2013 APS Cal/Nev Section Annual Meeting
1-2 November 2013
CSU Sonoma
Rohnert Park, CA

A DFT Study of Tetragonal Rocksalt Copper Monoxide: A Proxy Structure for Understanding HTSC in the Copper Oxide Perovskites

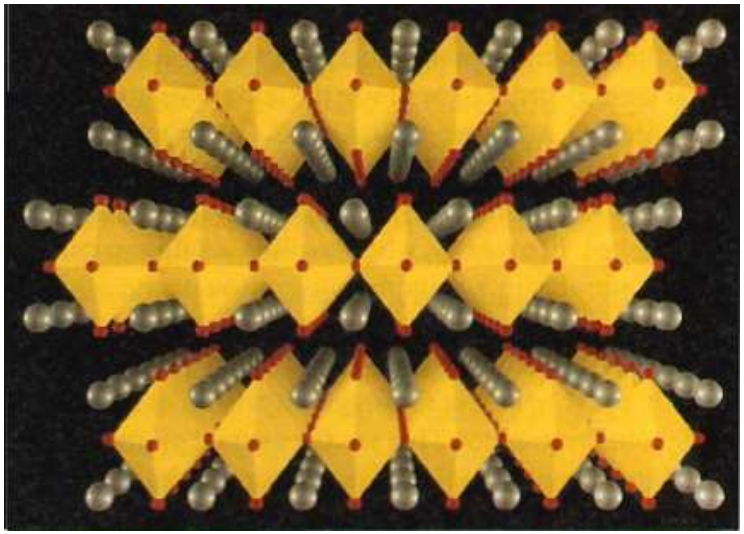
Paul Michael Grant

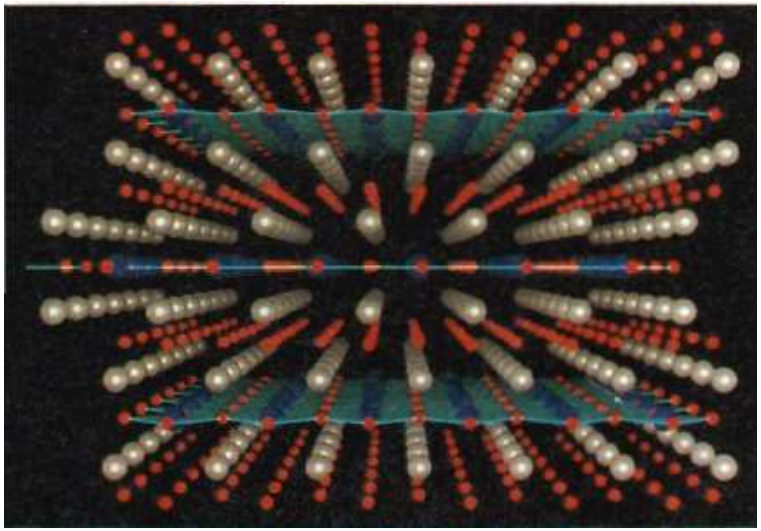
W2AGZ Technologies (www.w2agz.com)
APS Senior Life Fellow
Fellow, Institute of Physics, United Kingdom
EPRI Science Fellow (retired)
IBM Research Manager, Emeritus
...etc., etc., whatever...

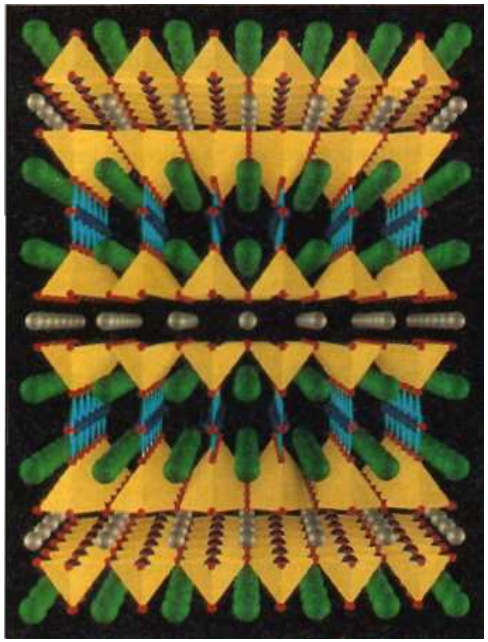
AGING IBM PENSIONER

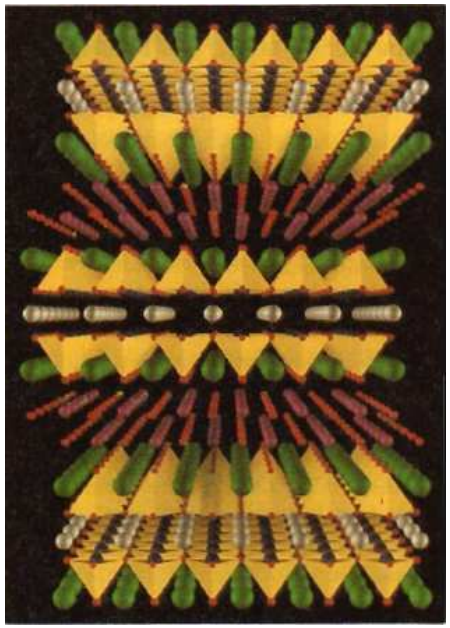
The Homework Problem

Some Copper Oxide Superconductors

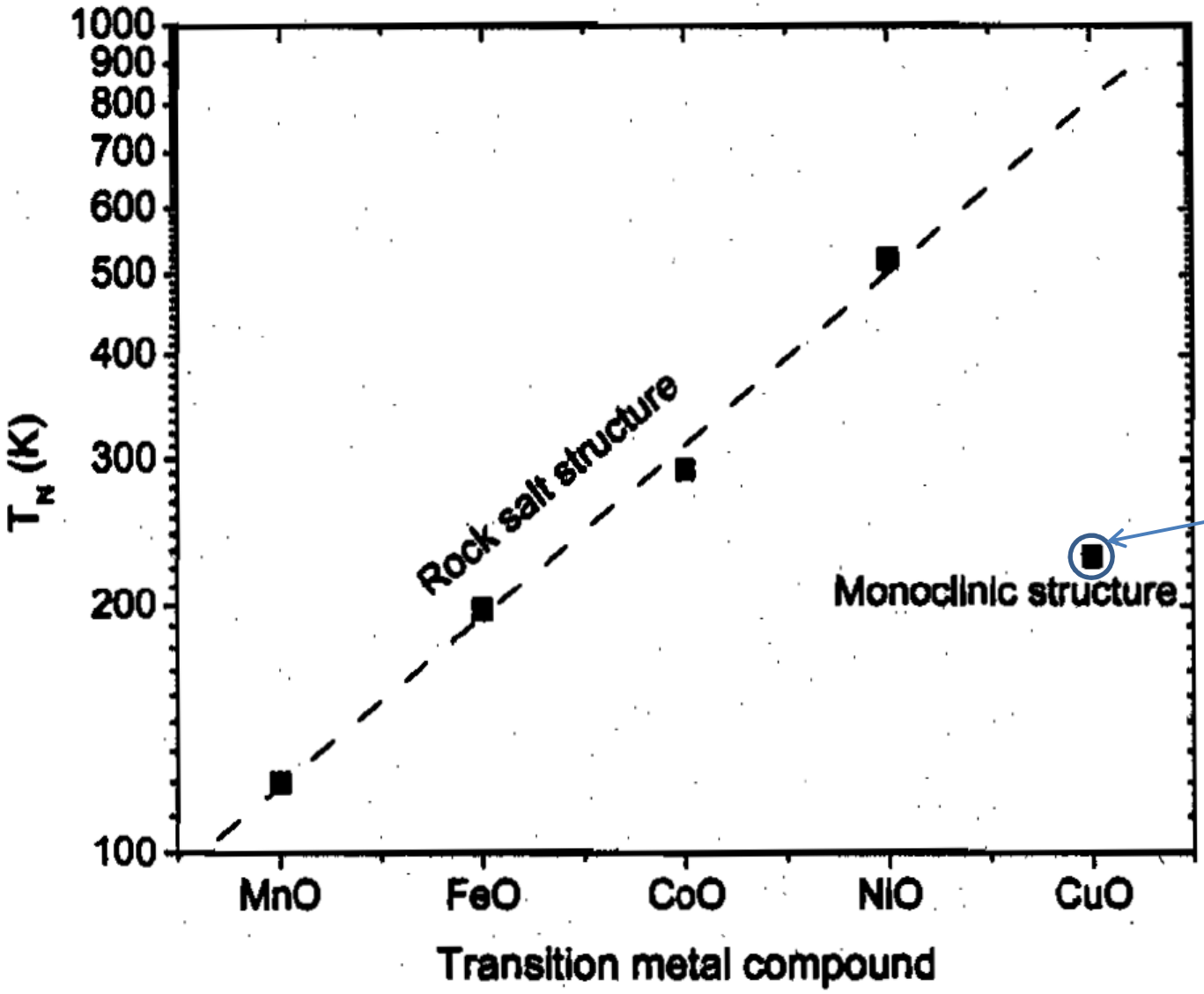






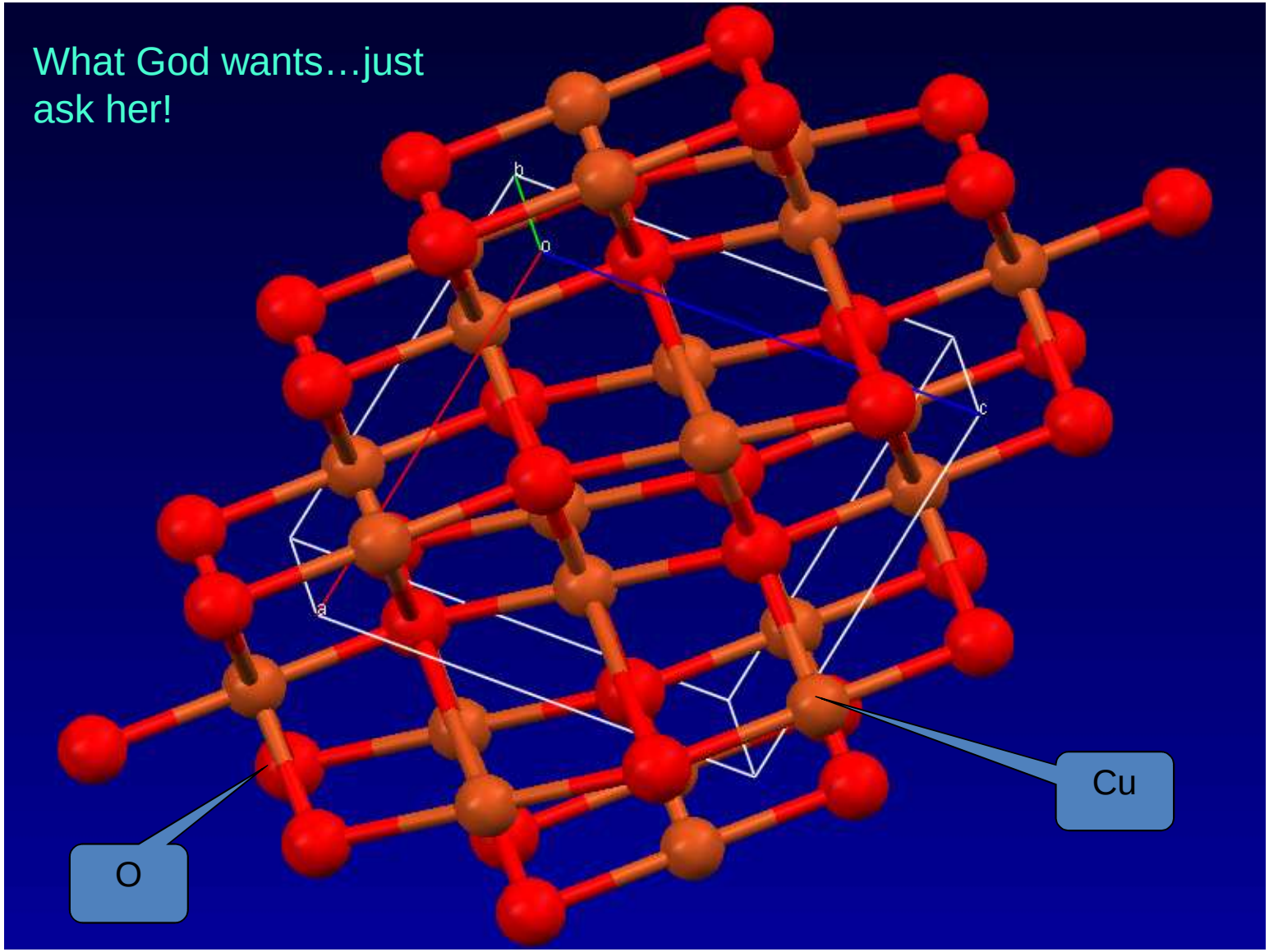


Néel Temperature vs. TMO Atomic Number



"Tenorite"
~225 K

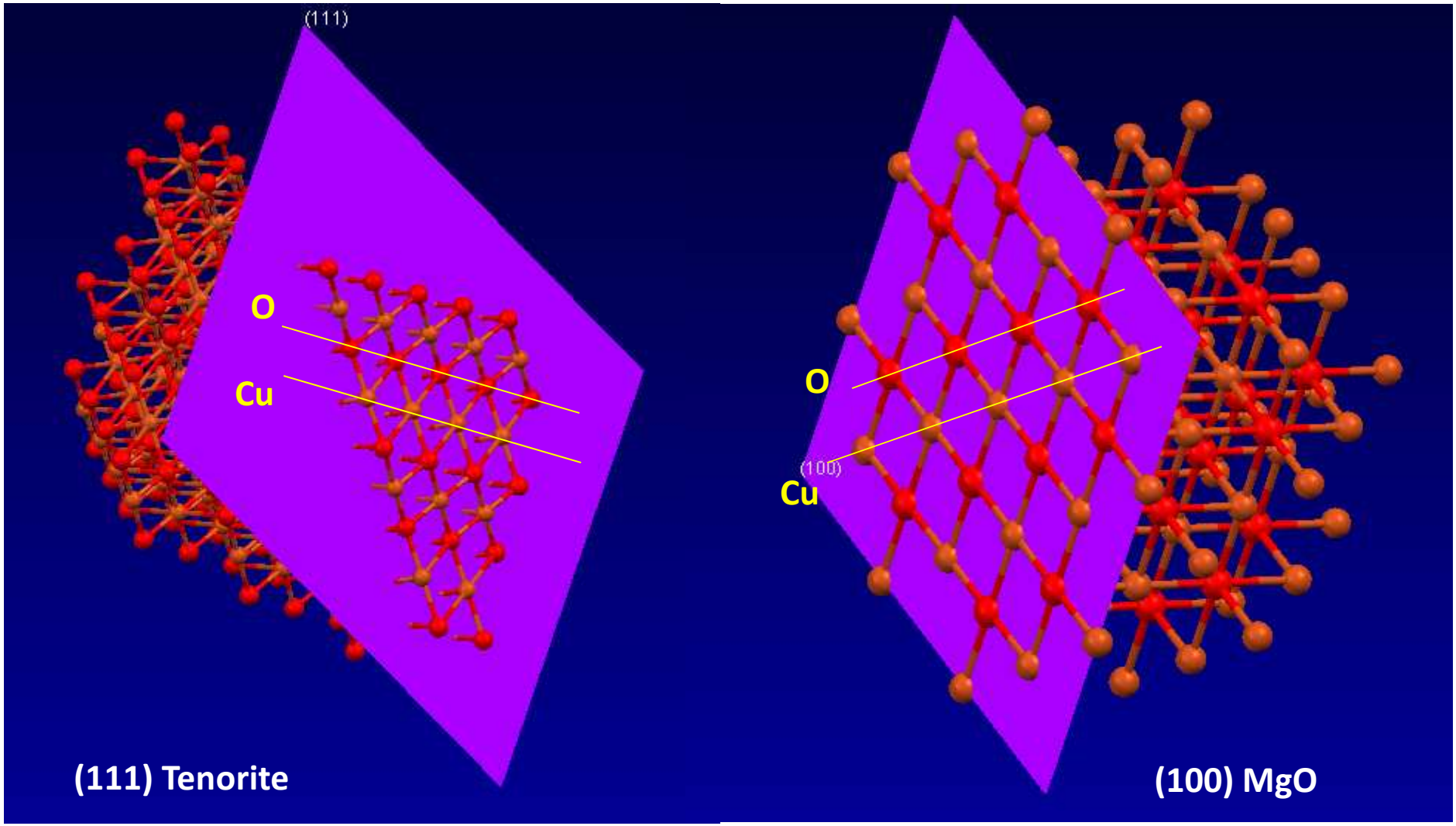
Tenorite (Monoclinic CuO)



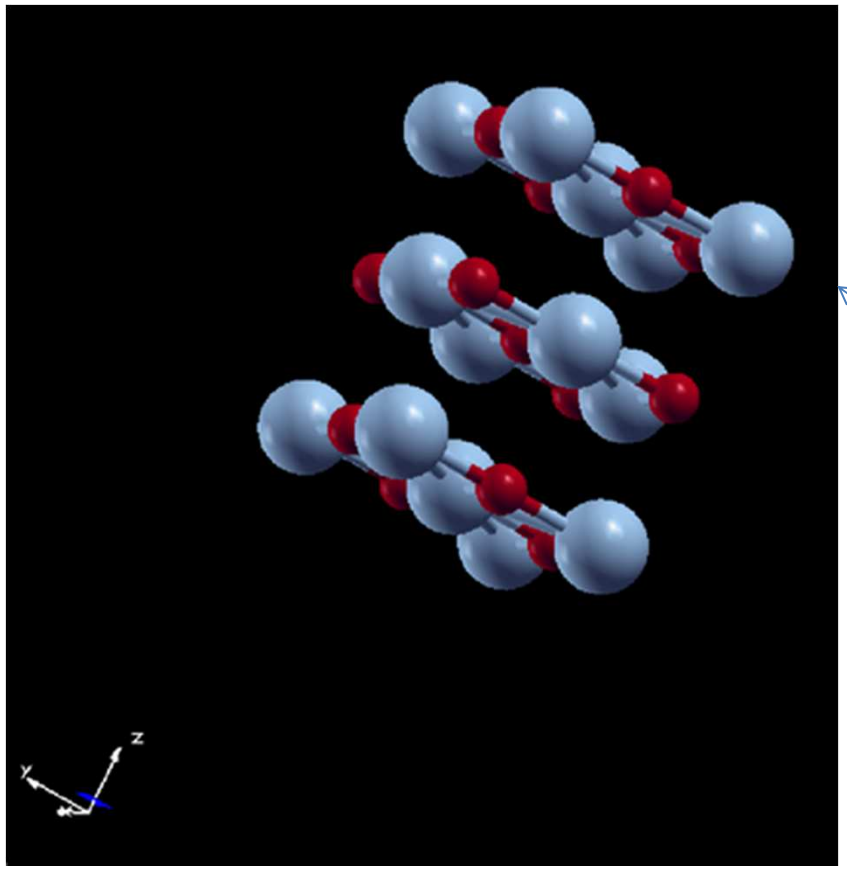
Tools

-Experimental-

Comparison of Tenorite (111) to CuO – MgO Proxy (100)



Attempt Growth by MBE Forced-epi on MgO or STO Substrates



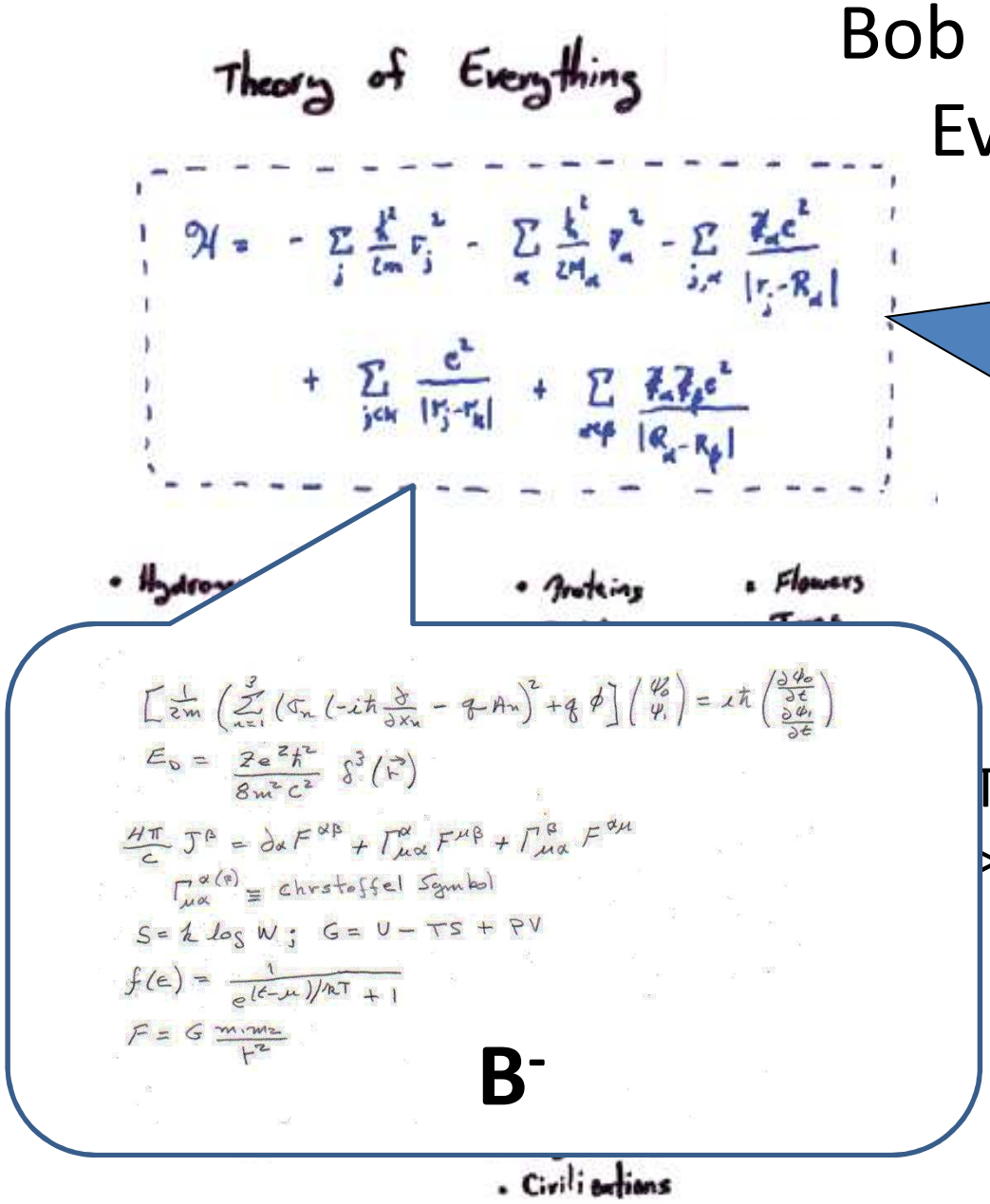
You get 5-6 monolayers of tetragonal CuO (c/a =1.36)

Siemons, et al.

Tools

-Computational-

Bob Laughlin's "Theory of Everything" (that matters)



Where's spin, Pauli and Darwin? Ya screwed up, Bob!
Oh yeah, how about Maxwell, Boltzmann, Gibbs, Fermi,…and finally, Newton's Apple.

The crunch comes when Σ_i with i >= 3 -> "thermodynamic limit."

"Van Vleck Catastrophe (1936)"

"Size Matters !"

Extended Hubbard Hamiltonian

Qualitative Description of the Physical Properties of Antiferromagnetic Insulators

$$H = \sum_{\langle ij \rangle,\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{i} n_{i\downarrow} n_{i\uparrow} + \frac{V}{2} \sum_{\langle ij \rangle,\sigma,s} n_{i\sigma} n_{js}$$

One-electron "band" term

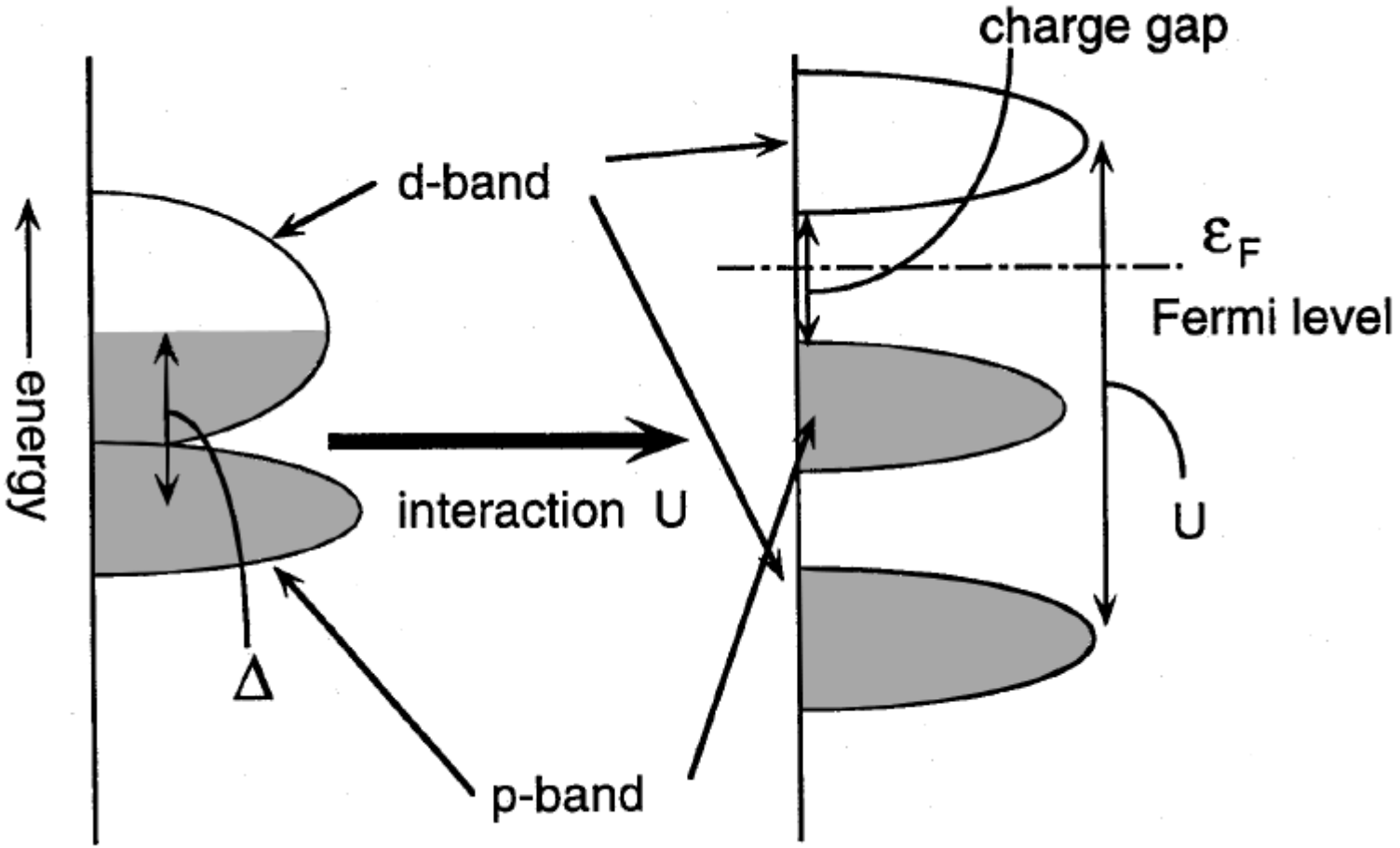
On-site "Hubbard" double occupation coulomb repulsion

Off-site repulsion

$$kT_N \approx 4t^2 / S^2 U$$

More Later!

Charge Transfer Insulator



After Imada, et al, RMP 70, 1039 (1998)

Density Functional Theory
Hohenberg – Kohn (NP Chemistry, 1998)

Kohn-Sham Equations (~1965)

$$(T + \hat{V} + V_H(n) + V_{xc}(n))\psi_i = \epsilon_i \psi_i$$

with charge density $n(\mathbf{r}) = \sum_i f_i |\psi_i(\mathbf{r})|^2$, i = combined $\mathbf{k}$ and band index,

f_i = occupancy of states, and orthonormality constraints $\langle \psi_i | \psi_j \rangle = \delta_{ij}$

Now minimize self-consistently:

$$E[\{\psi_i\}] = \sum_i f_i \langle \psi_i | T + \hat{V} | \psi_i \rangle + E_H + E_{xc}(n) + E_{ion-ion}$$

obtaining:

$$E = \sum f_i \langle \psi_i | T + \hat{V} | \psi_i \rangle + E_H + E_{xc}[n] + E_{ion-ion}$$

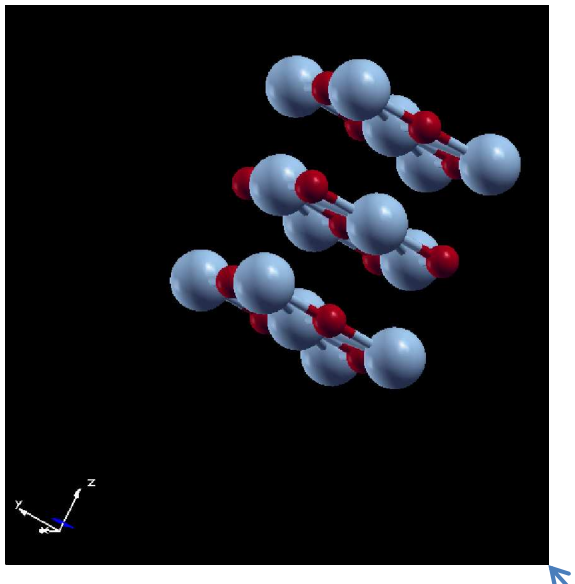
Looking into the future I expect that wavefunction-based and density-based theories will, in complementary ways, continue not only to give us quantitatively more accurate results, but also contribute to a better physical/chemical understanding of the electronic structure of matter. ***W. Kohn***

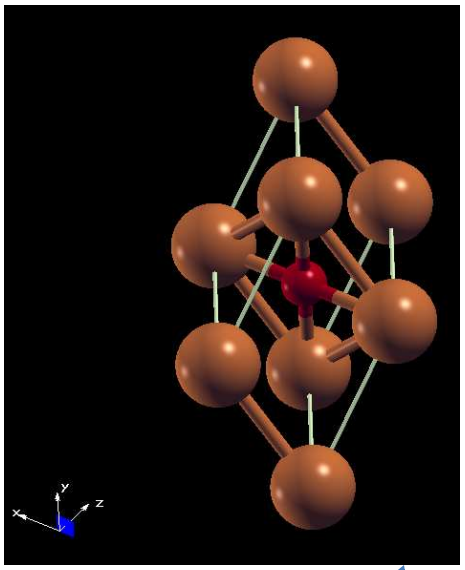
So...

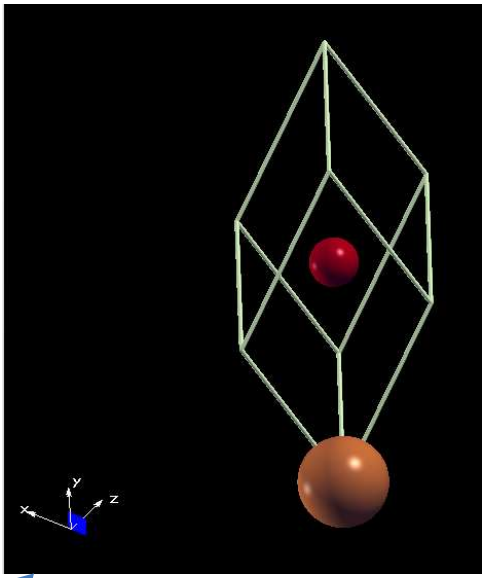
Let's "Shut up and start calculating."

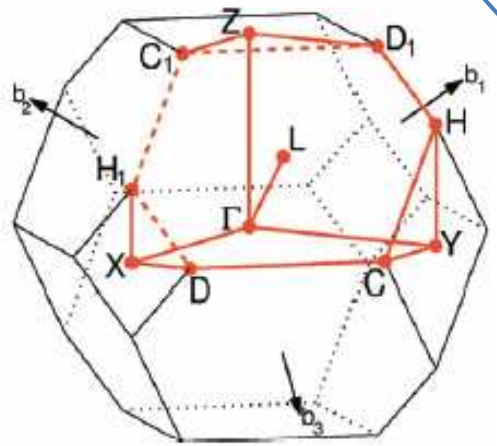
- David Mermin, Cornell, as quoted by yours truly in,
("The Great Quantum Conundrum," Nature 4 August 2011)

“Zone-ology” of “nm_Tet-CuO”









Conventional lattice
$\mathbf{a}_1 = (a, 0, 0)$
$\mathbf{a}_2 = (0, b, 0)$
$\mathbf{a}_3 = (0, 0, c)$

Primitive lattice
$\mathbf{a}_1 = (0, b/2, c/2)$
$\mathbf{a}_2 = (a/2, 0, c/2)$
$\mathbf{a}_3 = (a/2, b/2, 0)$

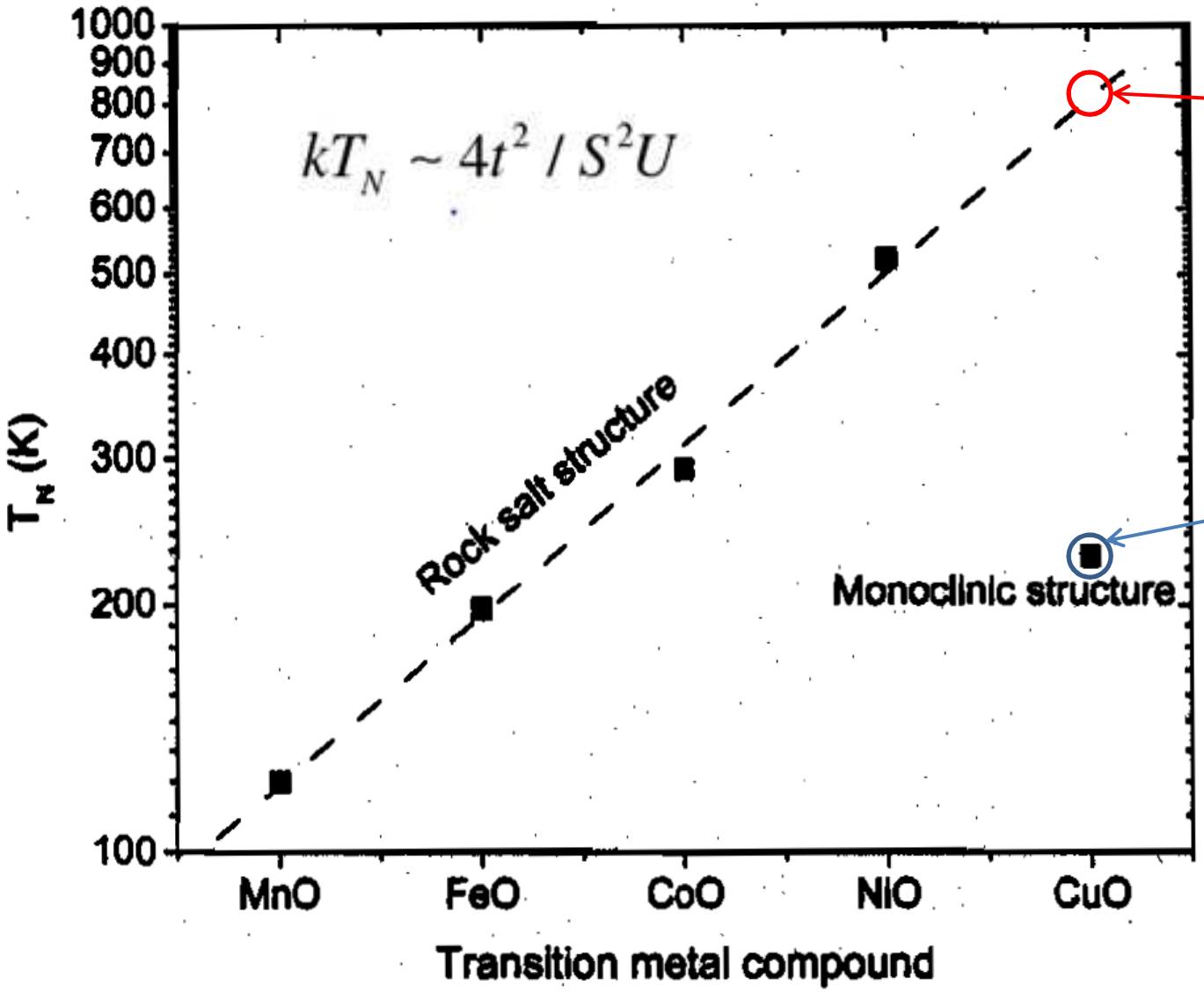
Actually, “Tet-CuO” really “Ortho-fcc CuO” with a = b

oh...btw...the red balls are O

Fig. 10. Brillouin zone of $ORCF_2$ lattice. Path: Γ–Y–C–D–X–Γ–Z–D_1–H–C|C_1–Z|X–H_1|H–Y|L–Γ. An example of band structure using this path is given in Fig. 34.

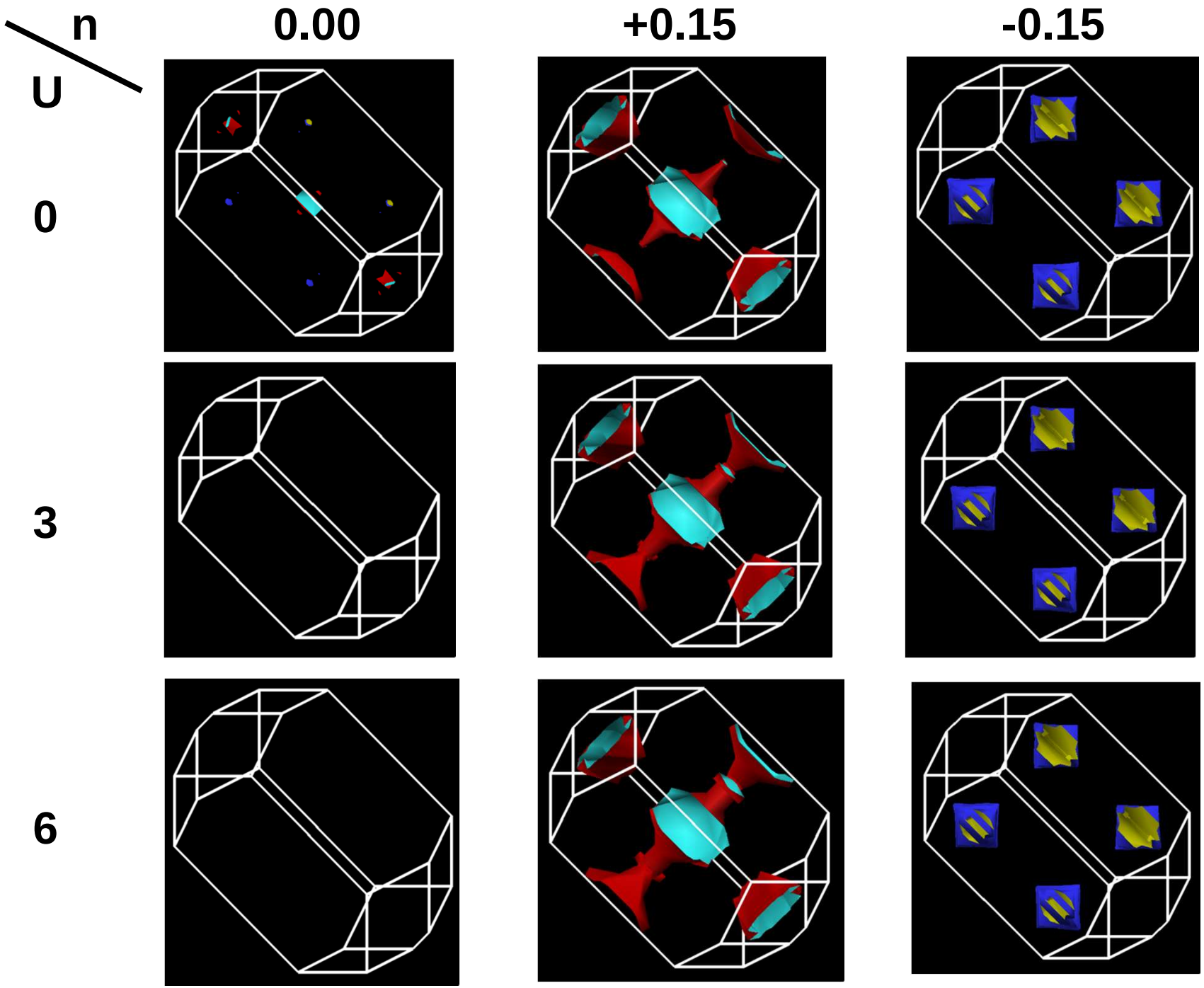
W. Setyawan, S. Curtarolo / Computational Materials Science 49 (2010) 299–312

Néel Temperature vs. TMO Atomic Number

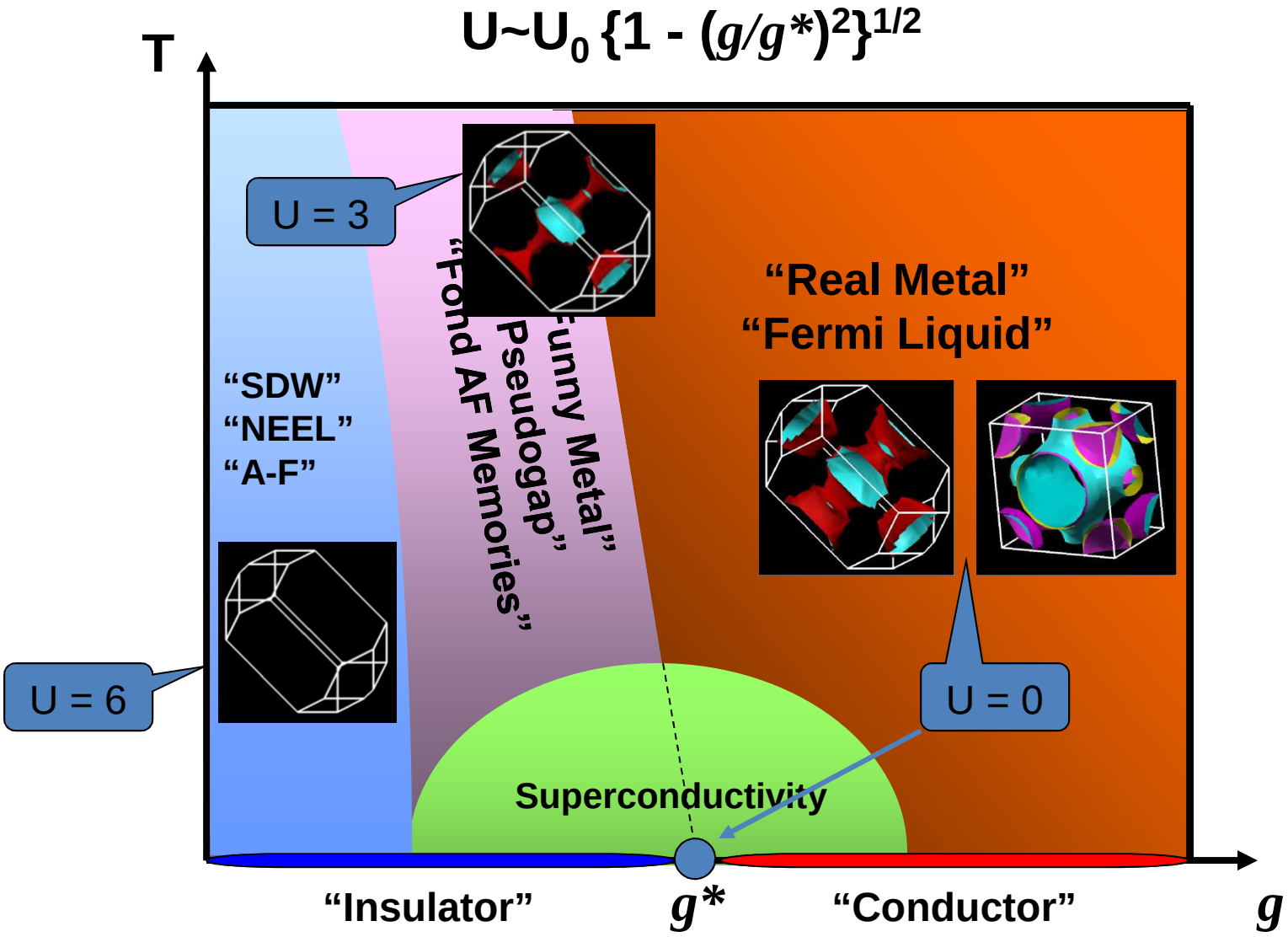


"Face-Centered, Rock Salt CuO" ~850 K (wow!)

"Tenorite" ~225 K


n
U
0.00
+0.15
-0.15
0
3
6

The Colossal Quantum Conundrum



Somewhere in here there has to be "BCS-like" pairing!

Shakes or Spins or Both?

Are They Copacetic, Competitive…or…

…just another Conundrum?

What formalism is the HTSC analogy to Migdal-Eliashberg-McMillan?

(In other words, how do I calculate the value of the BCS gap?)

- Original Strong Coupling, Eliashberg *(JETP, 1960), McMillan (PR, 1968)*
- Generalized Linhard Response Function (RPA + fluctuations) *Hu and O'Connell (PRB 1989)*
- Dielectric Response Function *Kirznits, Maximov, Khomskii (JLTP 1972)*

McMillan Strong Coupling

(Computationally implemented by Wierzbowska, et al., cond-mat/0504077, 2006)

$$T_c = \frac{\Theta}{1.45} \exp\left[-\frac{1.04(1+\lambda)}{\lambda-\mu^*(1+0.62\lambda)}\right]. \qquad (18)$$

$$\lambda = 2\int \frac{d\omega\, \alpha^2(\omega) F(\omega)}{\omega} = \frac{N(0)\langle \mathcal{I}^2\rangle}{M\langle\omega^2\rangle}, \qquad (23)$$

$$\alpha^2(\omega) F(\omega) = \int_S \frac{d^2p}{v_F} \int_{S'} \frac{d^2p'}{(2\pi\hbar)^3 v_{F'}} \sum_\nu g_{pp'\nu}{}^2 \delta(\omega-\omega_{p-p'\nu}) \Big/ \int_S \frac{d^2p}{v_F}, \qquad (19)$$

where the integral $\int d^2p$ is taken over the Fermi surface and the electron-phonon matrix elements are given by[14]

$$g_{pp'\nu} = (\hbar/2MNV\omega_{p-p'\nu})^{1/2} \mathcal{I}_\nu(p, p'), \qquad (20)$$

where $\mathcal{I}_\nu(pp')$ is the electronic matrix element of the change in the crystal potential $\mathfrak{U}$ as one atom is moved:

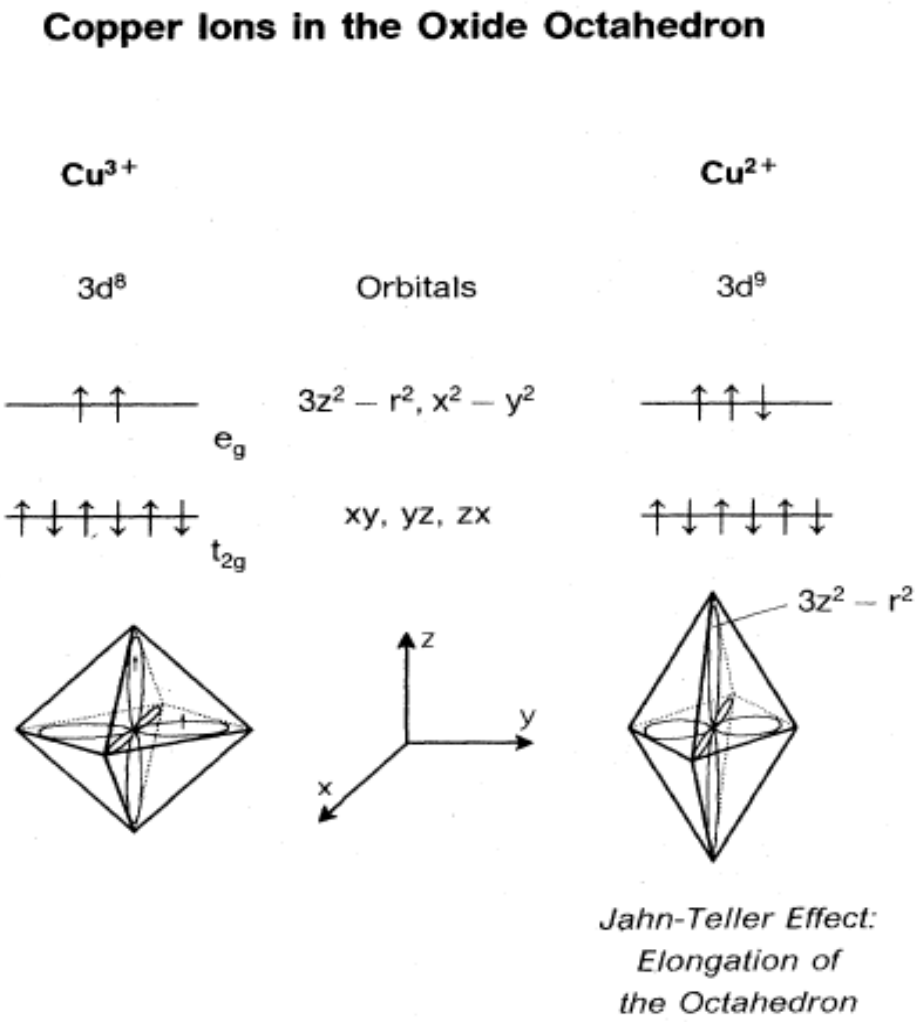
$$\mathcal{I}_\nu(pp') = \int \psi_p{}^*(\varepsilon_{p-p'\nu} \cdot \nabla\mathfrak{U})\psi_{p'} d\mathbf{r}. \qquad (21)$$

What's the HTSC equivalent?

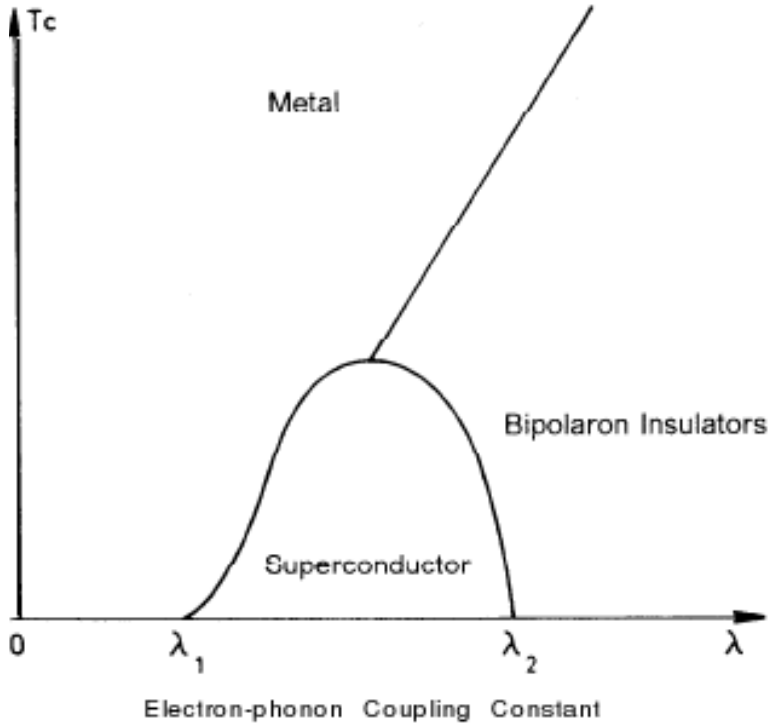
Well!
What do I "move?"

Phonons?

Bednorz-Mueller Nobel Lecture



Jahn-Teller Effect: Elongation of the Octahedron

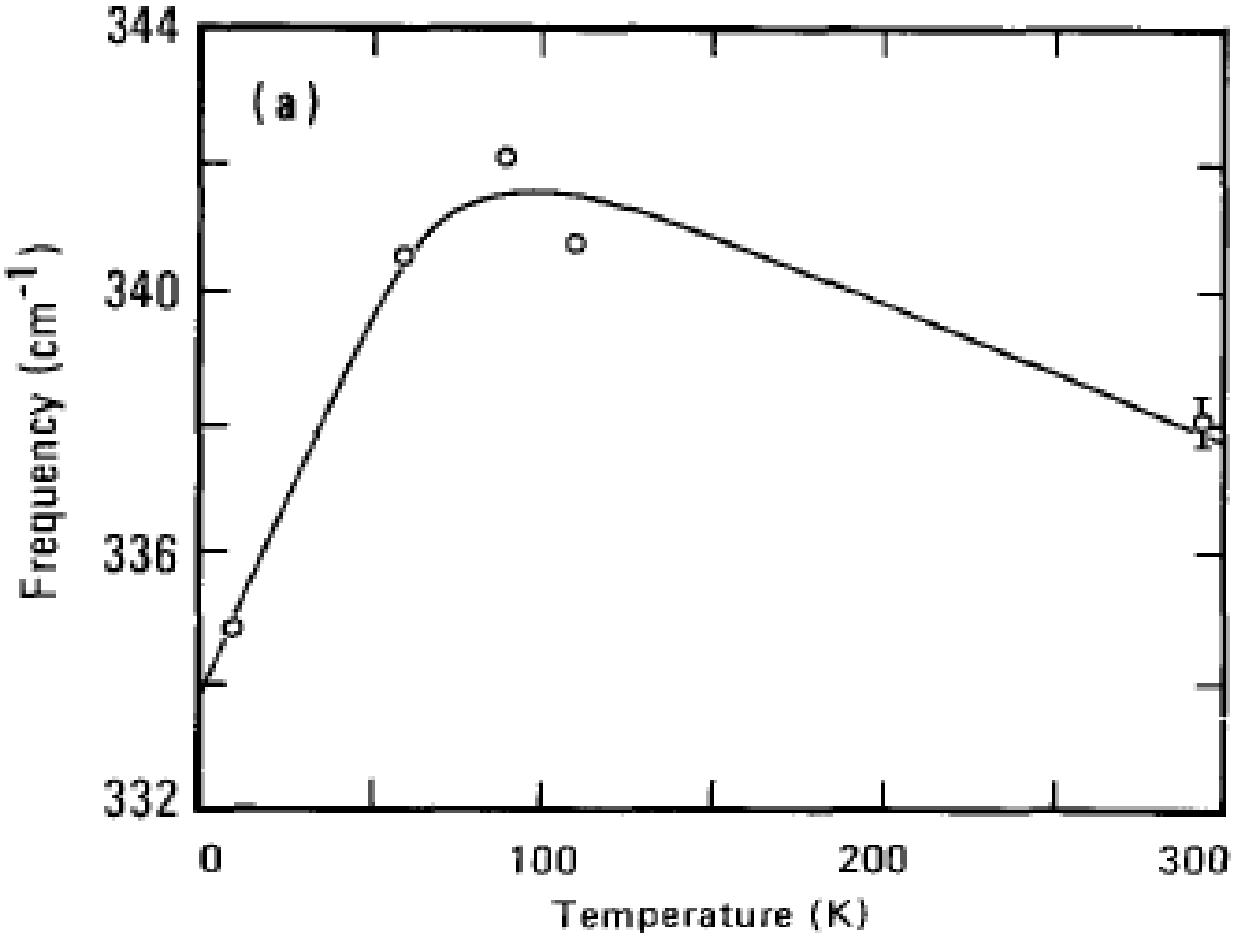


After Chakravarty, (1979)

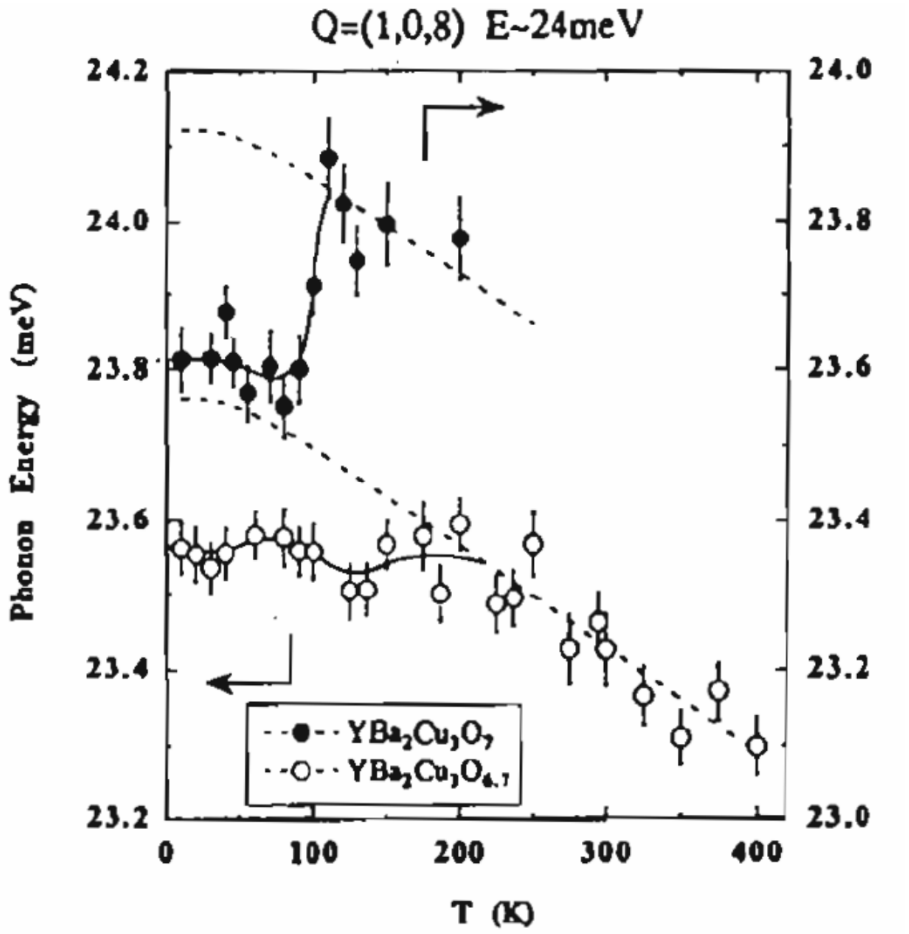
Indeed, they're there!

Macfarlane, Rosen, Seki, SSC 63, 831 (1987)

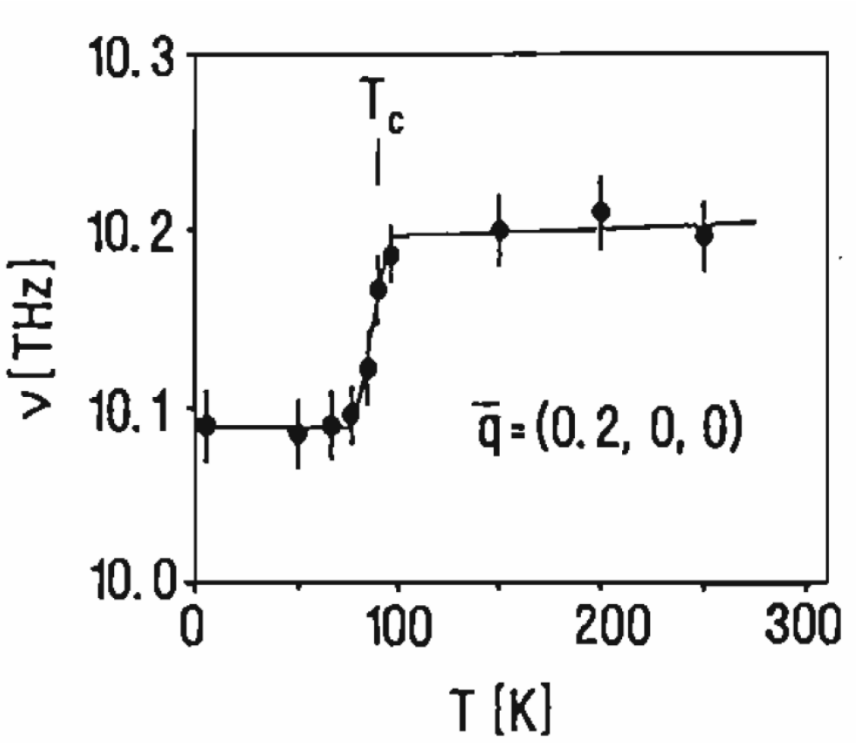
Raman Spectroscopy of YBCO



More Evidence



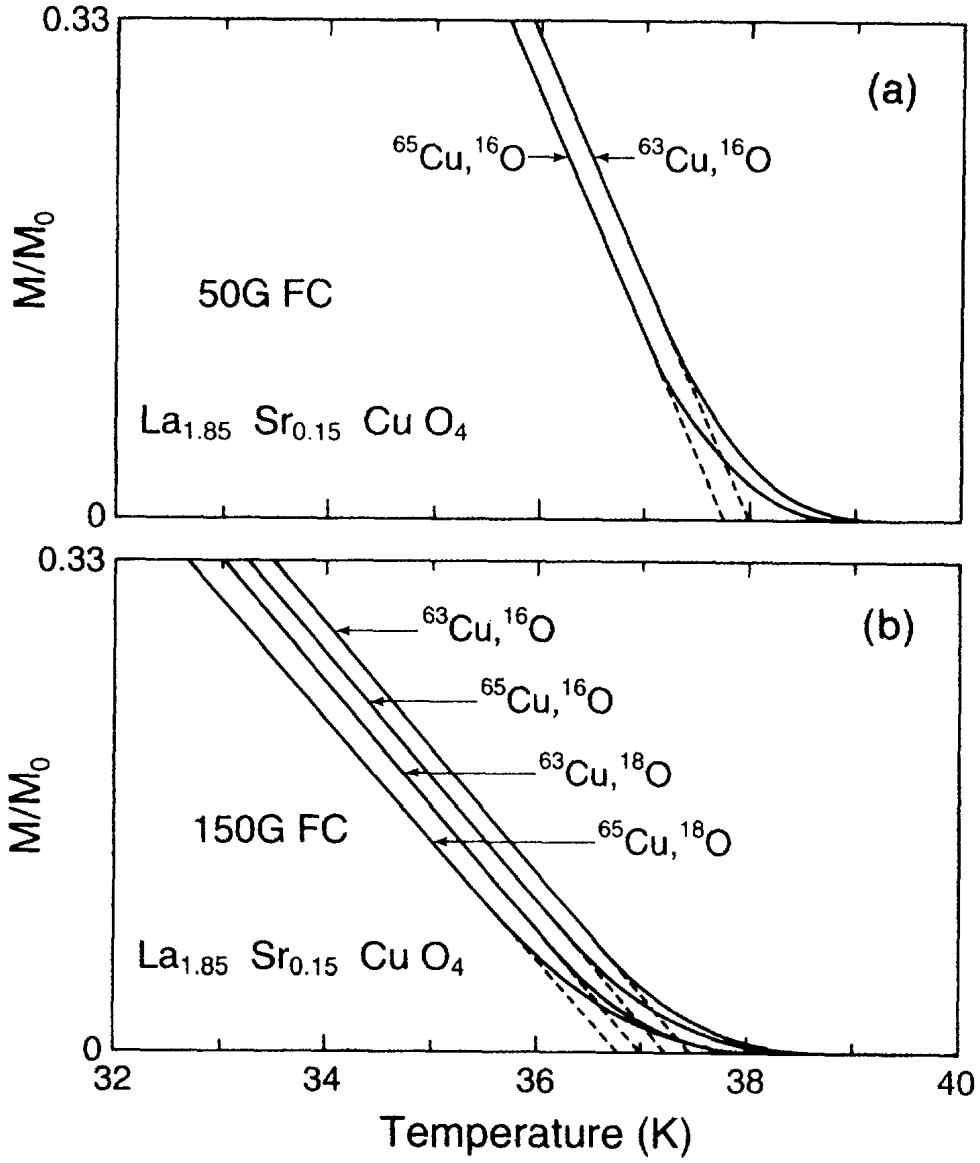
Harashima, et al., Physica C263, 257 (1996)



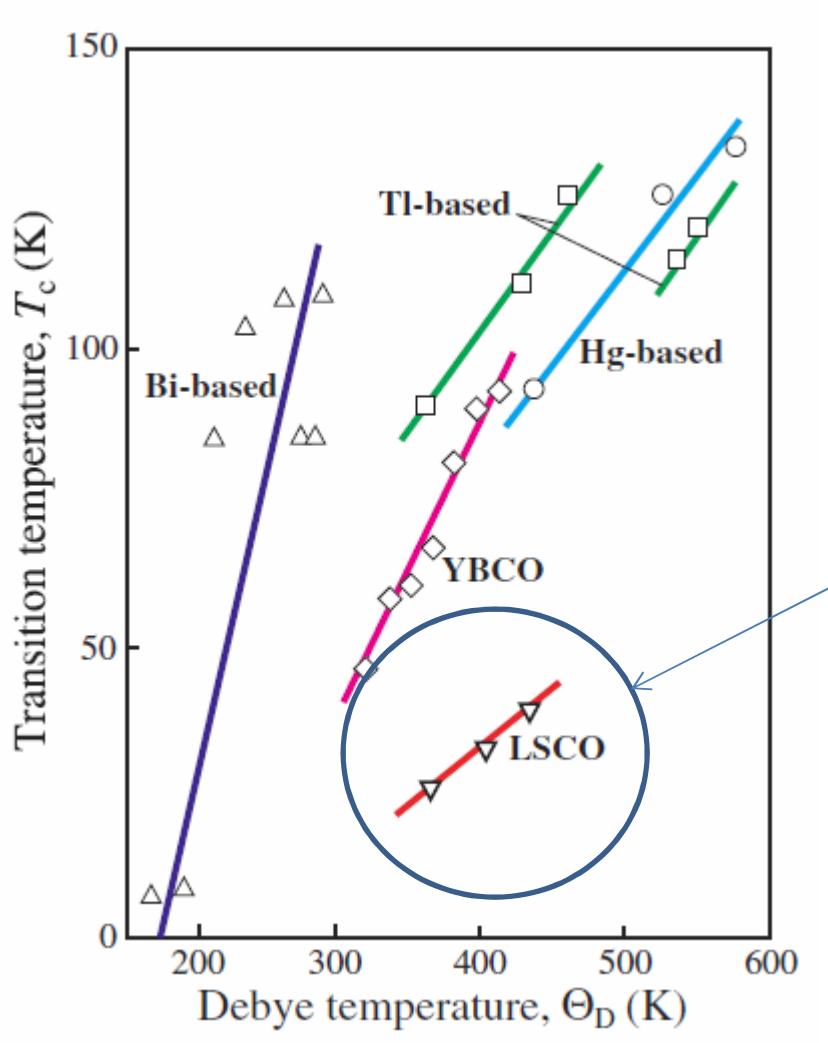
Pyka, et al., PRL 70, 1457, (1993)

Copper and Oxygen Isotope Effects in $La_{2-x}Sr_xCuO_4$

J. P. Franck,[1] S. Harker,[1] and J. H. Brewer[2]



Finally, T_C scales (roughly) with Θ_D



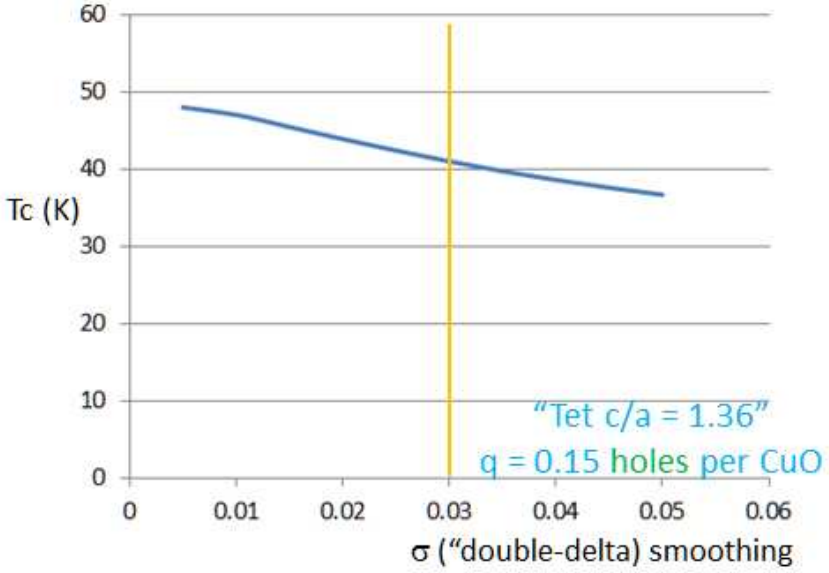
Nota Bene!

Ledbetter, Physica C 235, 1325 (1994)

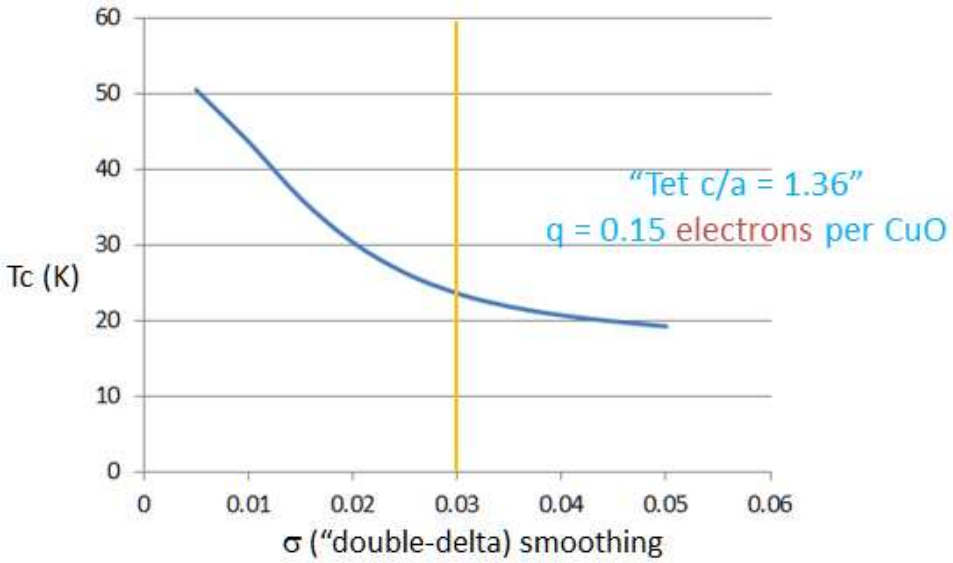
Eliashberg-McMillan-Allen-Dynes

$\Theta_D \approx 440$ K, $\mu^* \approx 0.05$

Holes

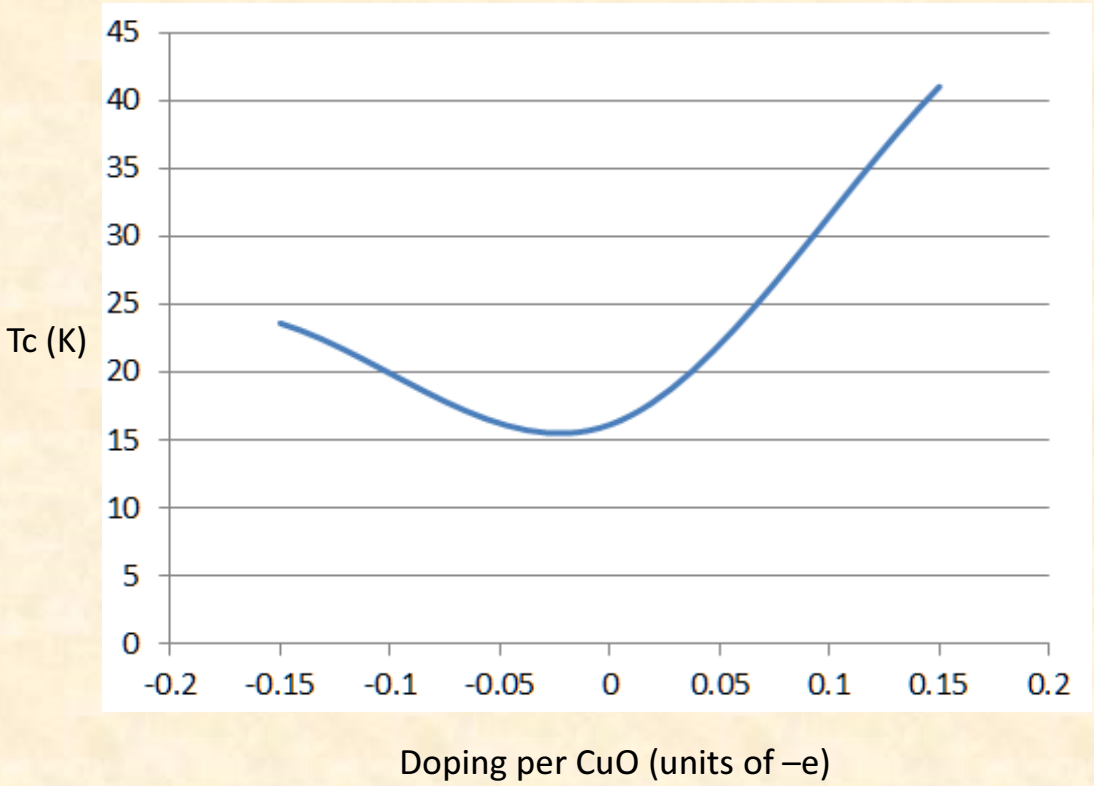


Electrons



Note Differences
in Tc Scale

Conclusions



- Phonons can yield “credible” values of Tc in the cuprates
- Holes are better than electrons
- Can’t account for higher Tc’s in “1-2-3 +” layered compounds (Yet...but stay tuned!)

Computers and the Study of Proxy Structures may finally resolve the mystery of High-Tc...a Future NP for someone in the audience...much younger than me!

The End