms vs magnetic mechanism of superconductivity.
- Conclusion: magnetic mechanism. A metallic layer has infinite polarizability and should have increased Tc.
- A lot more will be learned by looking at this compound more carefully, exploiting the fact that a calculable internal field couples to the different orbitals of the active iron pnictide layer. MONODOMAIN sample, stripe order, magnetic domains……

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- Exhibit 3: Understanding Tcmax, and a new prediction of a superconducting material. Hg(CaS)2 (CuO)2

Phys. Rev. B 43, 2968–2982 (1991)

Apex oxygen and critical temperature in copper oxide superconductors: Universal correlation with the stability of local singlets

Abstract | References | Citing Articles (126) | Page Images

Download: PDF (3,064 kB) Buy this article Export: BibTeX or EndNote (RIS)

Y. Ohta, T. Tohyama, and S. Maekawa
Department of Applied Physics, Nagoya University, Nagoya 464-01, Japan

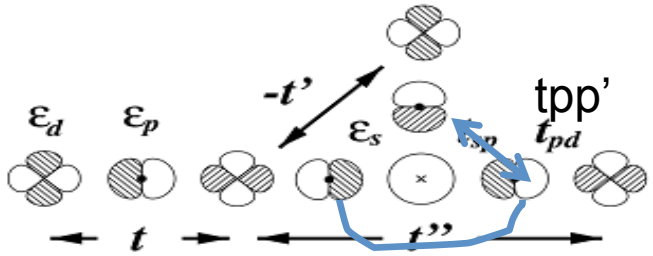
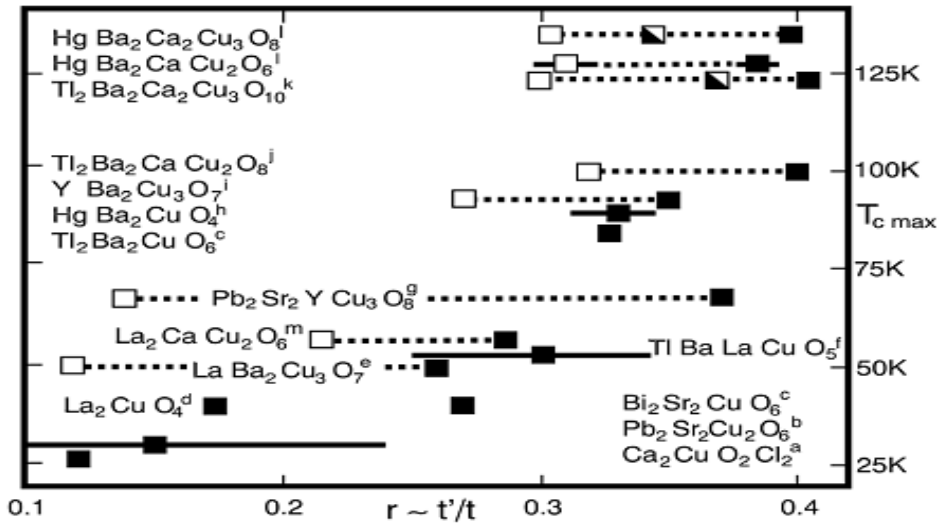


FIG. 1. Relation between the one-orbital model ($t, t', t'', \ldots$) and the nearest-neighbor four-orbital model [4] ($\varepsilon_d - \varepsilon_p \sim 1$ eV, $t_{pd} \sim 1.5$ eV, $\varepsilon_s - \varepsilon_p \sim 4.16$ eV, $t_{sp} \sim 2$ eV).



- Significant scatter, but correlation is clear: $T_{c,max}$ increases with larger hopping range.

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

See also Raimondi et. al. **Phys. Rev. B 53, 8774–8788 (1996)**

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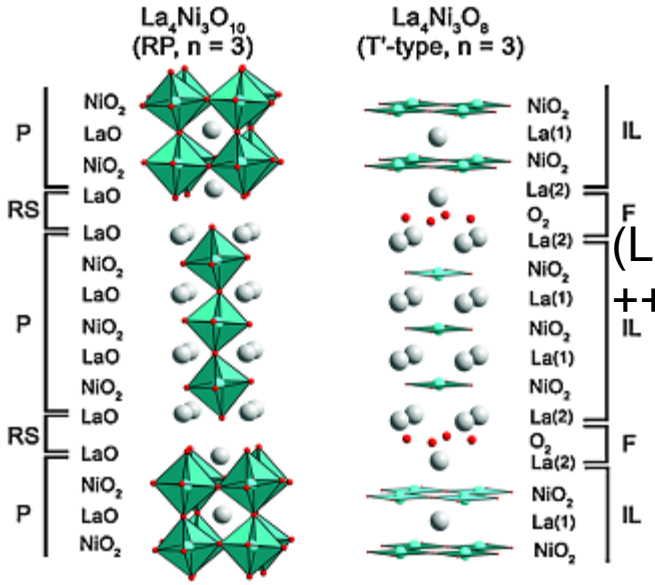


Ni+ d9
Ni++
d8

(La+++)3 (O--)8 (Ni3)+
+++

2/3 Ni(d9) +
1/3 Ni(d8)

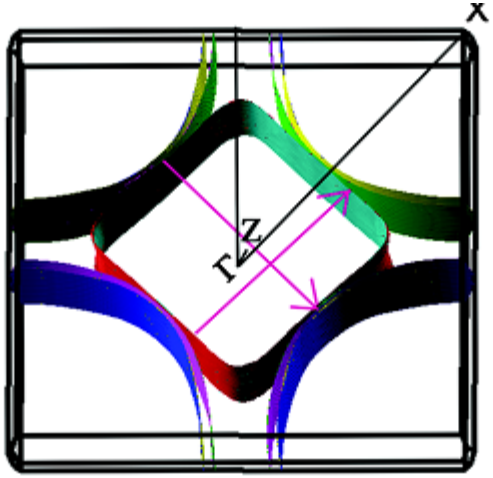


FIG. 4 (color online). Fermi surface of $La_4Ni_3O_8$ in recipro space with nesting vectors (arrows).

Larger t'/t than cuprates but no Tc

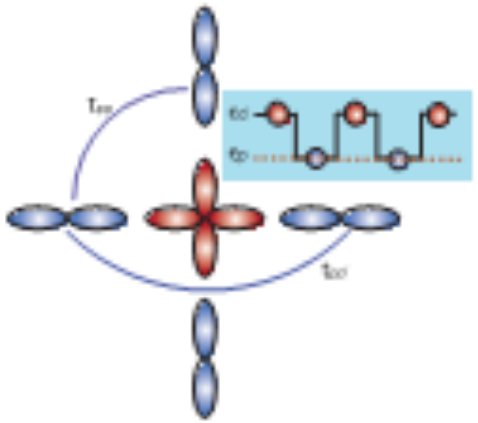
PRL **104,** 206403 (2010) PHYSICAL REVIEW LETTERS week ending 21 MAY 2010

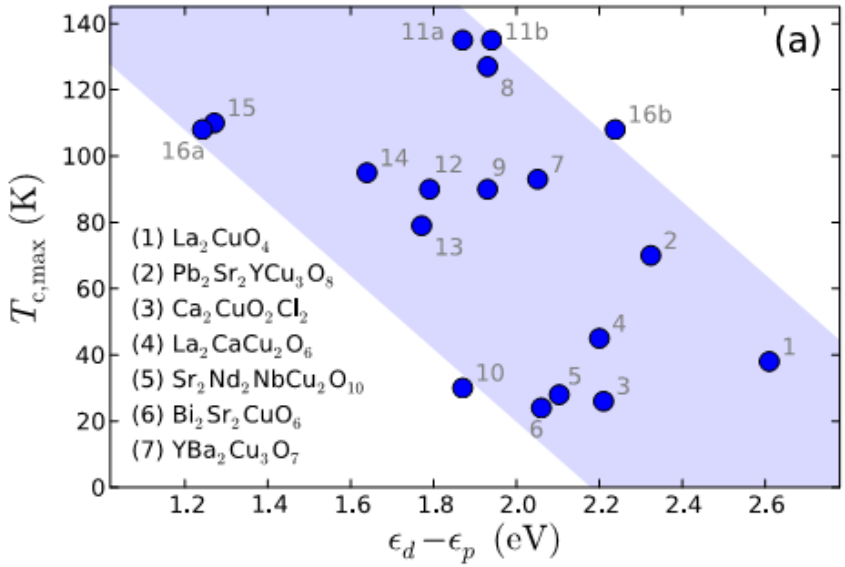
Bulk Magnetic Order in a Two-Dimensional Ni^{1+}/Ni^{2+} (d^9/d^8) Nickelate, Isoelectronic with Superconducting Cuprates

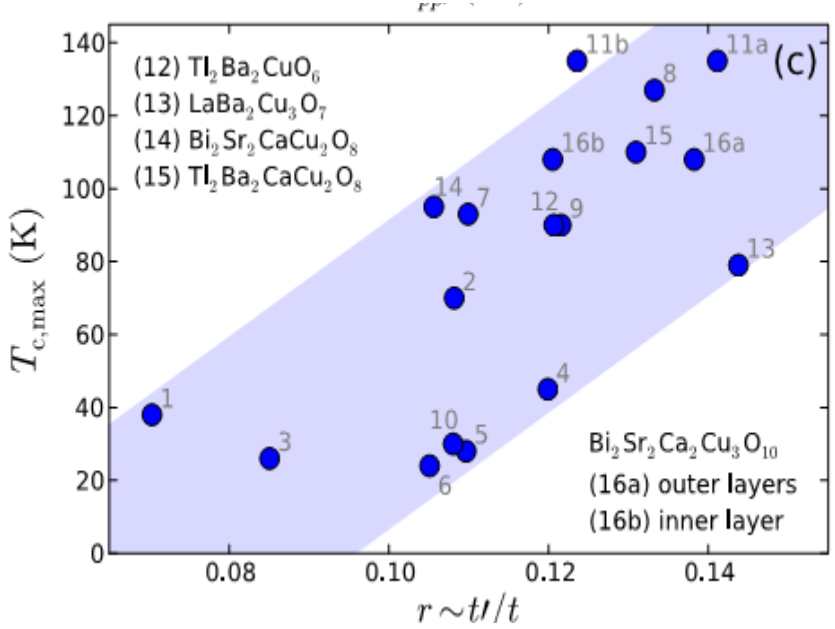
Viktor V. Poltavets,[1,2] Konstantin A. Lokshin,[3] Andriy H. Nevidomskyy,[4] Mark Croft,[4] Trevor A. Tyson,[5] Joke Hadermann,[6] Gustaaf Van Tendeloo,[6] Takeshi Egami,[3,7,8] Gabriel Kotliar,[4] Nicholas ApRoberts-Warren,[9] Adam P. Dioguardi,[9] Nicholas J. Curro,[9] and Martha Greenblatt[1]

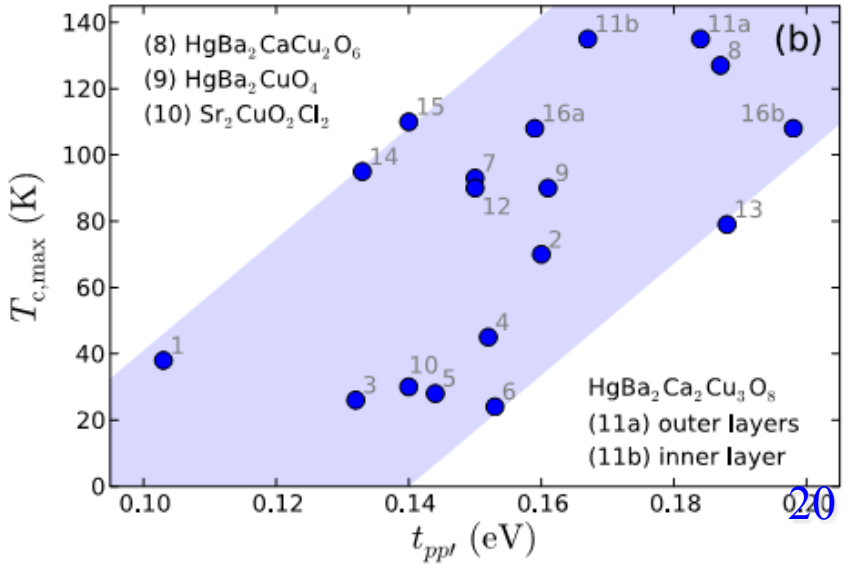
C. Weber C. Yee and G.K.

Eur. Phys. Lett. 100, 37001 (2012)

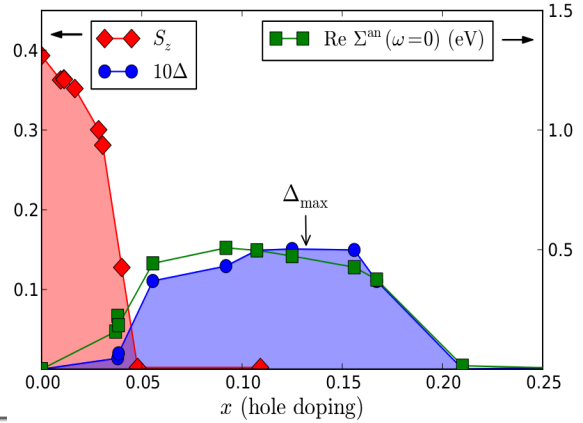


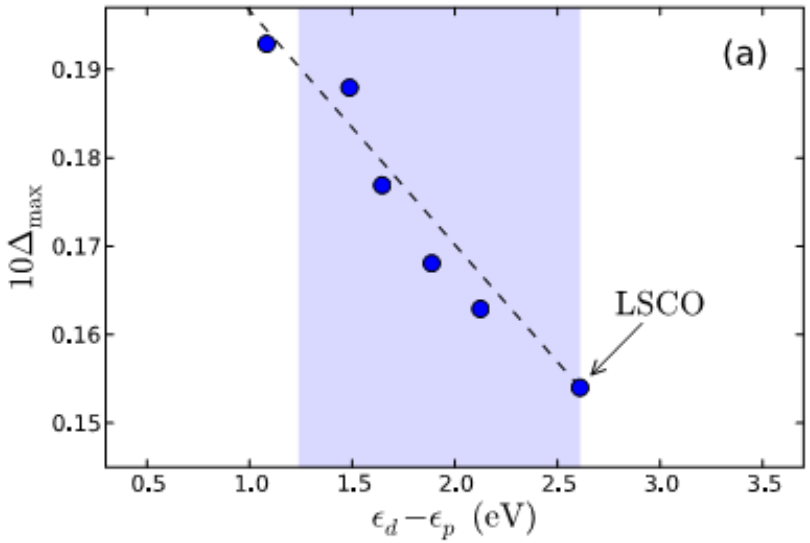


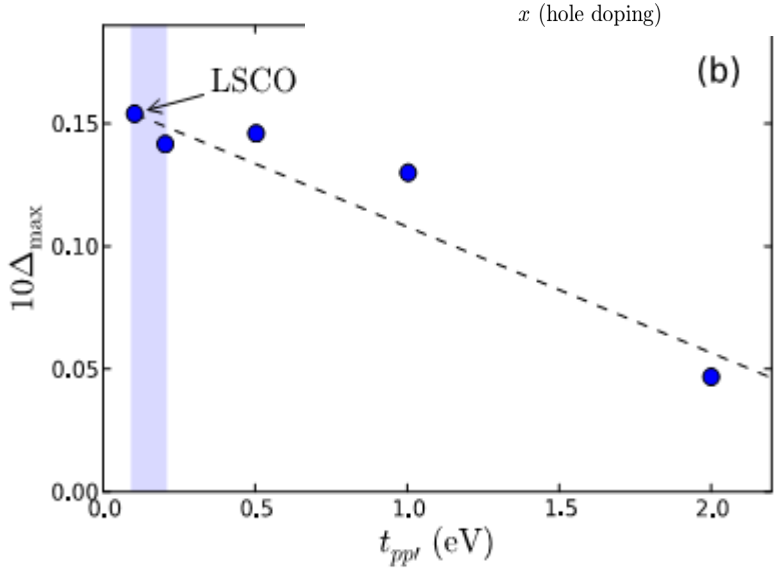




Causation: Reducing ed-ep helps Tc
(pushing apical away from the plane)







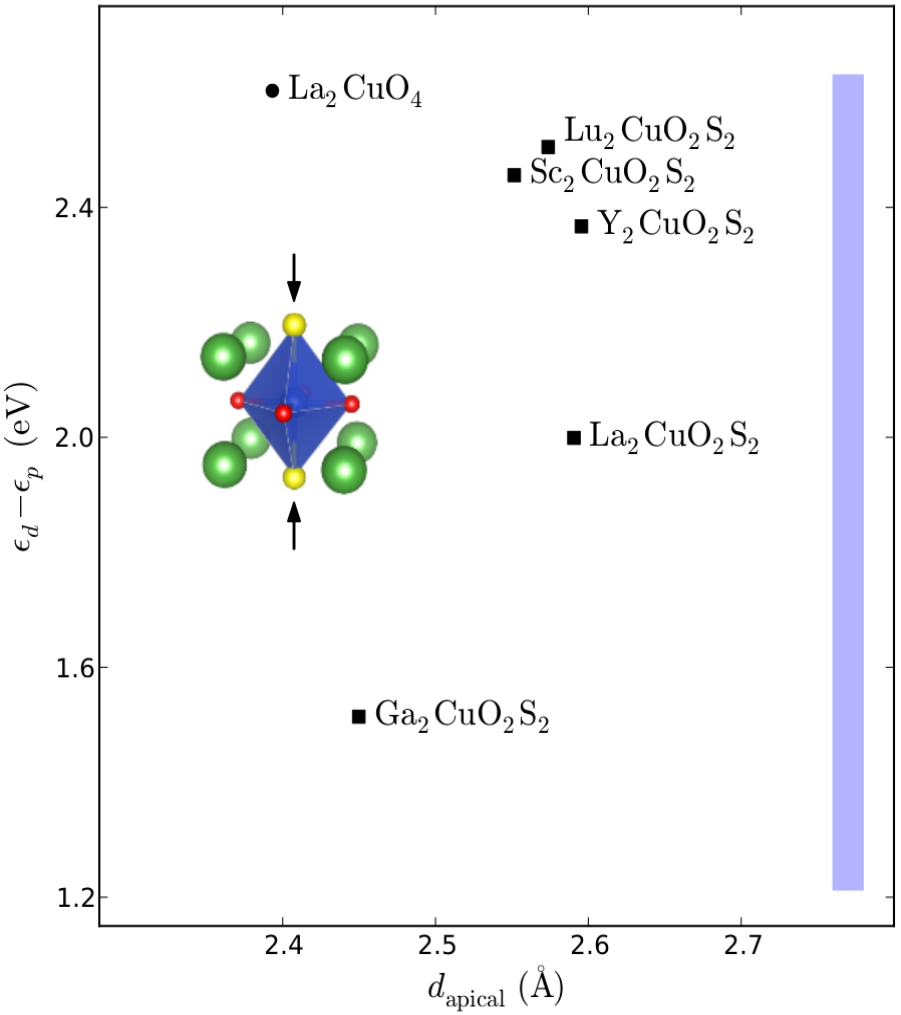
Increasing tpp' hurts Tc

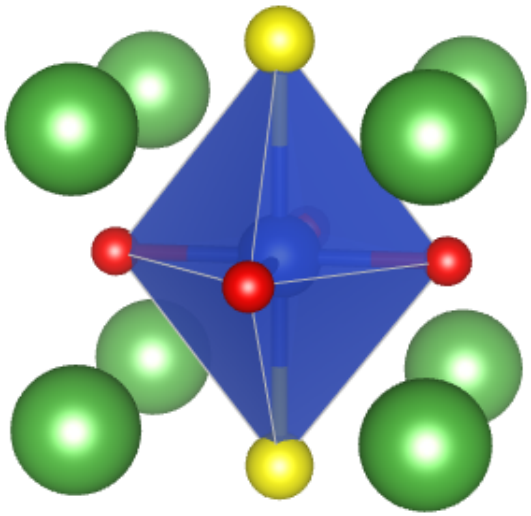
Moving the apical oxygen away form the plane reduces ed-ep but also increases tpp' . We believe the reduction of ep-ed is dominant

How can we reduce CTE ? Simplest way would be layer by layer depostio
*R*CuO2S2 family C. Yee and GK Phys. Rev. B 89, 094517 (2014)

Chuck Yee

- Apical oxygen → sulfur; La





Not so easy to make. Layer by layer methods ?

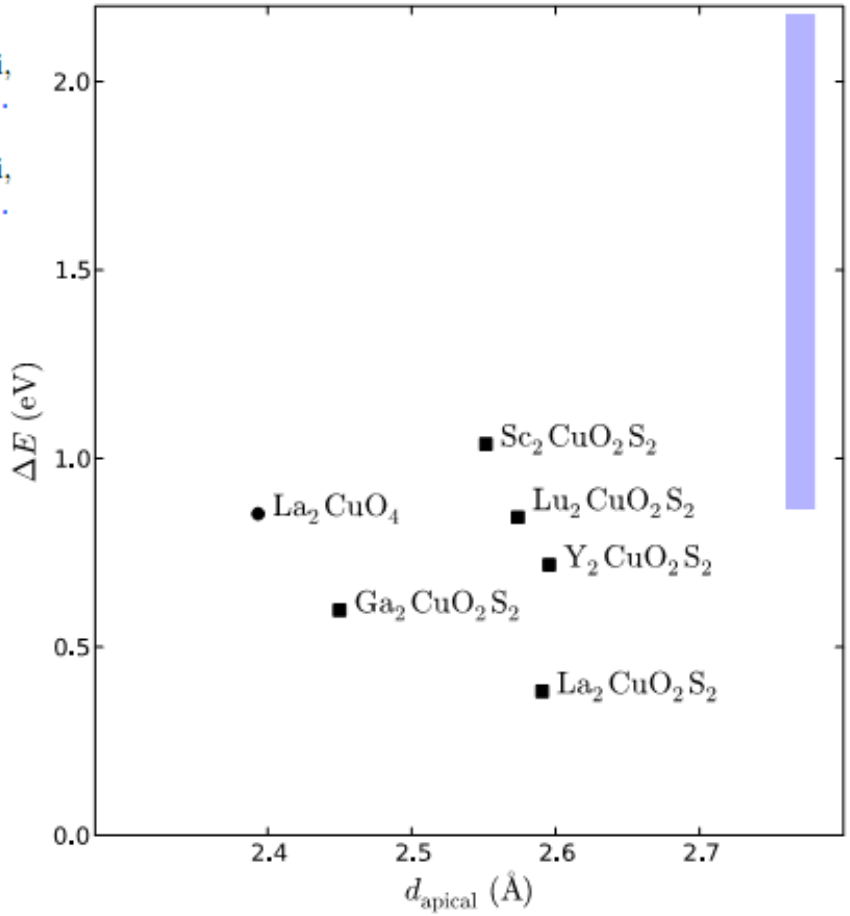
ΔE	ΔV	Synthesis pathway
141	-7.3	$La_2O_2S + CuS \rightarrow La_2CuO_2S_2$
223	-3.4	$Y_2O_2S + CuS \rightarrow Y_2CuO_2S_2$
267	-5.0	$Lu_2O_2S + CuS \rightarrow Lu_2CuO_2S_2$
356	-3.0	$Sc_2O_2S + CuS \rightarrow Sc_2CuO_2S_2$
101	-4.9	$La_2O_2S_2 + Cu \rightarrow La_2CuO_2S_2$
148	-3.3	$La_2O_3 + CuS \rightarrow La_2CuO_3S$
454	-0.7	$Sc_2O_3 + CuS \rightarrow Sc_2CuO_3S$
97	-4.9	$La_2O_2S + CuO \rightarrow La_2CuO_3S$
269	2.8	$Sc_2O_2S + CuO \rightarrow Sc_2CuO_3S$
28	-5.1	$La_2O_3 + CuO \rightarrow La_2CuO_4$

If one can avoid distortions, buckling, etc, this family will help decide if the d_{z2} splitting or the CT energy is the right variable that controls Tc.

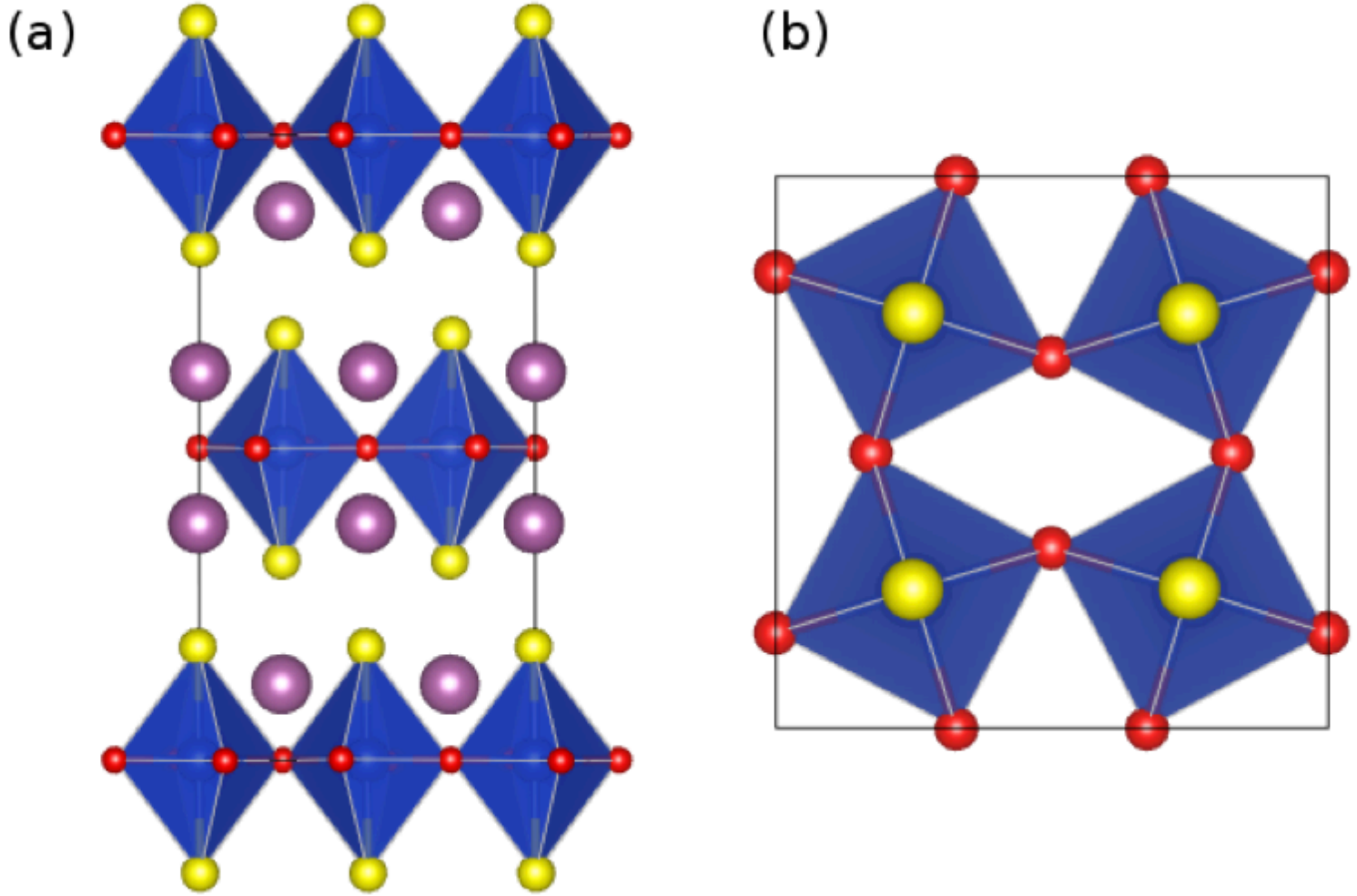
[10] H. Sakakibara, H. Usui, K. Kuroki, R. Arita, and H. Aoki, Phys. Rev. Lett. **105**, 057003 (Jul 2010), http://link.aps.org/doi/10.1103/PhysRevLett.105.057003.

[11] H. Sakakibara, H. Usui, K. Kuroki, R. Arita, and H. Aoki, Phys. Rev. B **85**, 064501 (Feb 2012), http://link.aps.org/doi/10.1103/PhysRevB.85.064501.

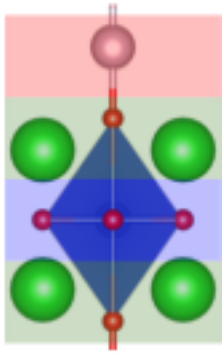
FIG. 5. The energy splitting $\Delta E = E_{x^2-y^2} - E_{z^2}$ between the onsite energies of the $d_{x^2-y^2}$ and d_{z^2} orbitals among the copper oxysulfide family (squares). For comparison is the actual compound La_2CuO_4 (circle). The physical range of ΔE spanned by the single-layer cuprates is shown with a shaded bar (from Sakakibara, *et. al.*) [11]. The ΔE in the oxysulfides are generally smaller, implying stronger mixing of the d_{z^2} orbital with the in-plane $d_{x^2-y^2}$ orbital. Thus, barring other competing orders, sulfur substitution should enhance $T_{c,max}$ according to the charge-transfer theory, while $T_{c,max}$ will be suppressed according to the two-orbital theory.



Interesting hypothetical materials, but…… they tilt in an unusual way so they are not cuprate like.



So recently Chuck and Turan undertook a little material design problem

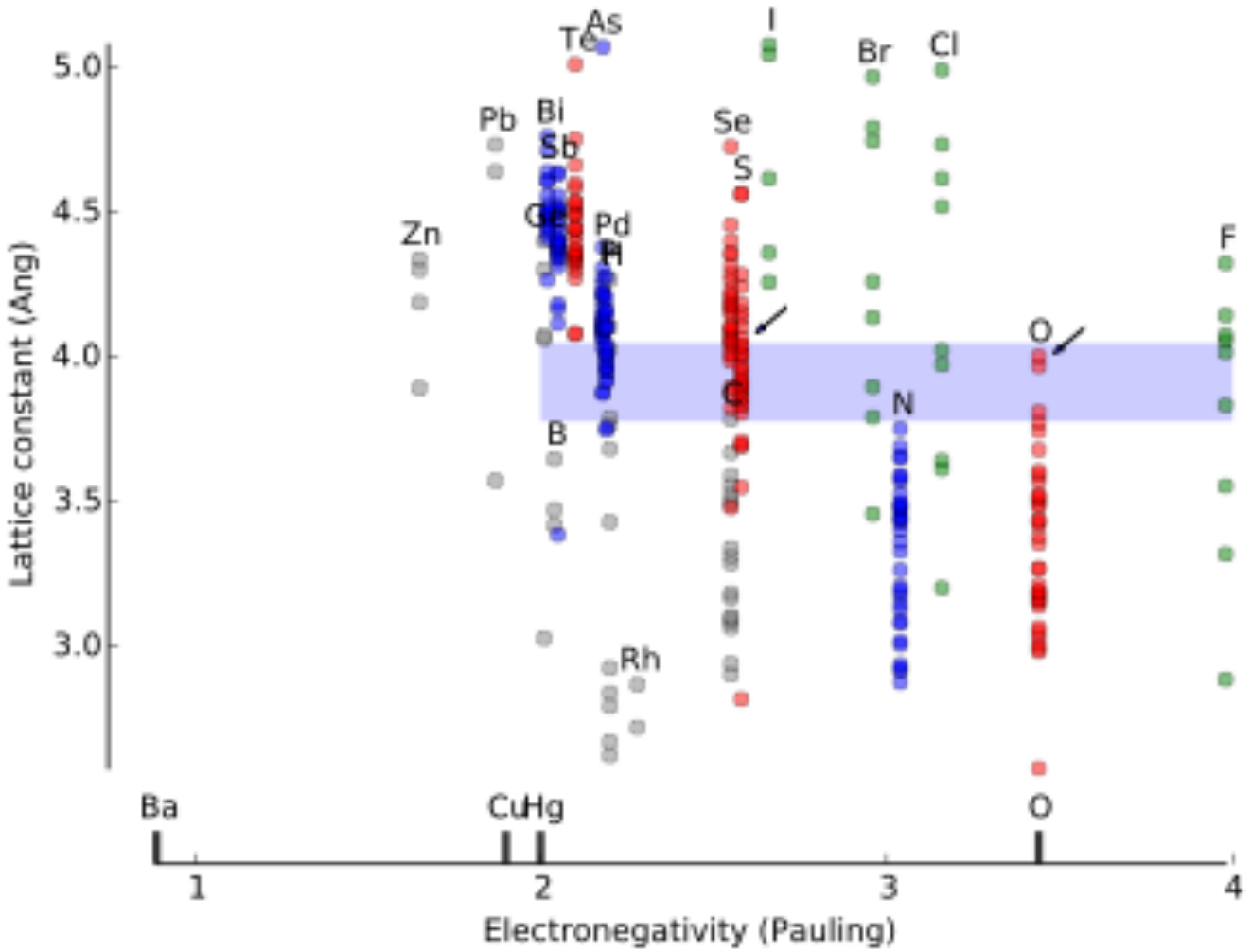


	charge	dopants	structure	hamiltonian
HgO_δ	balances -2 charge	supplies	harbors dopants	tunes chemical potential
BaO	neutral	inert	protects CuO_2 from disorder	tunes in-plane t, t', U
CuO_2	-2 charge/u.c.	accepts	roughly sets lattice const.	superconducts
BaO			(same as other CaS layer)	

FIG. 1. Each layer in the structural stack of $HgBa_2CuO_{4+\delta}$ performs a specific chemical, structural and electronic function. We focused on tuning the layers immediately adjacent to the CuO_2 plane which function to tune the in-plane hamiltonian, but must also be charge neutral and not interfere with doping.

Strategy : C. Yee T. Birol and GK.
Look for replacements of Ba and O by all possible elements XY

1) Use chemical arguments to restrict the search
2) Require local stability by checking all phonons.
3) Check for stability of the structure against multiple moves using genetic algorithms.
4) Look for compounds that are marginally stable against phase separation, within 250 mev of the zero of the convex hull.



Hg (XY)2 (CuO)2

C. Yee T. Birol and GK

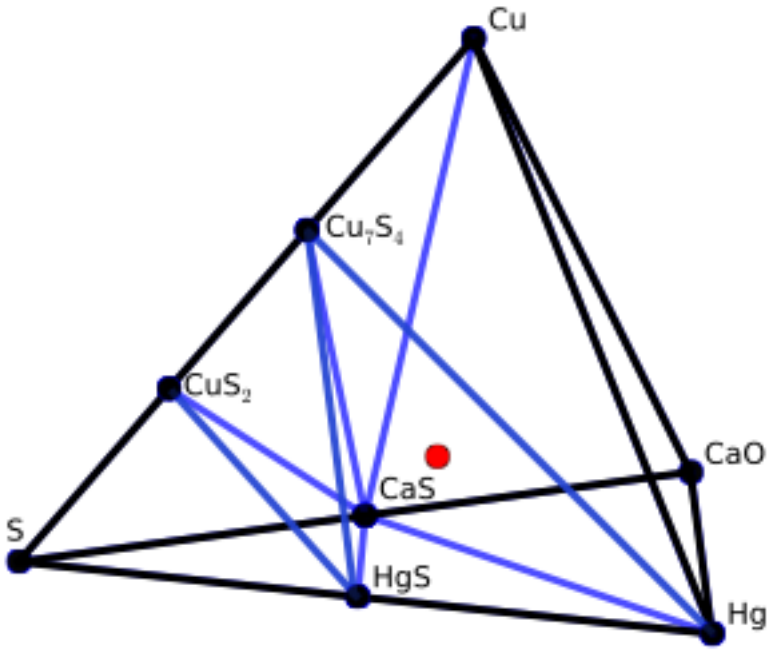
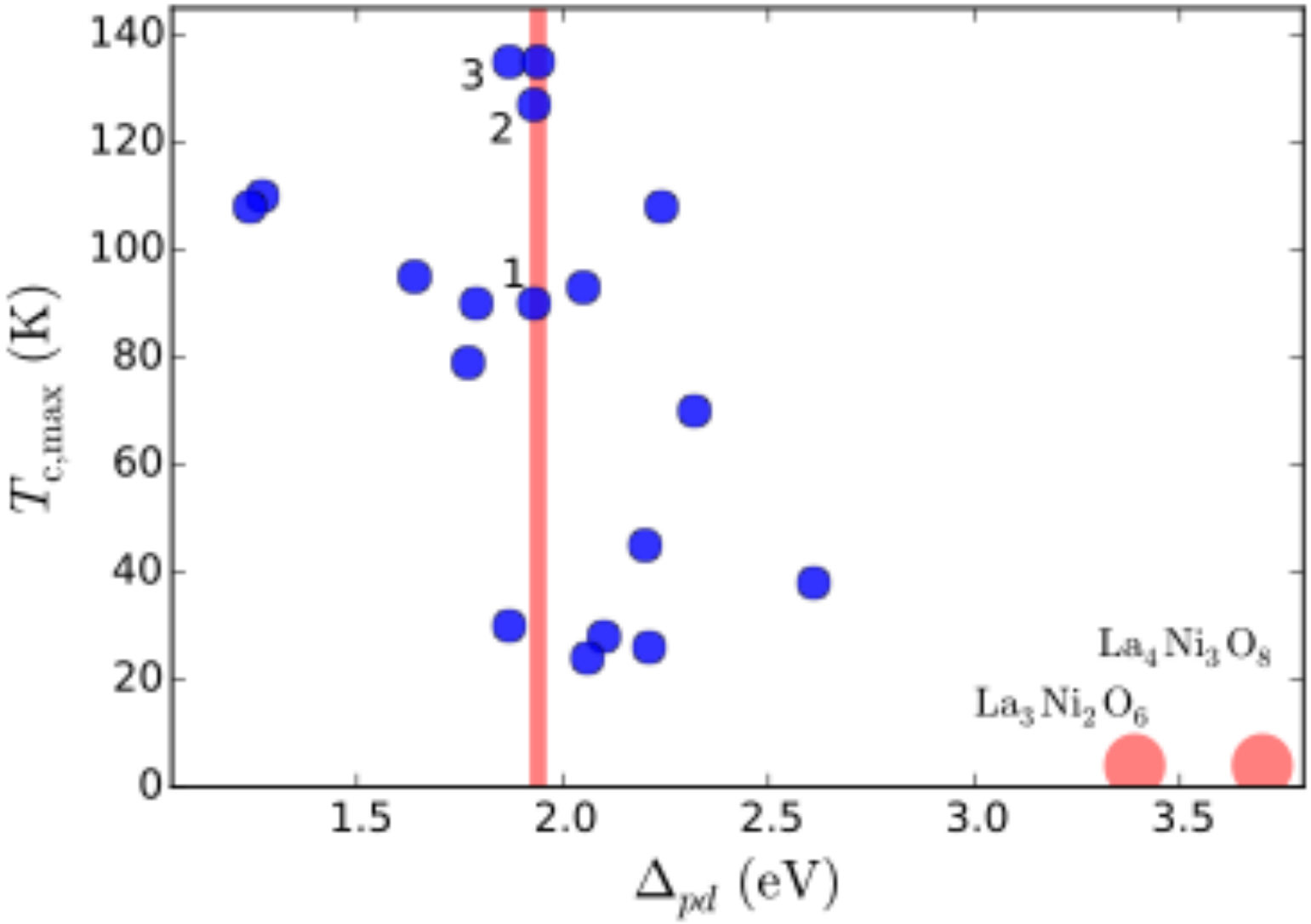


FIG. 3. The Gibbs phase diagram of the Hg-Ca-S-Cu system at an oxygen chemical potential of $\mu(O_2) = -16.48$ eV, chosen because $Hg(CaS)_2CuO_2$ (red dot) is least unstable at this value. The phase diagram forms a tetrahedron with S, Hg, Cu and CaO at the vertices (elemental Ca isn't stable under this oxygen environment). HCSCO lies in the interior of the tetrahedron, on the triangular face formed by Hg, Cu and CaS.

Test against phase separation.

CaO is about 175 mev above the convex hull



Hg (CaS)2 (CuO)2 is interesting Slightly shorter Cu-Cu distance !

Thank you for your attention!

I can also address the rest
of the questions in the list.