Cuprate High-Temperature Superconductors – How to Get Back to the Future with Phonons

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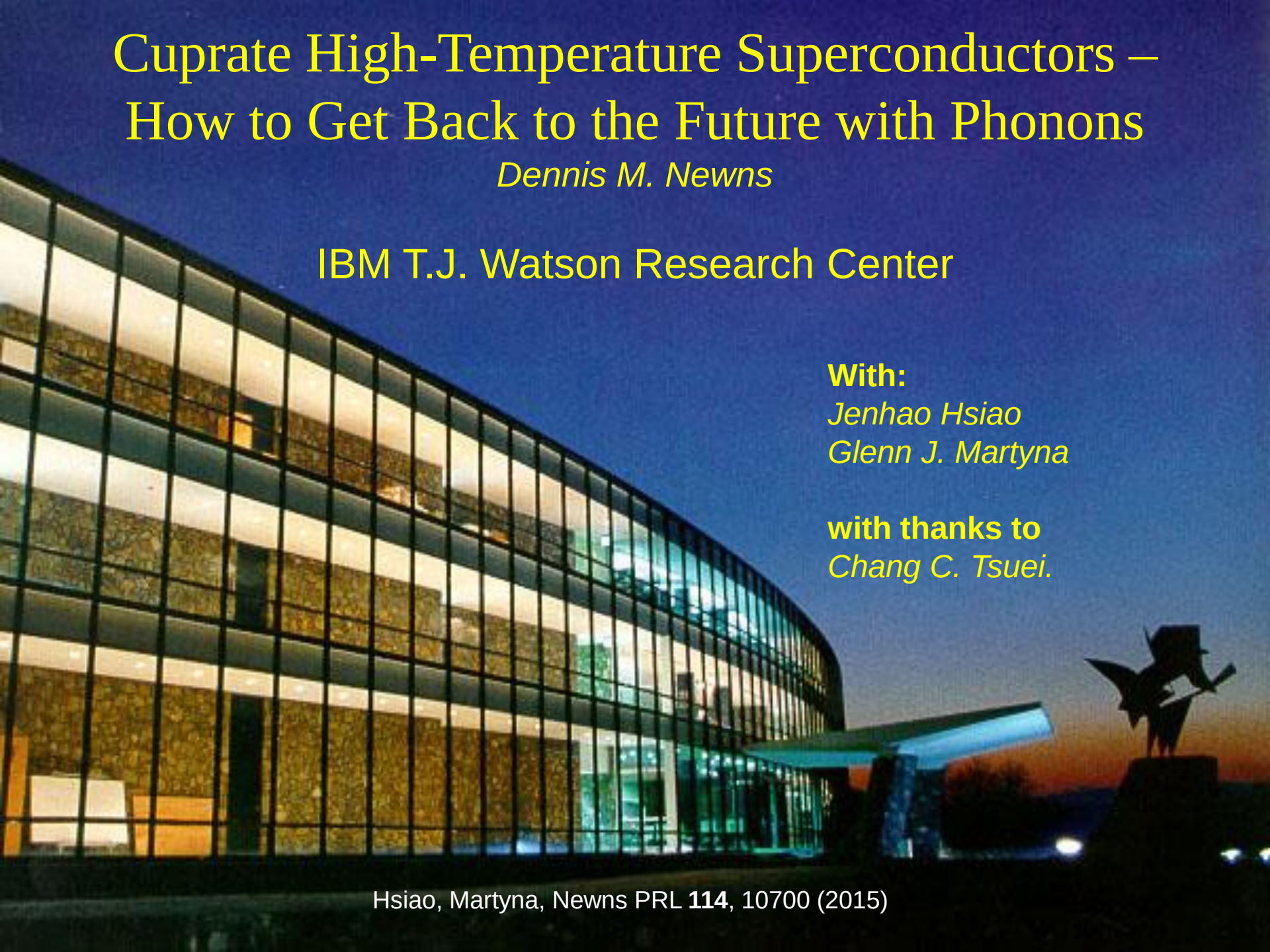


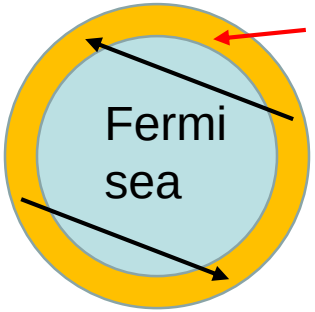
With:
Jenhao Hsiao
Glenn J. Martyna

with thanks to
Chang C. Tsuei.

Hsiao, Martyna, Newns PRL **114**, 10700 (2015)

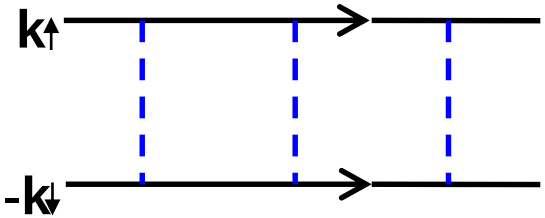
Nature of Superconductivity

• In a metal, electrons near the Fermi Energy are weakly (repulsively) interacting 'quasiparticles' (Landau)



Very few transitions conserving momentum and energy within k_BT

• A source of attraction, typically interaction between the electrons and the lattice, overcomes the repulsion and leads to the electrons pairing up into **Cooper Pairs**

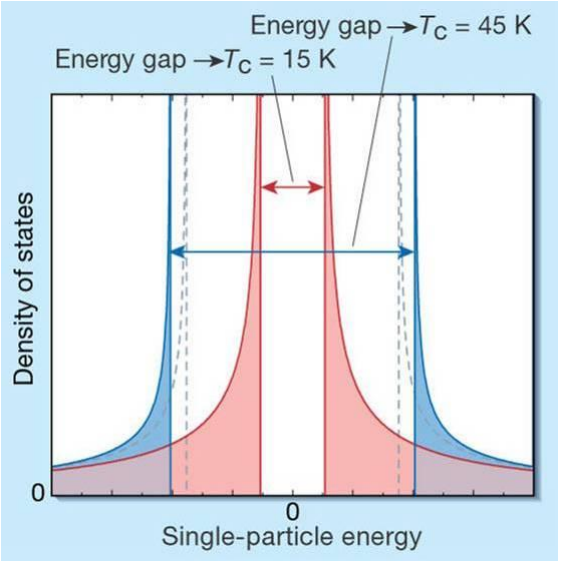


Bardeen, Cooper, Schrieffer (BCS)

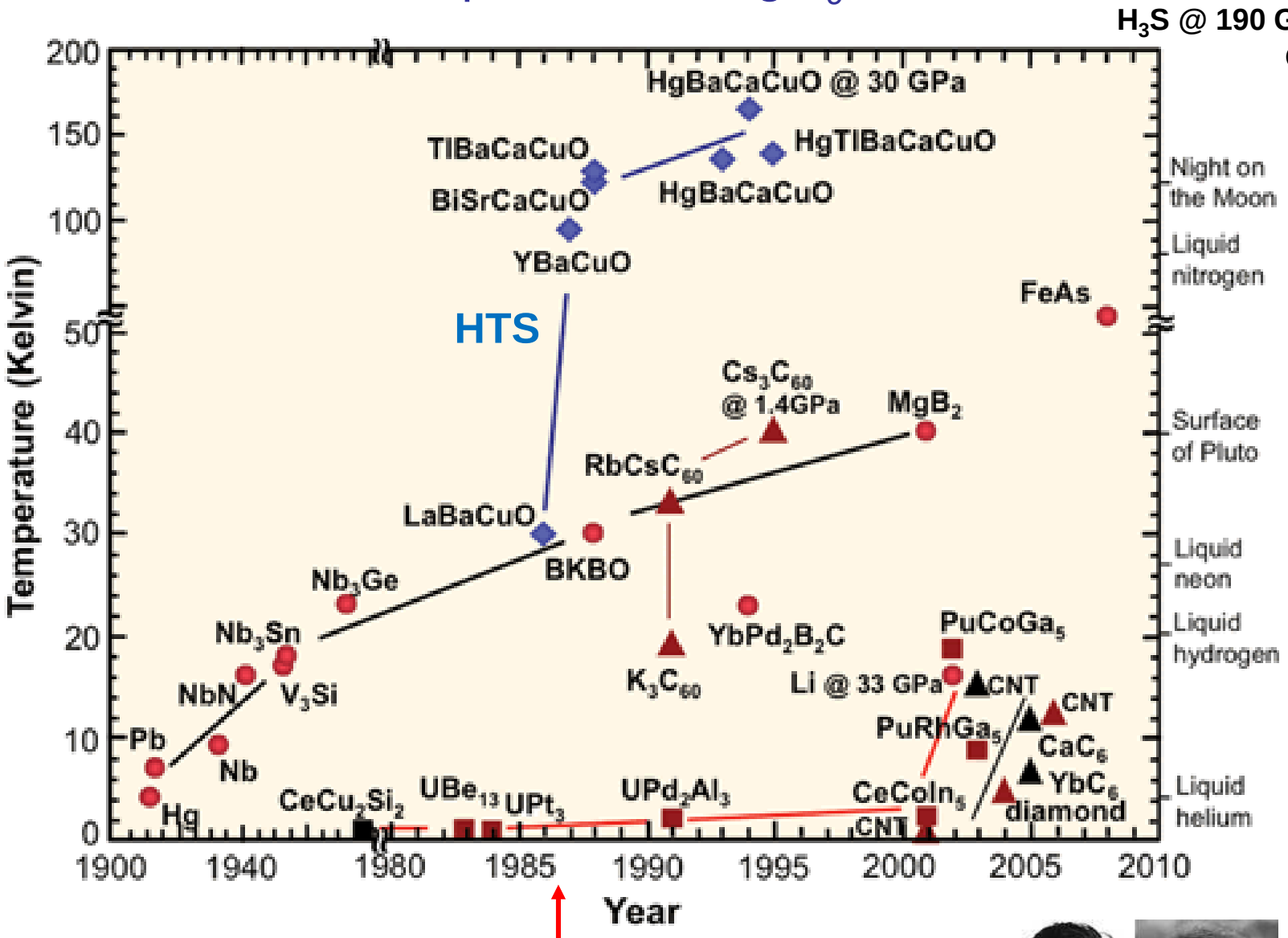
• The Cooper pairs are Bosons, and condense into a quantum coherent state – a superfluid – *simultaneously with their formation*, below T_c

• Current in a superconductor is carried by a macroscopic flow of the charged superfluid condensate, involving collective behavior of the electrons. Hence it does not encounter electrical resistance

• The formation of the condensate leads to an **energy gap** in the spectrum of electronic states at the Fermi level – which also carries a macroscopic *phase*.



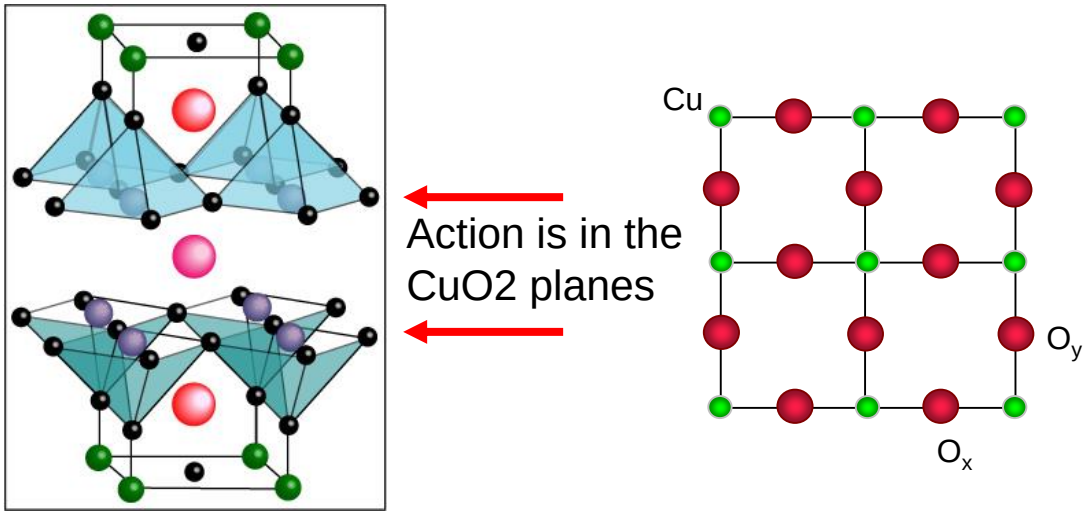
Increase in Superconducting T_c with Year



Discovery of LBCO HTS by Muller and Bednorz opened HTS field

The HTS materials: Quasi-2D metallic SC

• HTS are *layered perovskite materials* – they contain the O-Cu-O bond in a square symmetry environment



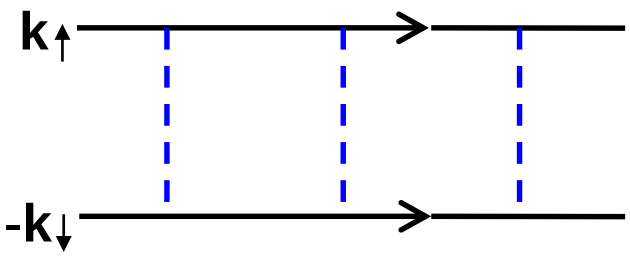
• Action is in the CuO_2 planes

• **Low-*T* state** metallic with de Haas-van Alphen Fermi Surface

C. Jaudet et al., Phys. Rev. Lett. **100**, 187005-187009 (2001),
S. Sebastian et al., Rep. Prog. Phys **75**, 102501 (2012).

Properties of a BCS Superconductor (violated by HTS)

1. Origin of Pairing is electron-phonon interaction

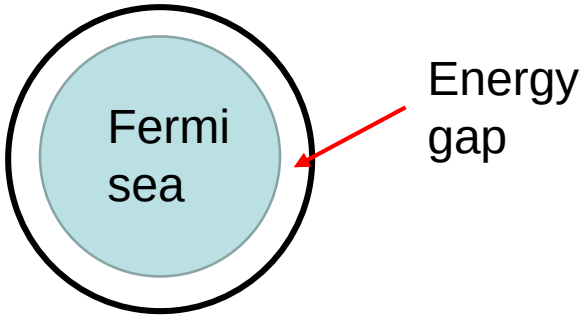


$$T_c = \omega_{ph} e^{-1/(gN(\varepsilon_F))}$$

Coupling constant

DOS at Fermi level

2. Energy gap is isotropic – *s*-wave



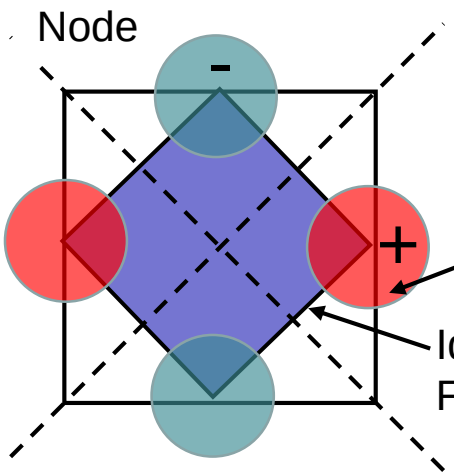
3. Energy gap $2\Delta / k_B T_c = 3.5$: universal value

4. Isotope shift $\alpha = -\dfrac{\Delta T_c / T_c}{\Delta M_O / M_O} = 0.5$: universal value

5. No ancillary phase transition expected

High Temperature Superconductivity Contrasts with BCS

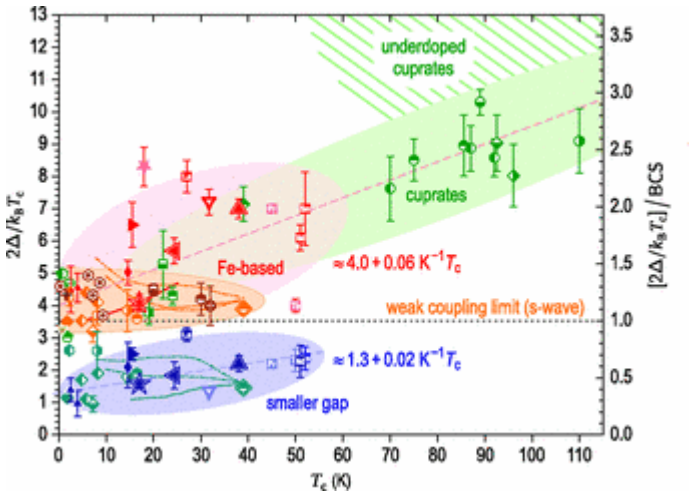
1. Origin of Pairing in dispute
2. Energy gap is *d*-wave
3. Energy gap/T_c ratio increases with T_c up to 10



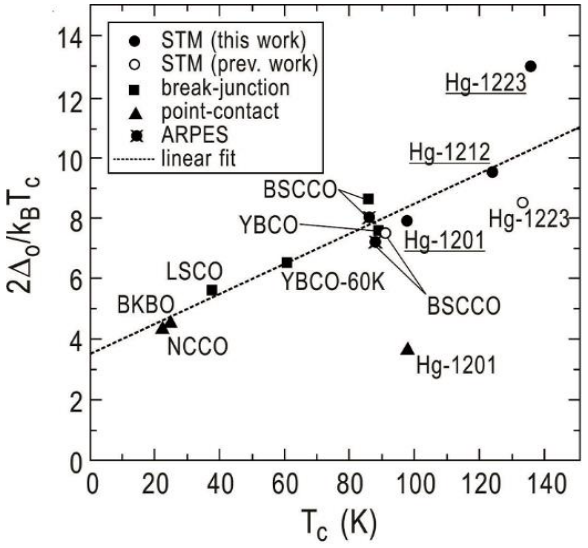
HTS gap has *d*-wave symmetry C.C. Tsuei et al., •PRL **73**, 593 (1994)

Idealized Gap function

Idealized Fermi Surface



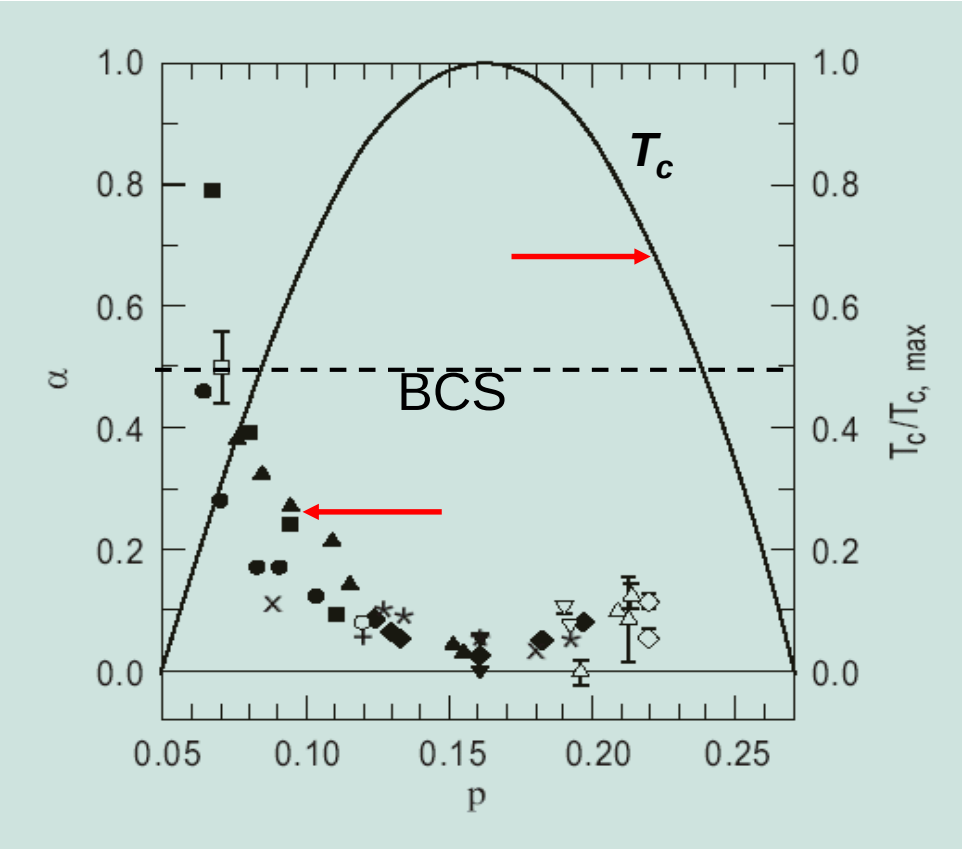
D. S. Inosov, J. T. Park, A. Charnukha, Yuan Li, A. V. Boris, B. Keimer, and V. Hinkov, Phys. Rev. B 83, 214520 (2011).



J. Wei, C. Tsuei, P. van Bentum, Q. Xiong, C. Chu, and M. Wu, Phys. Rev. B 57, 3650 (1998).

High Temperature Superconductivity

4. Isotope shift *large*, varies strongly with doping

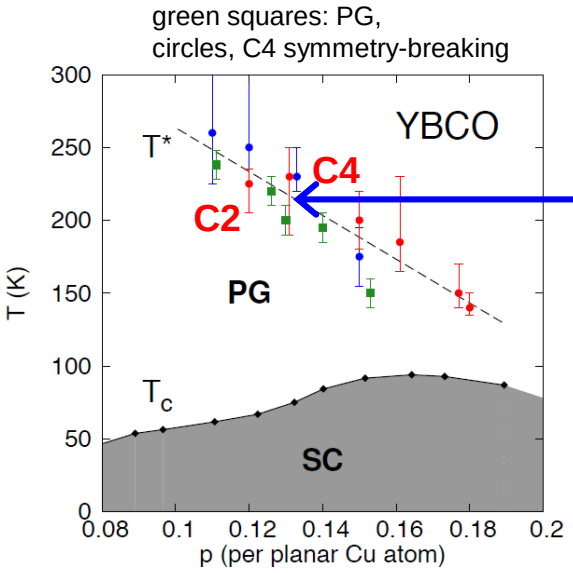


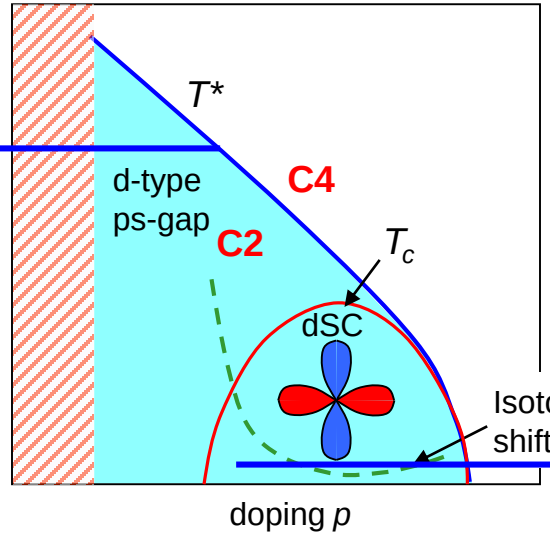
5. Ancillary phase transition, the *pseudogap*, involving C4→C2 symmetry breaking = *d*-wave CDW

Identity of *T** with C4 symmetry-breaking based on Nernst effect (R. Daou et al., Nature **463**, 519 (2010)).

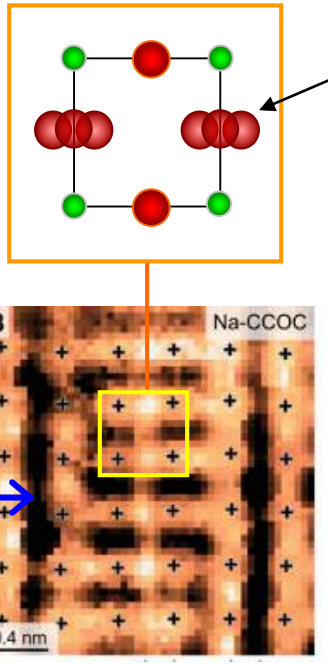
Phase Diagram

Low-T STM :Y. Kohsaka et. al. *Science* **315**, 1380 (2007), Y. Kohsaka et. al., Nature **454,** 1072 (2008).





Isotope shift α



+ other data …

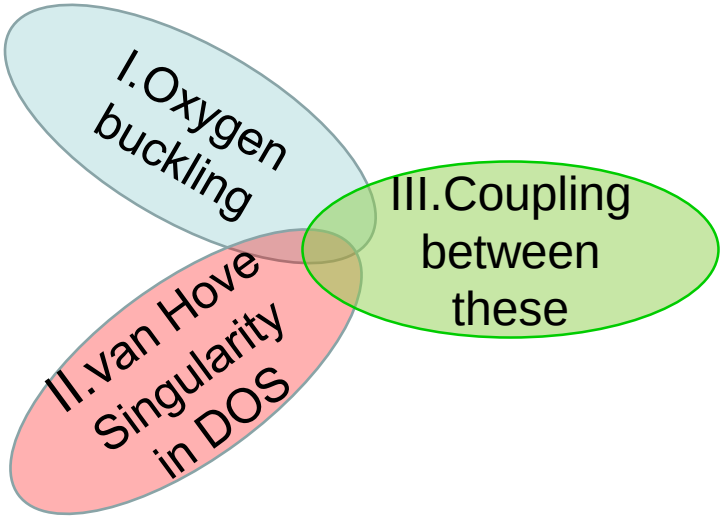
- The pseudogap transition is associated with a C4→C2 symmetry breaking (in most materials with *short coherence length*)
- The symmetry breaking includes the vibrational amplitude of the planar oxygens

Where does this lead us?

- What basic physics underlies the anomalous phenomenology of HTS?

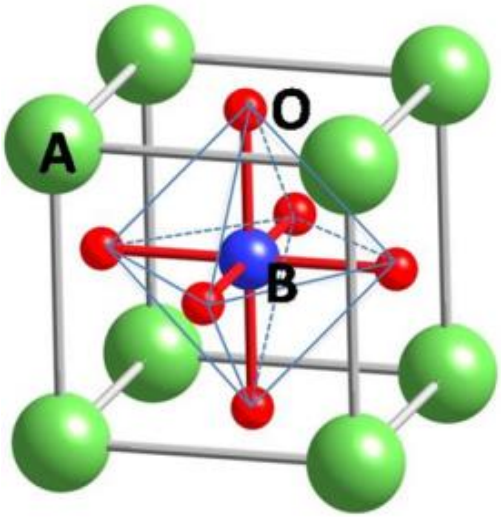
- There is a strongly felt view that it is spin-based, can be described by Hubbard model – but evidence shows this can't be the only component

- If we take into account *three basic phenomena:*



  - The phenomenology could be understood in a *modified conventional electron-vibration model.*

I. Oxygen Buckling in Cubic ABO_3 Perovskites leading to *Highly Anharmonic Potential*



tolerance factor **t**

e.g. from sum of radii

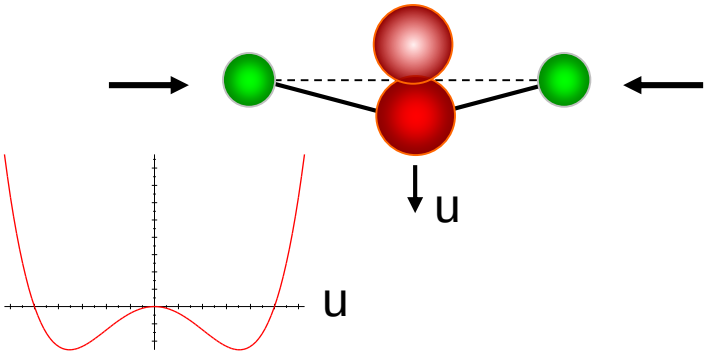
$$t = \frac{R_{A-O}}{\sqrt{2}\,(R_{B-O})}$$

Benedek & Fennie, J. Phys. Chem C, **117**, 13339 (2013)

t < 1

Cu-O-Cu bond under compression

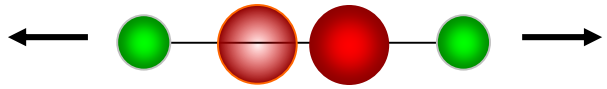
oxygens buckle - affects magnetism



t > 1

Cu-O-Cu bond under tension

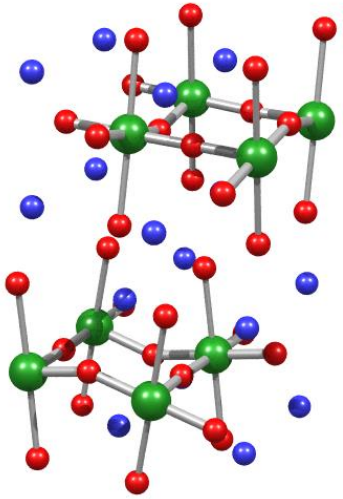
ferroelectricity



The HTS Cu-O-Cu bond also buckles (i.e. under effective compression)

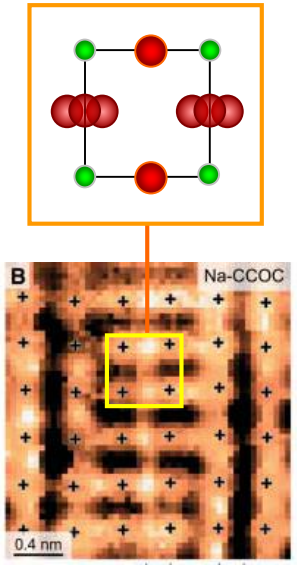
Oxygen Buckling in HTS Perovskites: Experiment and Theory

R. A. Nistor, et al.,
Phys. Rev. B **83**, 144503 (2011)
Predicted this structure theoretically

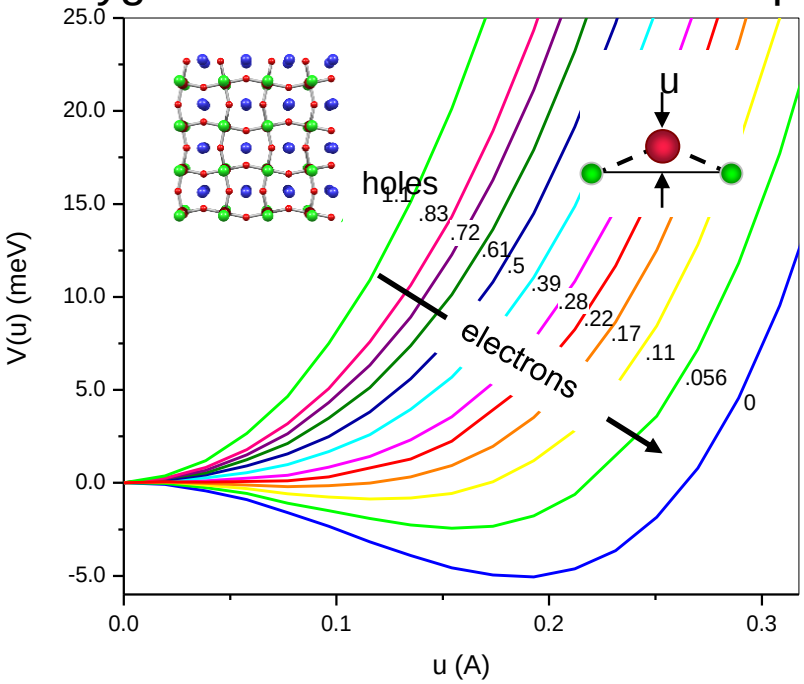


It is also seen Experimentally as the LTT structure.

Oxygen buckling

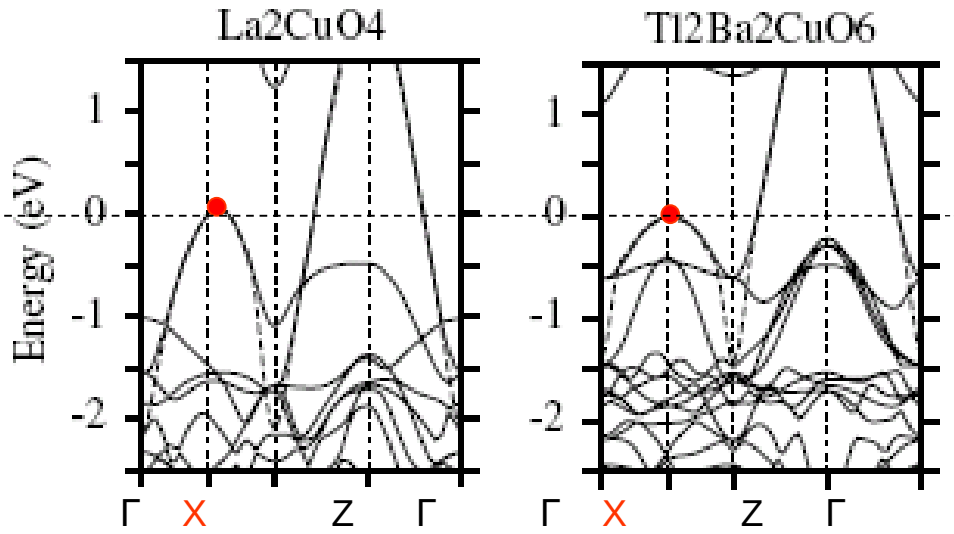


We did a detailed calculation of the Oxygen PE surface for different dopings

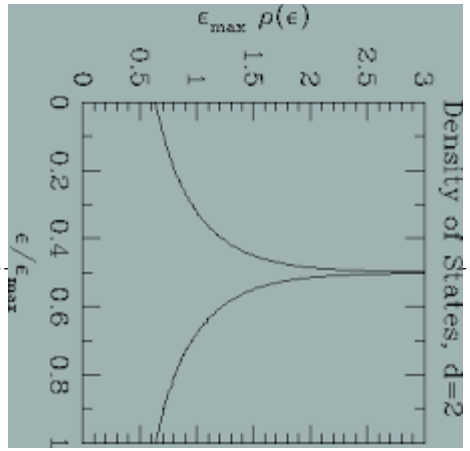


It clearly showed buckling towards the undoped side.

II. 2D Band structure has Log van Hove Singularity



E. Pavarini, et al., *PRL* **87,** 047003 (2001)

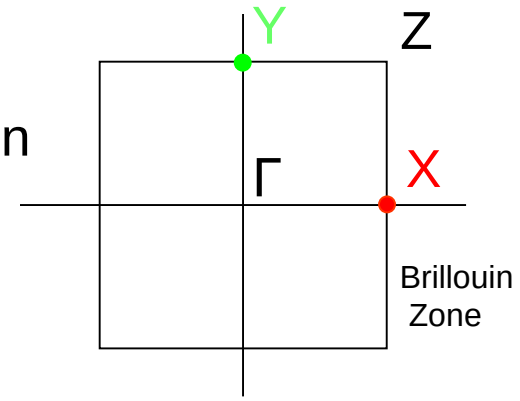


DOS

E_F

Theorem by van Hove –
Powerful effect when at E_F

Two vHs is located at points X and Y in Brillouin Zone (simplest type)



The log singularity in the DOS enhances superconductivity
- but can also lead to a Peierls distortion, the ancillary phase transition.

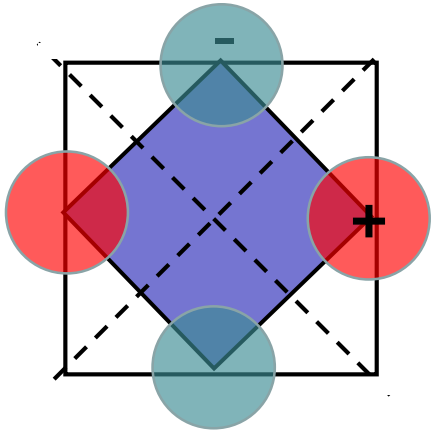
III. Coupling to Low Frequency Vibrational Modes

- From Eliashberg Equation:

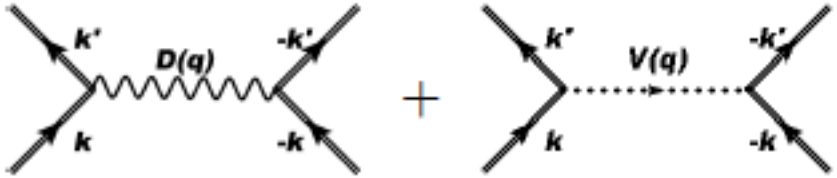
$$\nu_n Z(\mathbf{k},n) = \nu_n - T\sum_{\mathbf{q},m} W(\mathbf{k},\mathbf{k}+\mathbf{q},m) \times G_2(\mathbf{k}+\mathbf{q},n+m)\nu_{n+m} Z(\mathbf{k}+\mathbf{q},n+m),$$

$$\Phi(\mathbf{k},n) = -T\sum_{\mathbf{q},m} W(\mathbf{k},\mathbf{k}+\mathbf{q},m) \times G_2(\mathbf{k}+\mathbf{q},n+m)\Phi(\mathbf{k}+\mathbf{q},n+m),$$

$$G_2 = \left(\nu^2 Z^2 + \Phi^2 + \varepsilon_k^2\right)^{-1}; \quad \Phi = \Delta Z$$



W(***k***, ***k+q***) =

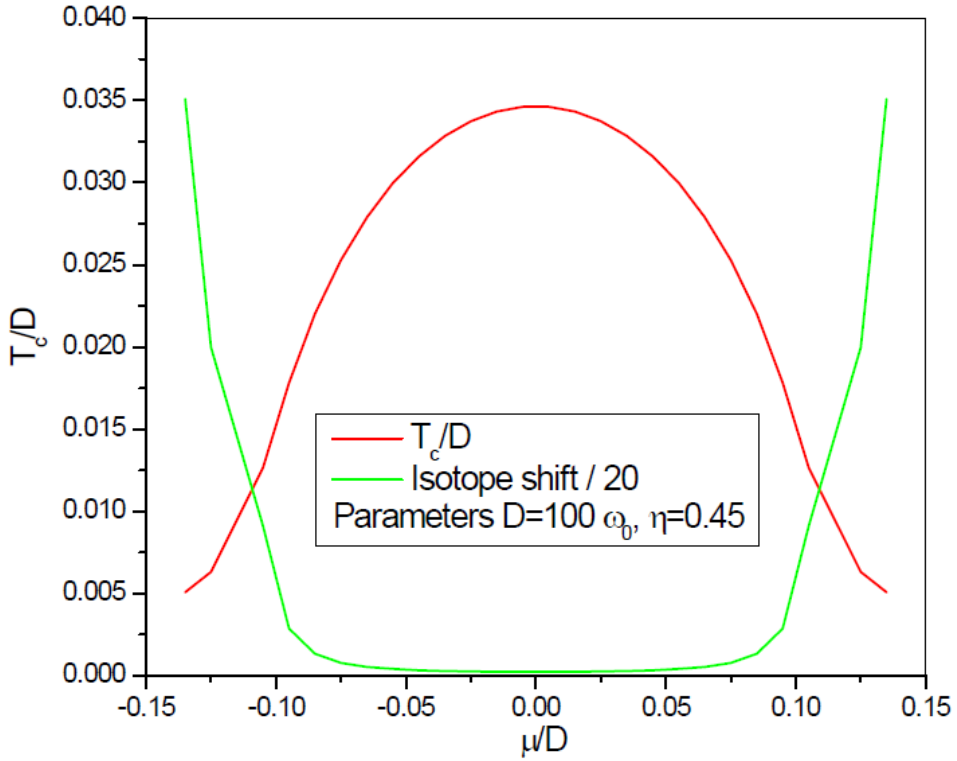


D(q) and *V* (q) being a phononic propagator and a repulsive electronic interaction. *d*-wave HTS is generated with a ***bond-centric*** D(q). *V* (q) is counter-*d*-wave.

- When pairing interaction *D(q)* is on a bond, leads to d-wave pairing

- Significant *d*-wave pairing can occur with coupling to *low frequency* vibrations (e.g. limit $\pi T > \omega_{phonon}$ vibrators classical, *d*-wave not *s*-wave).

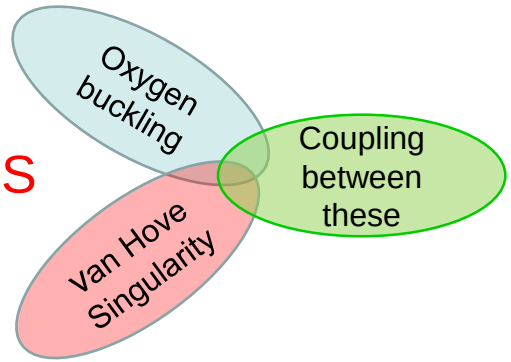
Coupling to Low Frequency Vibrational Modes



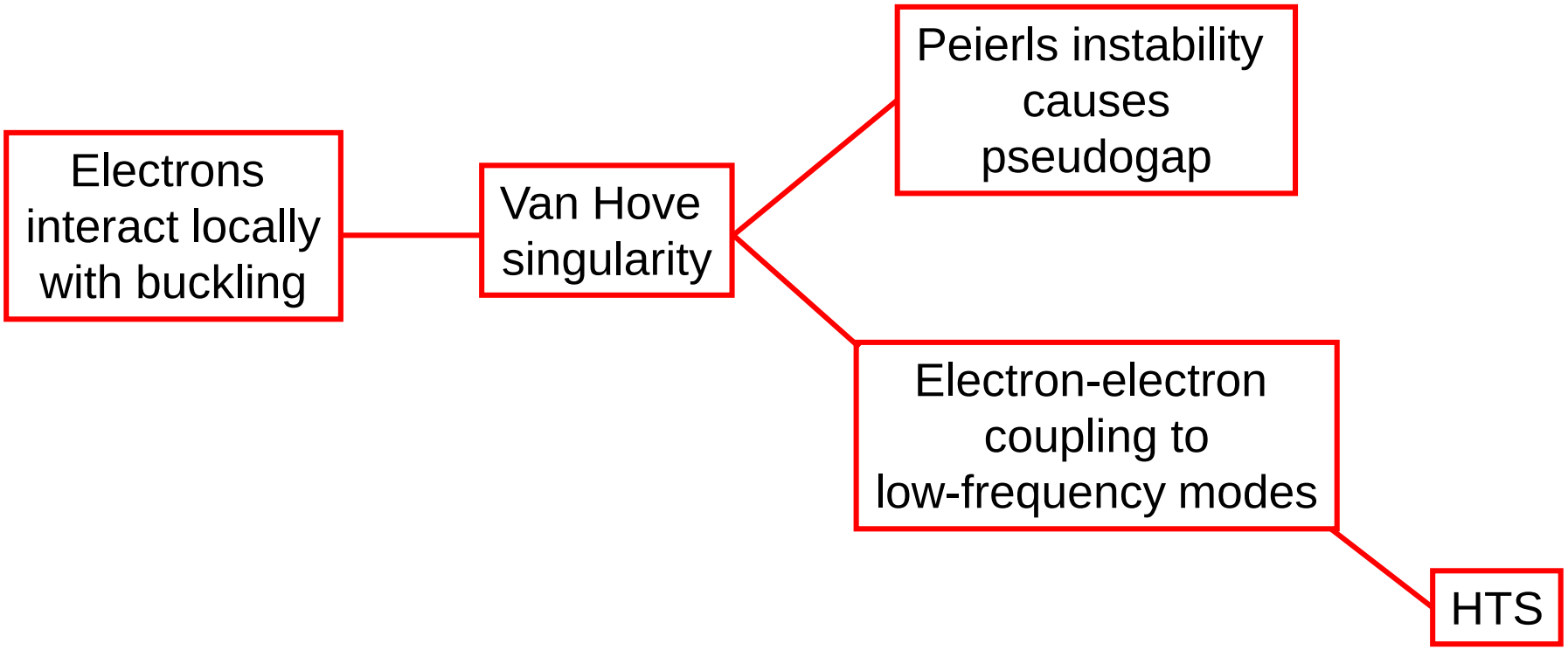
D = electronic bandwidth
η = dimensionless coupling

- If we look at the Eliashberg equation in this regime at a van Hove singularity, we see remarkably similar Tc and isotope shift behavior to that in the HTS experimental data.

These 3 concepts can generate the phenomenology of HTS

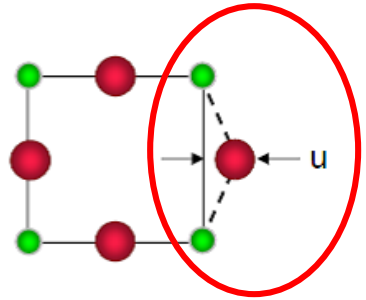


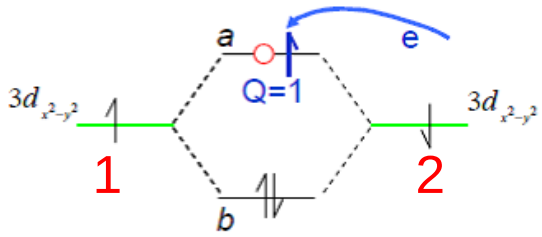
Fluctuating Bond Concept



Fluctuating Bond Model: Coupling Buckling to Electrons

One bond example





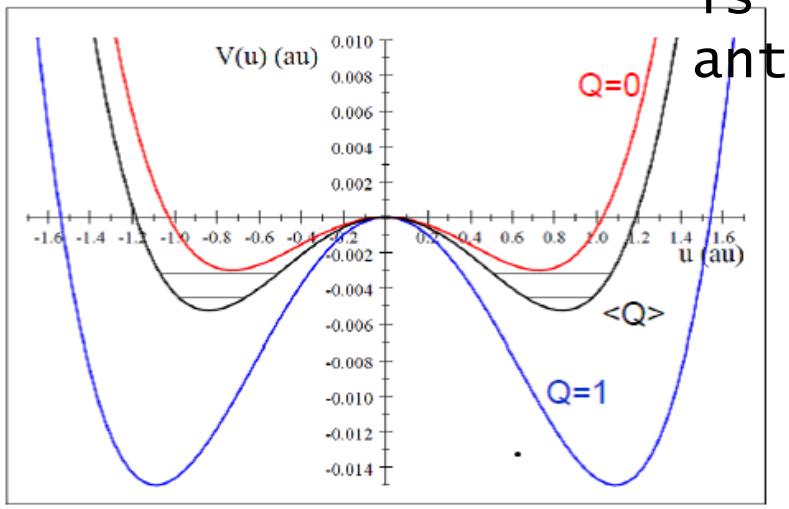
Oxygen vibrator coordinate *u* transverse to Cu-O-Cu bond.

Electronic energy levels of Cu-O-Cu bond (1-band picture), b = bonding, a = antibonding level.

$$Q = \frac{1}{2}\sum_{\sigma}\left(c_1^{+} - c_2^{+}\right)\left(c_1 - c_2\right) = n_a$$

is electronic occupation of antibonding level

Buckling strongly enhanced by electron occupation Q of antibonding level



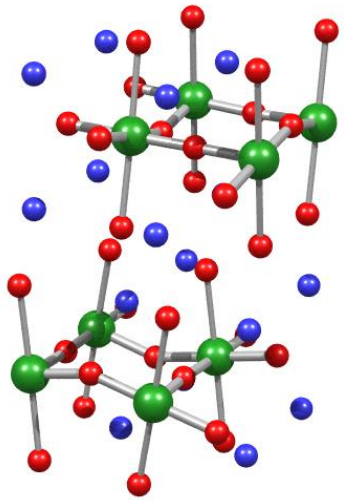
$$V(u) = \frac{1}{2}u^2 + \frac{1}{8}wu^4 - \frac{1}{\sqrt{2}}vu^2Q$$

Fluctuating Bond Model

$$H = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} n_{\mathbf{k},\sigma} + \sum_b \left[\frac{p_b^2}{2M_O} + \frac{\chi_0}{2} u_b^2 + \frac{w}{8} u_b^4 \right] - \frac{v}{\sqrt{2}} \sum_b u_b^2 n_b^a$$

band structure | O-vibrator: KE + PE + quartic term | quadratic electron-lattice coupling

Coupling *v* quantified by *ab initio* calculations



R. A. Nistor, et al., Phys. Rev. B **83**, 144503 (2011).

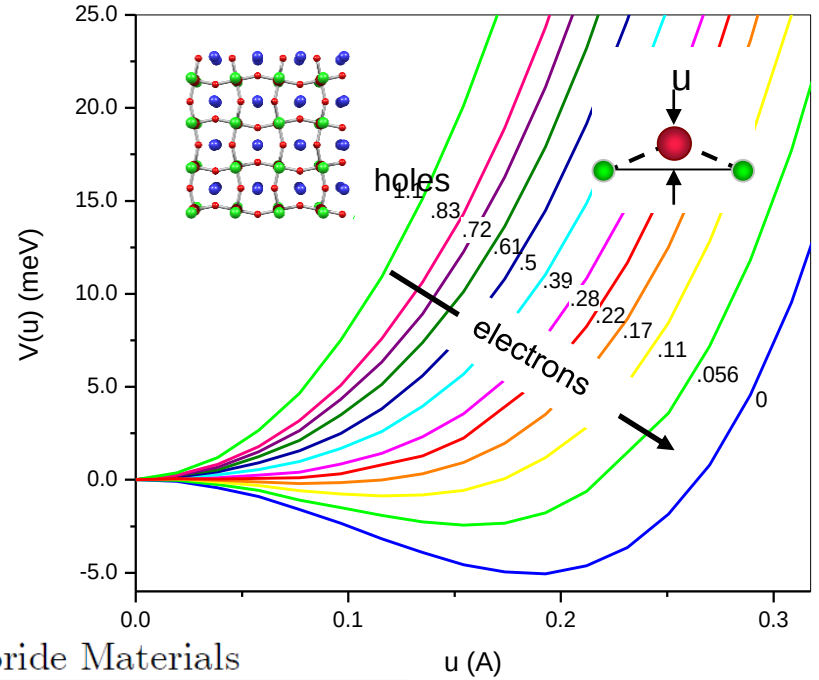
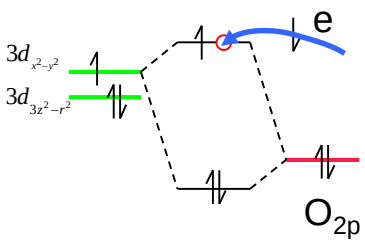


Table I: FBM Parameters for 214 and Oxychloride Materials

Polarization	v_{214} (au)	v_{oxy} (au)	w_{214} (au)	w_{oxy} (au)	K_{214} (eV)	K_{oxy} (eV)
$xy \perp$ to bond	0.0163	0.0182	0.053	0.090	0.14	0.10
$z \perp$ to bond	0.0174	0.0202	0.122	0.106	0.068	0.104

Mean Field Solution to the Fluctuating Bond Model



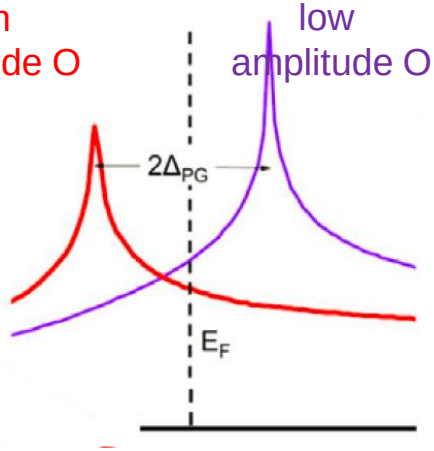
Leads to anharmonic oscillator where antibonding level occupation softens harmonic force constant

$$H_{vib} = \sum_b \left[\frac{p_b^2}{2M_O} + \left(\frac{\chi_0}{2} - \frac{v}{\sqrt{2}} \left\langle n_b^a \right\rangle \right) u_b^2 + \frac{w}{8} u_b^4 \right]$$

anharmonic oscillator with harmonic force constant controlled by $\left\langle n_b^a \right\rangle$

high amplitude O

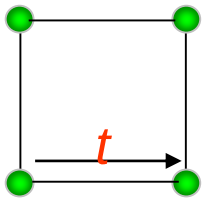
low amplitude O



Decouple interaction term in 2 possible ways

$$H = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} n_{\mathbf{k},\sigma} + \sum_b \left[\frac{p_b^2}{2M_O} + \frac{\chi_0}{2} u_b^2 + \frac{w}{8} u_b^4 \right] - \frac{v}{\sqrt{2}} \sum_b u_b^2 \left\langle n_b^a \right\rangle - \frac{v}{\sqrt{2}} \sum_b \left\langle u_b^2 \right\rangle n_b^a$$

band structure | O-vibrator KE + PE + quartic term | quadratic electron-lattice coupling



Leads to electronic Hamiltonian where vibrator amplitude modifies band structure (lowers t and hence reduces band width)

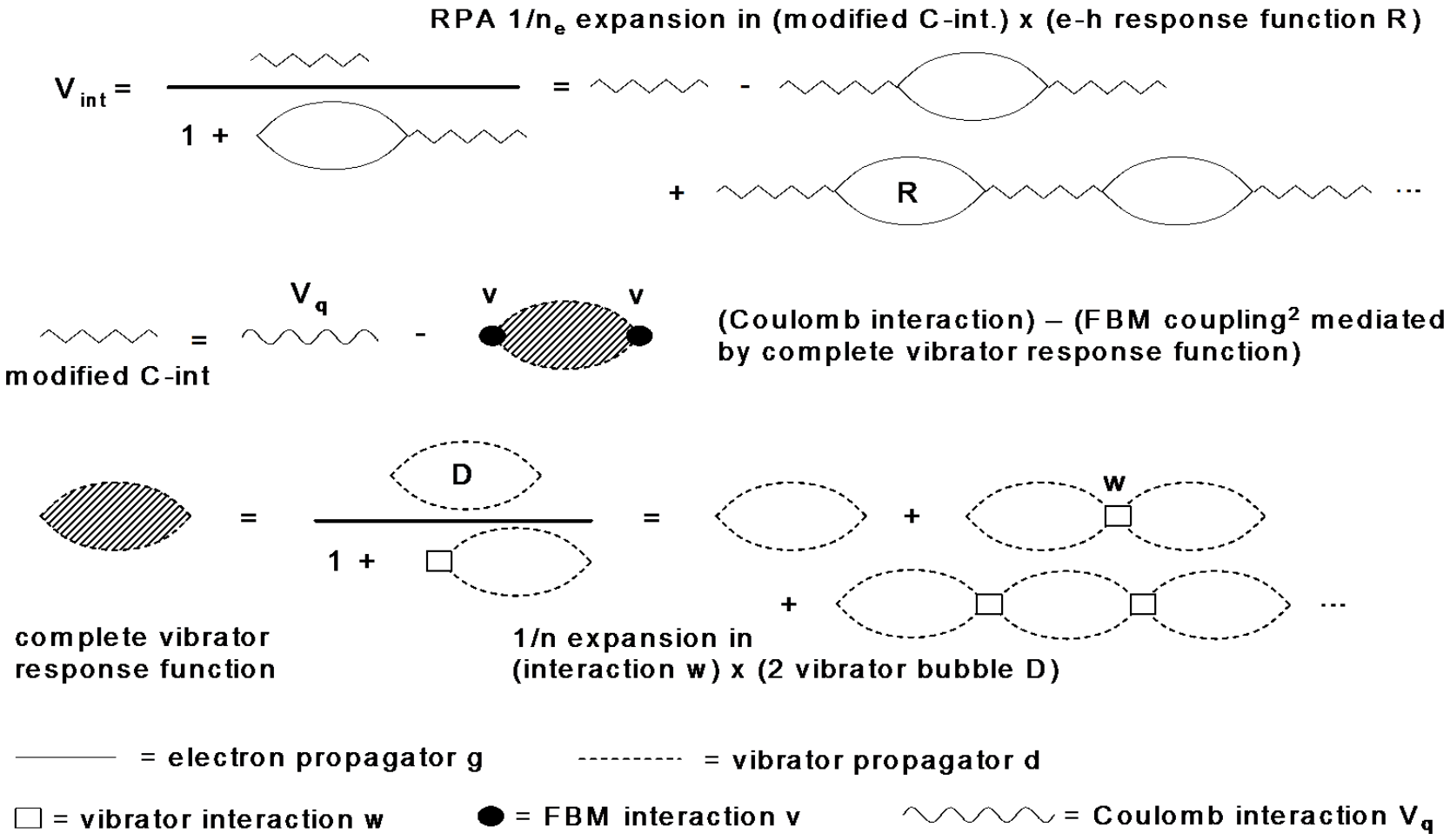
$$H_{el} = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} n_{\mathbf{k},\sigma} - \frac{v}{\sqrt{2}} \sum_b \left\langle u_b^2 \right\rangle n_b^a$$

band structure modified by term in $\left\langle u_b^2 \right\rangle$

- Assume spatially-uniform solution, then each piece, H_{vib} and H_{el} can be exactly solved.
- The electronic and vibrational problems are coupled via the expectation values $\langle n_b^a \rangle$ and $\langle u_b^2 \rangle$
- These are solved for self-consistently

R. A. Nistor, G. J. Martyna, D. M. Newns, C. C. Tsuei, and M. H. Muser, Phys. Rev. B 83, 144503 (2011).

A Generalized RPA Defines the Interaction *W(**k**, **k+q**, m)*

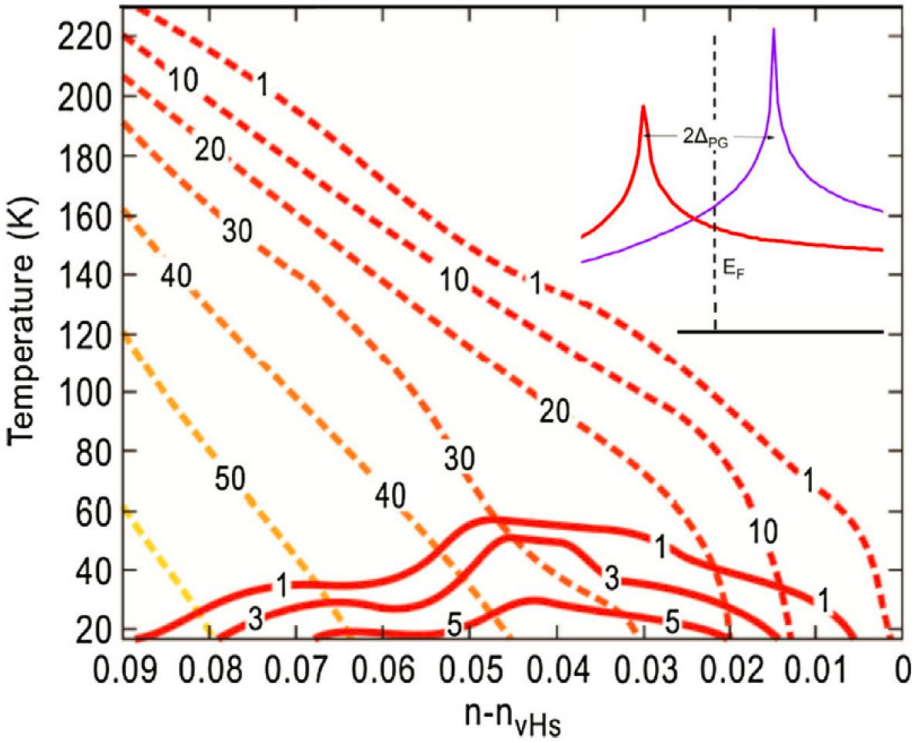


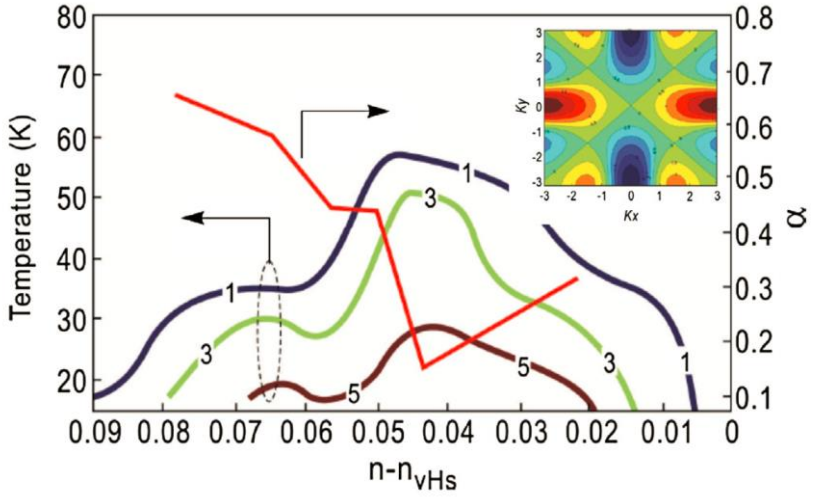
Generates low frequency coupled vibrational/electronic modes associated with pseudogap formation

Solve Eliashberg Equation with this interaction

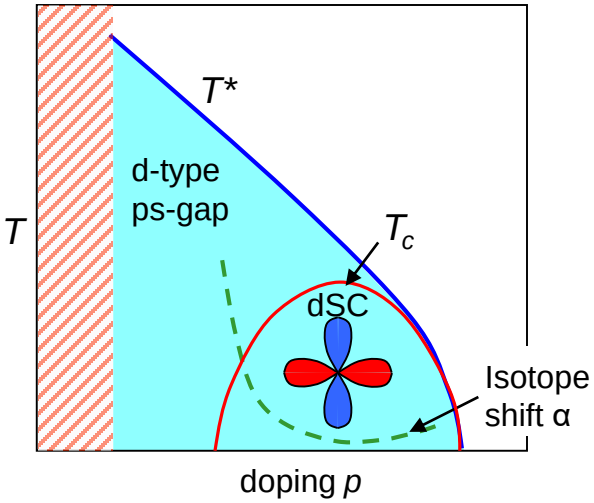
Hsiao, Martyna, Newns, PRL **114**, 107001 (2015)

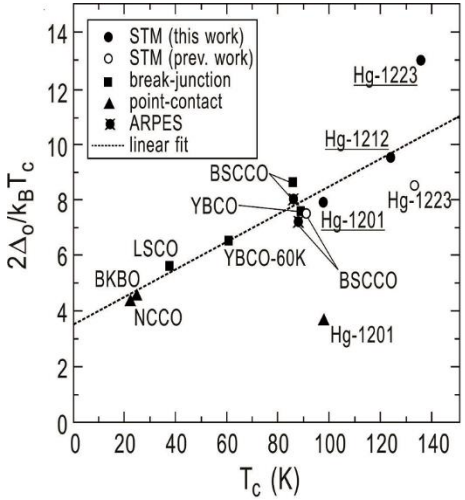
Phase Diagram with all gaps, symmetries reproduced

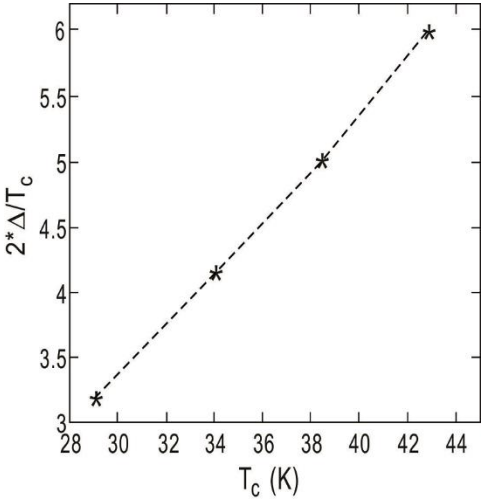




Anomalous Gap/T_c ratio reproduced – T_c varied via increased *v*







Conclusion

• The FBM, based on anharmonic oxygens coupled nonlinearly to the electron gas, captures the key pseudogap and SC properties of the cuprate HTS.

• The model produces a *d*-wave SC gap distorted by the C4→C2 symmetry breaking of the pseudogap, on average it is *d*-wave. There is some evidence for this.

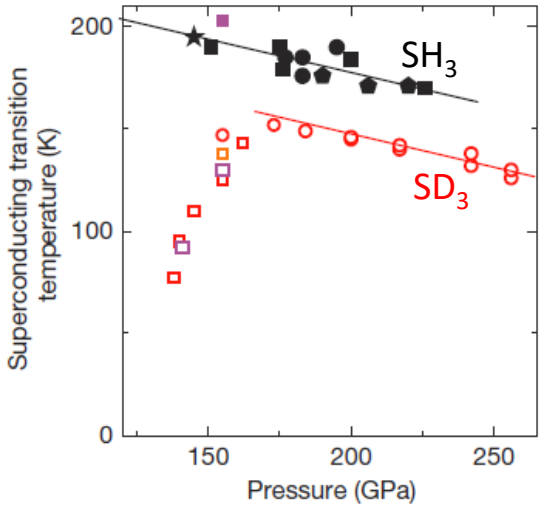
• The model has no spatial variation of the pseudogap – like certain YBCO compositions. As in YBCO, a double-hump T_c is predicted.

• A more accurate minimum isotope shift value should be produced by going beyond the quasi-harmonic mean-field + RPA approximation

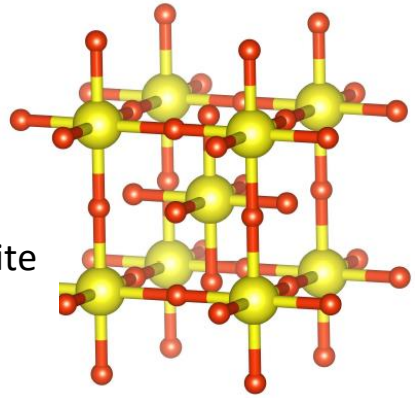
• It is important to calculate dynamics for comparison e.g. with the shift of O vibration frequencies with temperature below Tc.

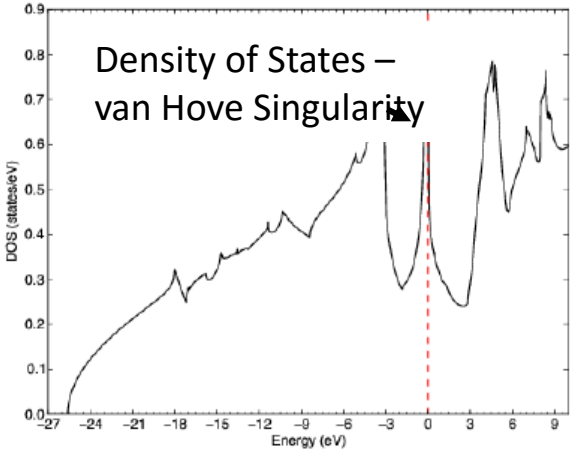
• A key next step is to incorporate the on-site Cu Hubbard U to complete the picture.

Conventional superconductivity at 203 kelvin at high pressures in the sulfur hydride system



Perovskite Planes





Anharmonicity

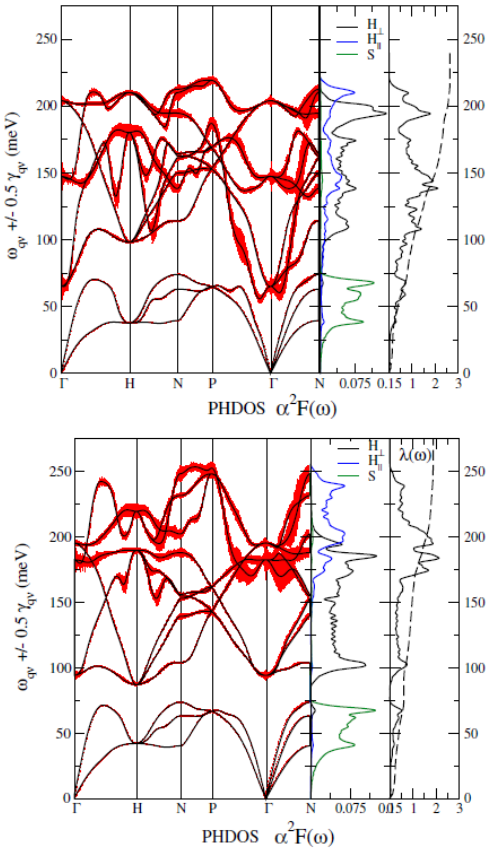
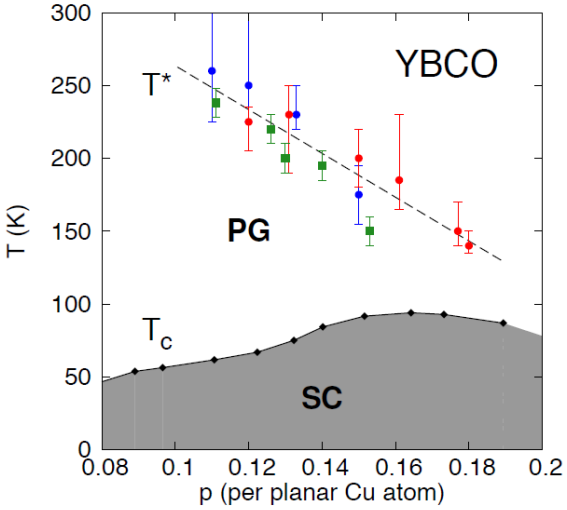


FIG. 2 (color online). Phonon dispersion, phonon density of states projected onto selected atoms and directions, and the Eliashberg function of H_3S in the harmonic approximation (top) and with the inclusion of anharmonic effects (bottom) for H_3S at 200 GPa. $H_\perp$ and $H_\parallel$ label displacements of an H atom in the

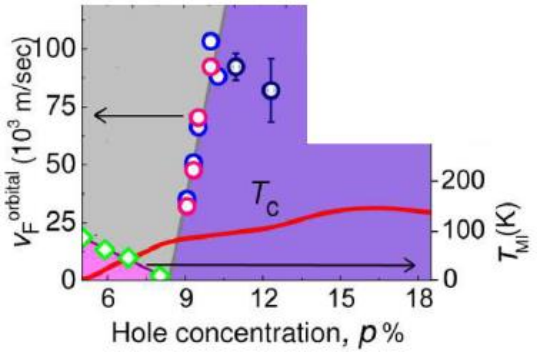
has some features in common with HTS - ? relevance

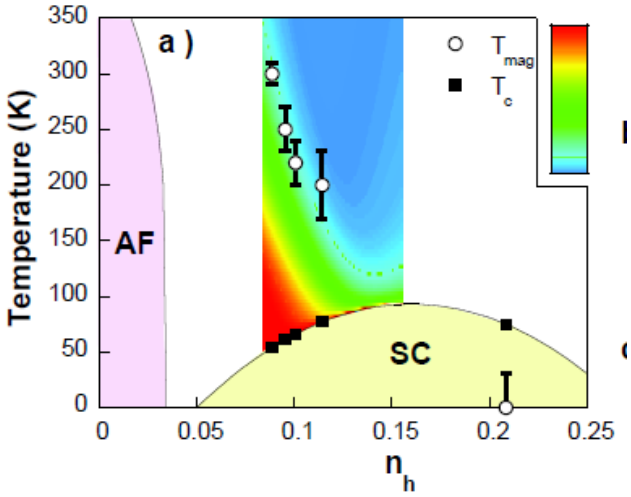
Backup Foils

Magnetism in Metallic Phase only near Mott Transition

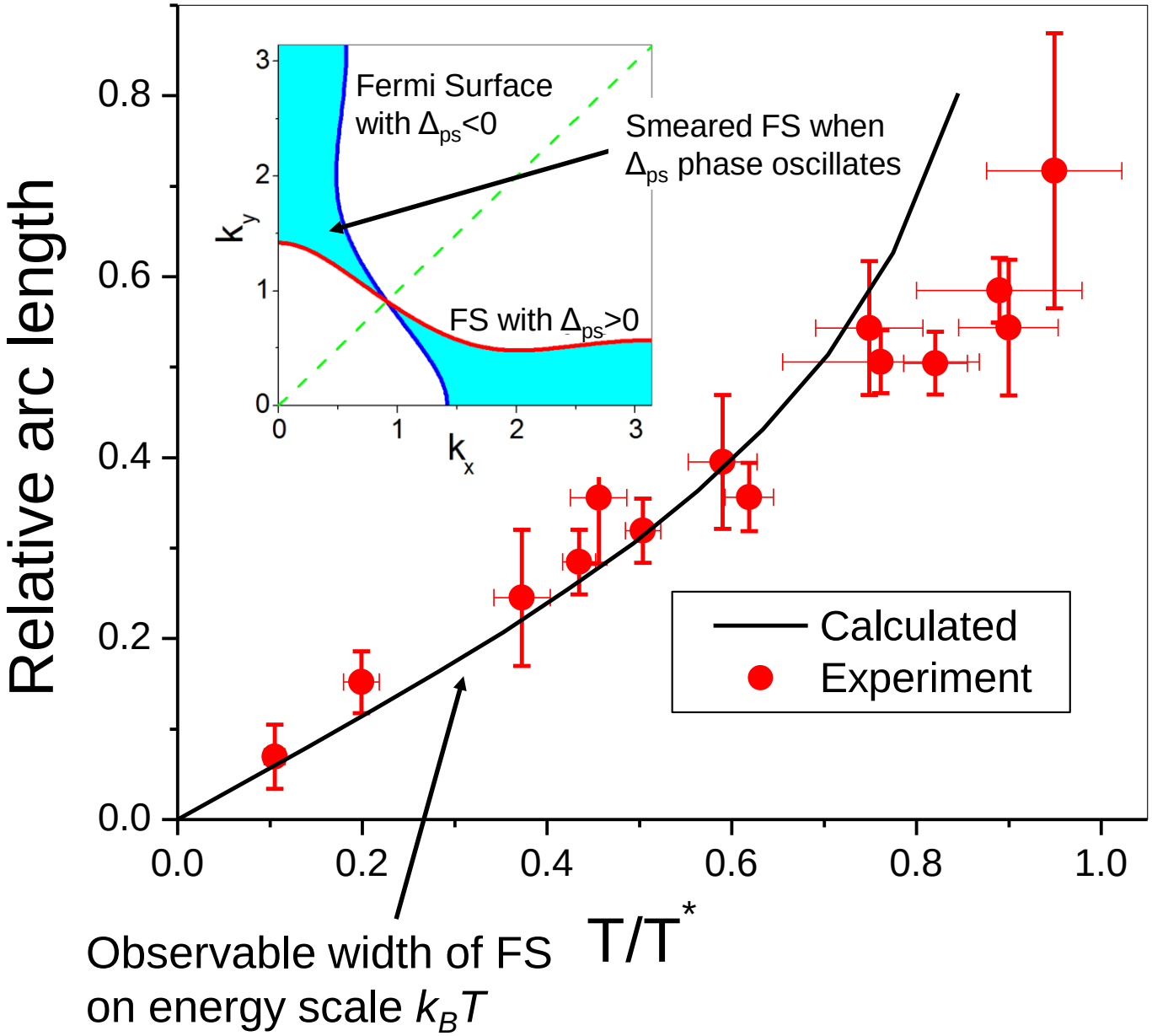


Identity of *T** with C4 symmetry-breaking based on Nernst effect (R. Daou et al., Nature **463**, 519 (2010)).

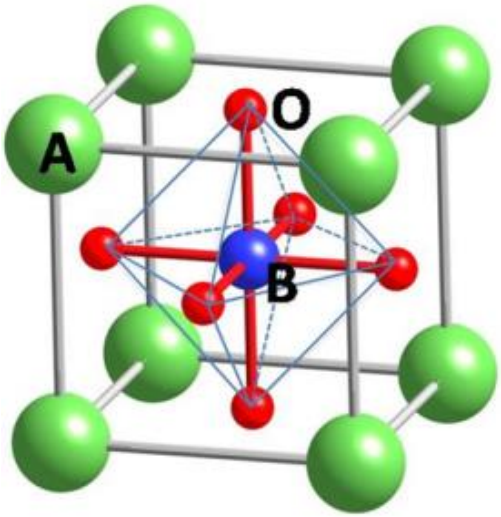




Fermi Surface Arc



I. Oxygen Buckling in Cubic ABO_3 Perovskites leading to *Highly Anharmonic Potential*

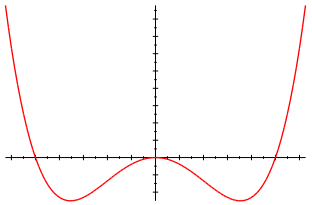


tolerance factor **t**

e.g. from sum of radii

$$t = \frac{R_{A-O}}{\sqrt{2}\,(R_{B-O})}$$

Benedek & Fennie, J. Phys. Chem C, **117**, 13339 (2013)



t < 1

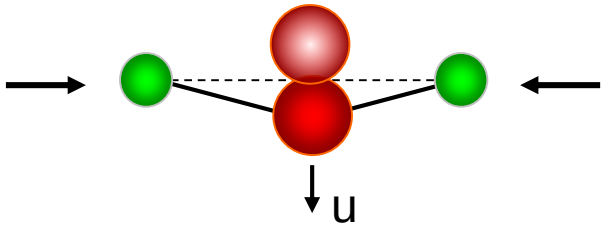
Cu-O-Cu bond under compression

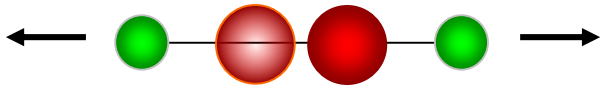
oxygens buckle - affects magnetism

t > 1

Cu-O-Cu bond under tension

ferroelectricity





The HTS Cu-O-Cu bond also buckles (i.e. under effective compression)