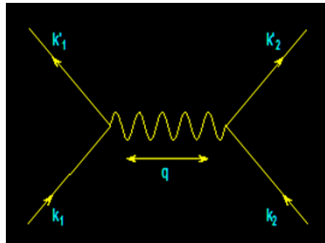
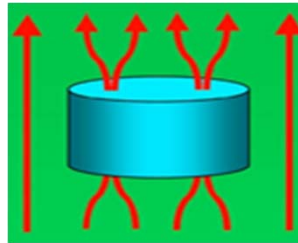


Opening...

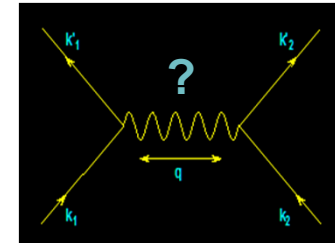
**From
Electrons
Paired**



**To
Electric
Power**



**...And...
Back
Again**



**-- A Personal Journey in Superconductivity --
-- IBM, EPRI, and Beyond --**

**Paul M. Grant
www.w2agz.com**

AGING IBM PENSIONER

IBM Almaden Research Center
650 Harry Road
San Jose, CA

ARC Auditorium
10:30AM – 11:30AM
Friday, 6 May 2011

PMG Timeline

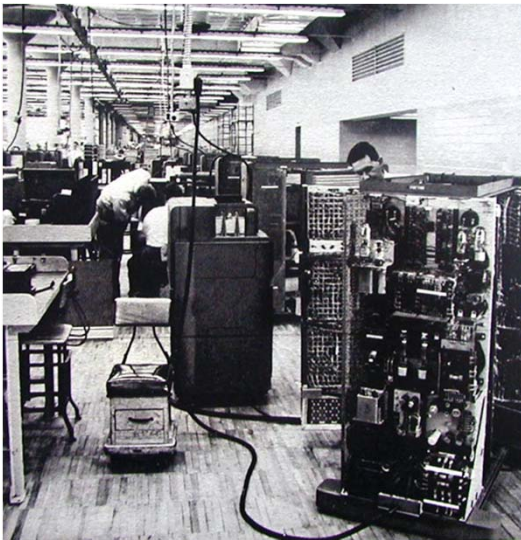
- IBM (1953-1993)
 - Project SAGE (IBM, MIT, USAF) (1953-56)
 - IBM Education Plan (1956-65)
 - San Jose/Almaden (1965-90)
 - Sabbatical @ UNAM (1990-93)
- EPRI (1993-2004)
 - Science Fellow (Superconductivity, Power Electronics Devices, Fusion, “Novel Concepts”)
- W2AGZ Technologies (2004-?)
 - Visionary Energy Societies (SuperCity, SuperSuburb, SuperGrid)
 - “Due Diligence” Consulting
 - **Uncovering the Nature of HTSC !**

IBM

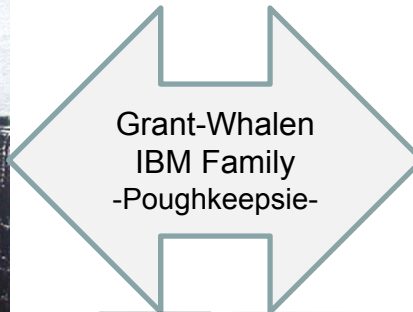
IBM – 100 Years



1952



604 (1948)



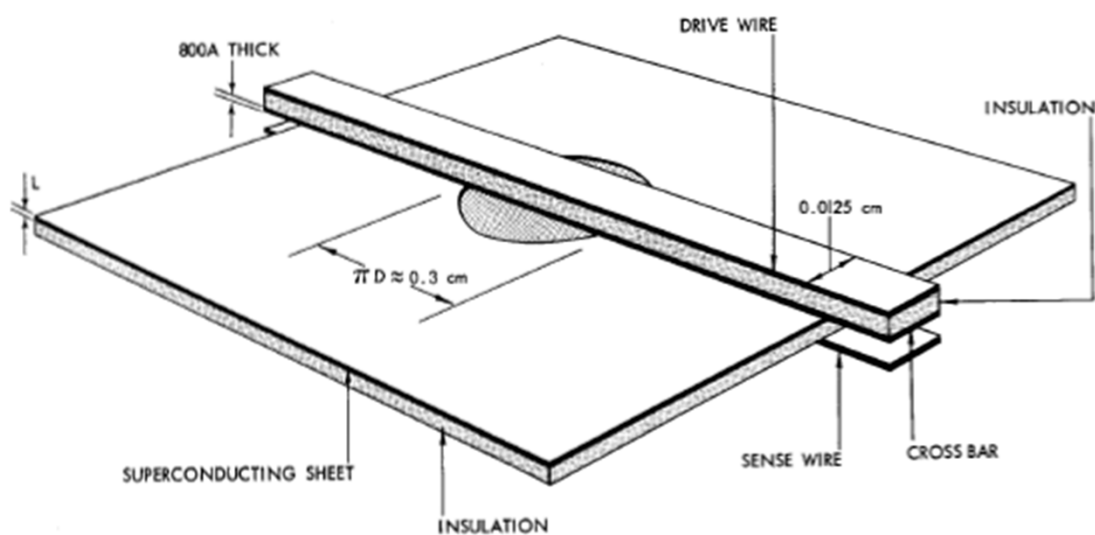
701 (1952)

1953
Project Sage – IBM/MIT



Trapped-Flux Superconducting Memory*

Abstract: A memory cell based on trapped flux in superconductors has been built and tested. The cell is constructed entirely by vacuum evaporation of thin films and can be selected by coincident current or by other techniques, with drive-current requirements less than 150 ma. The short transition time of the trapped-flux cell indicates its possible use in high-speed memories. The superconductive film memory does not exhibit the problems of "delta noise" in core memories resulting from the difference in half-select pulse outputs.



Out into the Cold: Early Experiences with Superconductivity

by Dr. Paul Michael Grant, W2AGZ Technologies, w2agz@w2agz.com, www.w2agz.com



The following article is part of a year-long series celebrating the 100th anniversary of the discovery of superconductivity. Contact CSA if you have ideas for submissions: theresa@cryogenicsociety.org.



One of my earliest memories was watching my parents ice skate on frozen Wappingers Pond where they had taken me swimming for my first time only a few months before. The mid-Hudson Valley was, and still is, notorious for its temperature extremes, the river itself usually completely freezing over between its banks. In mid-winter the outside temperature could approach -50°F (-46°C , 228K). I was reminded of the rigors and discomfort of my boyhood cold climate experiences this past July at ICEC-ICMC held in Wrocław, Poland, as one of a group of attendees who underwent a "cryotherapy" session at a nearby spa, where "room temperature" was approximately -100°C . Thomas Wolfe was wrong...You can go home again!

Ice was the base cryogenics technology of my childhood years throughout the early 1940s, delivered daily, sawdust covered, in carts drawn by horses due to the wartime rationing of gasoline for automobiles and trucks [1]. Household refrigeration didn't really arrive for working class folks until after WWII. However, while I was in grammar school, although we didn't have formal science classes, we had occasional "science demonstrations," usually conducted by engineers from the nearby IBM plant. I remember two in particular, one on something called "dry ice," really cold to the touch, which just sat there and smoked and didn't melt; the other by a gentleman who brought what looked like a large thermos bottle containing "liquid air" into which was dunked a tomato, which was then withdrawn and struck with a hammer, shattering it as if it were glass. Pretty impressive to a seventh grade male (~1948).

My next encounter with cryogenics didn't occur until I was 18. My high school grades were atrocious, to put it mildly, not good enough to get me into college, and I did not want to go anyway—I wanted a job so I could buy a car. So I did what Wappingers Falls boys usually did: I went to work at IBM, first setting pins in the employee bowling alley and then as a mail boy in the mail room of a new IBM lab in downtown Poughkeepsie. I really wanted to be a bench technician, so between delivery runs I hung out with the engineers. One day one of them called to me, "Hey, kid. Come over here and I'll show you something really cool." (He didn't actually say "cool.") His name was Jim Crowe [2].

Jim splattered some solder on his bench top, scraped it off, cut out a small rectangle with his "dikes," wired it in series with a flashlight battery and a resistor of unknown (to me) size, and also hooked up in parallel with leads to a Hewlett-Packard vacuum tube voltmeter. Next to his bench was a huge stainless steel container which Jim told me held liquid helium, saying it was the coldest substance known to man. He dropped the wired up solder chip through a small opening in the top of the "dewar" and we watched the voltage across it slowly drop...and then suddenly disappear! At the time, I knew enough about electricity and Ohm's Law to complain, "The leads must have come off!" Jim said, "No, that's 'superconductivity'." The resistance of the lead-tin in the solder goes away under liquid helium." I thought to myself, "Yeah, sure!"

That evening I had dinner at home with another IBM engineer, my dad. I told him about my experience, and he replied, "Humm. I've heard some talk about making a superconducting computer. But I don't know...you would have to fill up a whole building with liquid helium." This was 1953.

That was my first and last experience with superconductivity for some time to come. Shortly after turning 21, IBM decided I was worth educating and sent me (as an employee!) to college and graduate school for nine years, and I wound up with a physics doctorate from Harvard (superconductivity was not taught at Harvard in the early 60s!). IBM assigned me to the San Jose, now Almaden, Research Lab, and in 1972, Rick Greene (now at UMD) and I teamed up to start working on organic metals as possible room temperature superconductors, both of us having become disciples of Bill Little's

dream that properly prepared polymeric chains might exhibit really high (> 500K) superconductivity, and in 1975 the group indeed discovered the world's first 300 degree superconductor, the inorganic polymer polysulfur nitride...alas, the units were millikelvin!



Paul Grant at 17. This photo shows him about six months before he went to work for IBM.

In 1986, 25 years ago, Bednorz and Mueller taught us we should have been spending our time looking at layered copper oxide perovskites instead.

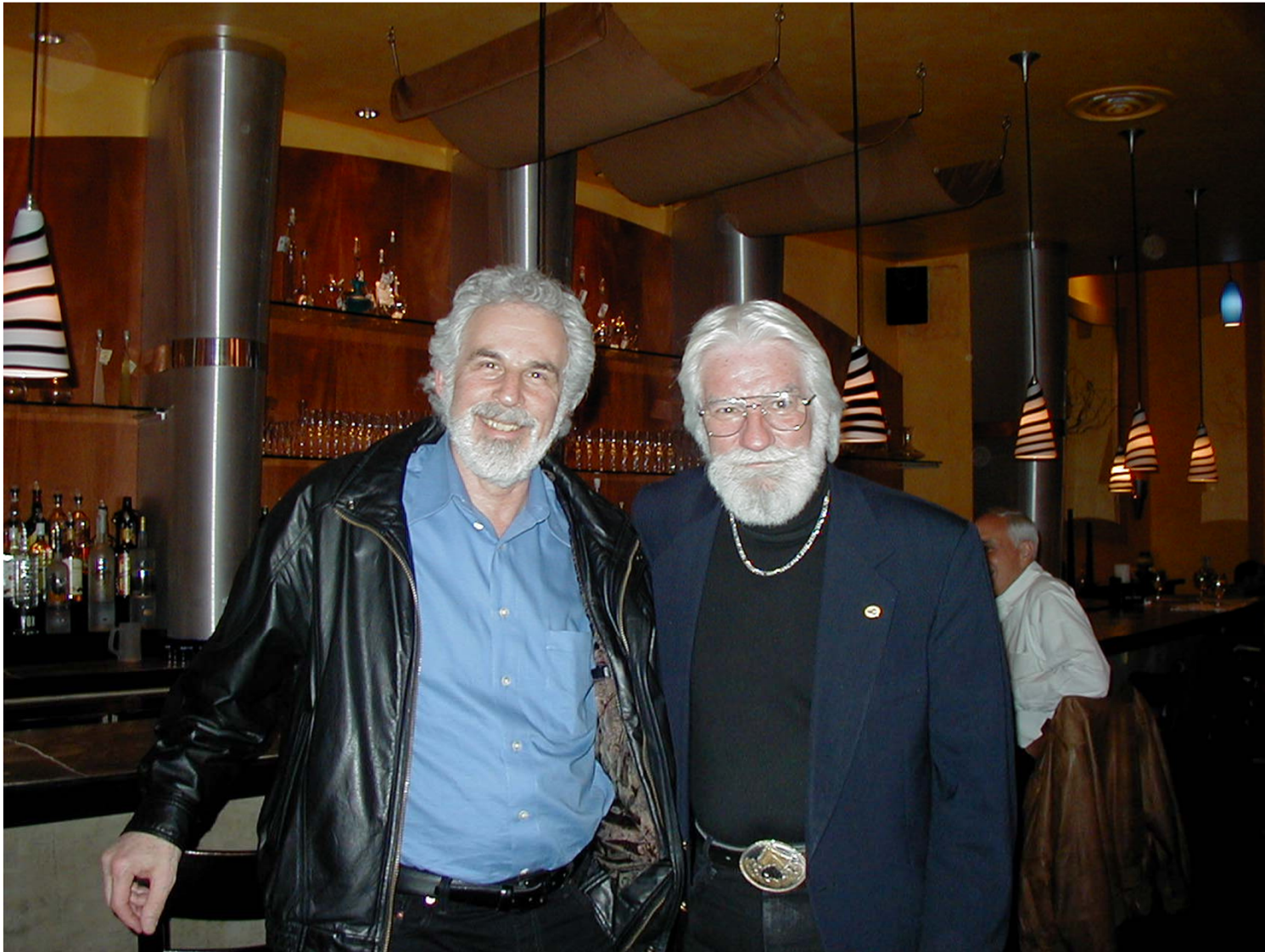
Nevertheless, I remain an ardent fan of the Little/Ginzburg exciton-mediated BCS-pairing proposal to enable superconductivity well above 300K. In 1998, I wrote a "sci-fi" piece for *Physics Today* predicting its fulfillment by 2028 [3]. Maybe then I can finally come in from the cold.

References

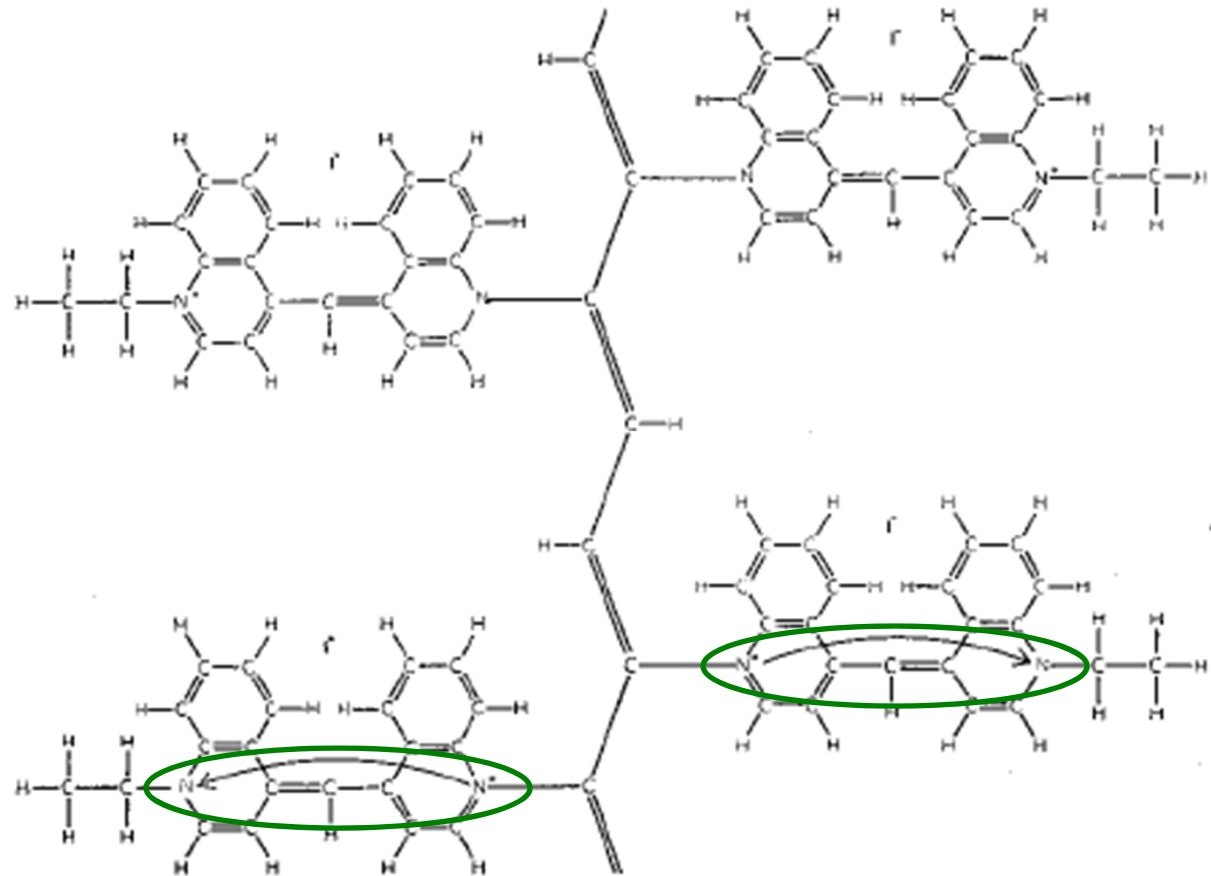
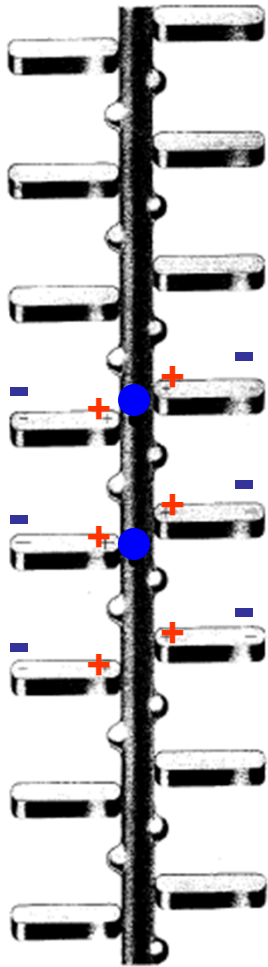
1. A fascinating tale of pre-industrial cryogenics technology can be found in Gavin Weightman's book, "The Frozen Water Trade," (ISBN 0-7868-6740-X), the story of two New England brothers who "farmed" almost every northeastern pond and lake each winter to cool the cocktails of Caribbean resorts in the 19th century.
2. Jim Crowe invented one of the very first superconducting memory elements, and arguably the first to employ trapped flux. See J. W. Crowe, "Trapped-Flux Superconducting Memory," *IBM Journal*, October 1957, p. 295. Jim Crowe became a good friend, mentor and my manager when I returned to work at IBM summers during my college years.
3. P. M. Grant, "Researchers Find Extraordinarily High Temperature Superconductivity in Bio-Inspired Nanopolymer," *Physics Today*, May 1998. Nineteen more years to go. [http://www.w2agz.com/Publications/Popular%20Science/Bio-Inspired%20Superconductivity,%20Physics%20Today%2051,%2017%20\(1998\).pdf](http://www.w2agz.com/Publications/Popular%20Science/Bio-Inspired%20Superconductivity,%20Physics%20Today%2051,%2017%20(1998).pdf)

G² !

THE BORSCHT BELT BOYS



Little, 1963



Diethyl-cyanine iodide

“Bill Little’s BCS”

$$T_C = a\Theta e^{-\frac{1}{\lambda - \mu^*}}$$

Where

Θ = Exciton Characteristic Temperature ($\sim 22,000$ K)

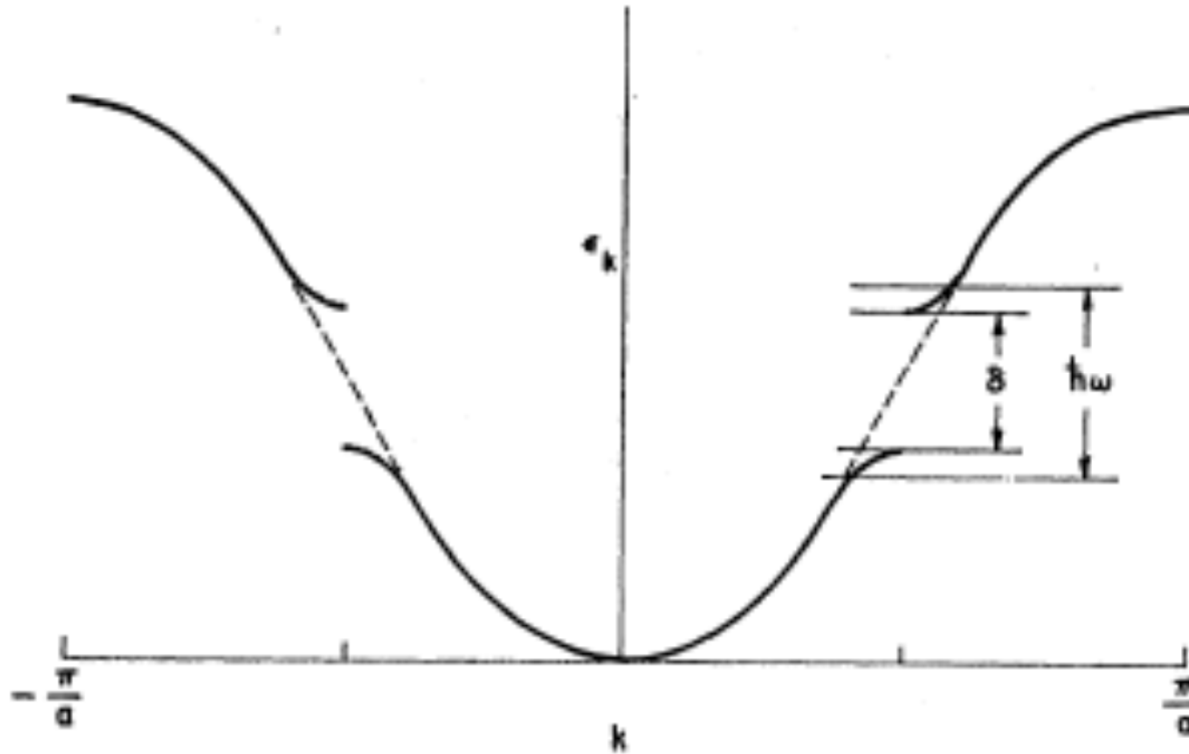
λ = Fermion-Boson Coupling Constant (~ 0.2)

μ^* = Fermion-Fermion Repulsion (?)

a = “Gap Parameter, $\sim 1-3$ ”

T_C = Critical Temperature, ~ 300 K

Spine can be a Semiconductor!



False Alarm:

SUPERCONDUCTING FLUCTUATIONS AND THE PEIERLS INSTABILITY IN AN ORGANIC SOLID*

L.B. Coleman, M.J. Cohen, D.J. Sandman, F.G. Yamagishi, A.F. Garito and A.J. Heeger

Department of Physics and Laboratory for Research on the Structure of Matter,
University of Pennsylvania, Philadelphia, Pennsylvania 19174, U.S.A.

(Received 20 February 1973 by E. Burstein)

Temperature Dependence of the Near-Infrared Optical Properties of Tetrathiofulvalinium Tetracyanoquinodimethane (TTF-TCNQ)

P. M. Grant, R. L. Greene, G. C. Wrighton,* and G. Castro

IBM Research Laboratory, San Jose, California 95114

(Received 13 August 1973)

We report the near-normal-incidence reflectivity spectrum of single-crystal TTF-TCNQ in the range 0.2–2.0 μm . A Drude-like edge, persisting through the metal-insulator transition at 60°K, is observed near 1.3 μm for light polarized parallel to the conducting axis. The temperature dependence of the optical parameters ϵ_0 , τ , and ω_p are discussed in conjunction with Hopfield's relation for the electron-phonon coupling constant.

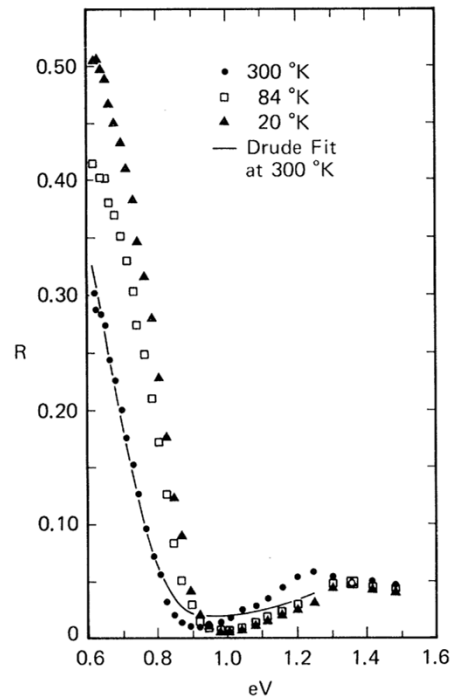


TABLE I. Summary of Drude parameters and the optical conductivity obtained from fitting the data of Fig. 2. At room temperature $\sigma_{\text{dc}} \approx 250 \Omega^{-1} \text{cm}^{-1}$.

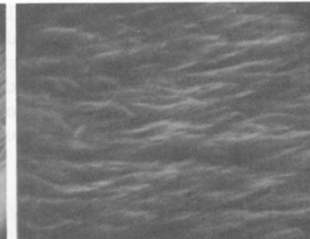
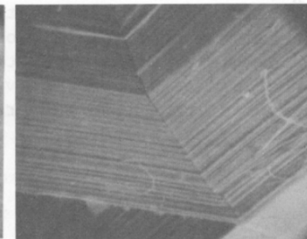
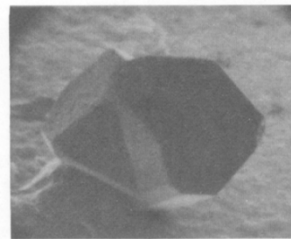
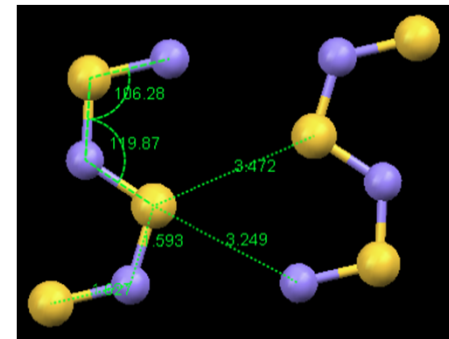
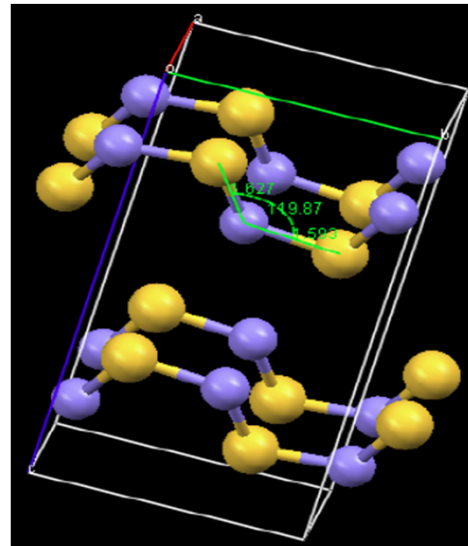
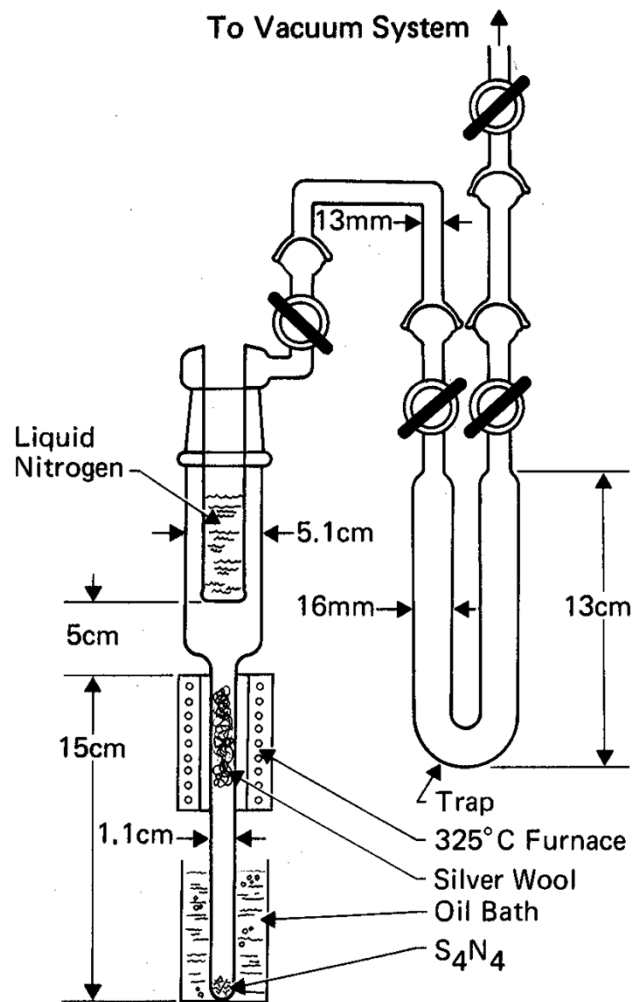
| T (°K) | ϵ_0 | ω_p (eV) | τ (10^{-15} sec) | σ_{op} ($\Omega^{-1} \text{cm}^{-1}$) |
|-------------|--------------|--------------------|-----------------------------|--|
| 300 | 3.3 | 1.38 | 2.3 | 900 |
| 84 | 2.8 | 1.41 | 2.5 | 1020 |
| 67 | 2.9 | 1.44 | 2.7 | 1170 |
| 57 | 3.0 | 1.46 | 3.0 | 1300 |
| 20 | 3.2 | 1.52 | 3.0 | 1430 |

$$\lambda_1 = (\hbar/2\pi kT) \langle \tau_{ep}^{-1} \rangle, \quad \lambda_2 = (\hbar/2\pi k) \omega_p^2 \partial \rho / \partial T.$$

$$\lambda_1 = 1.8, \quad \lambda_2 = 6.1$$

Polysulfur Nitride, (SN_x)

F. B. Burt (1910)
M. Boudeulle (1974)
G. B. Street (1974)



a

b

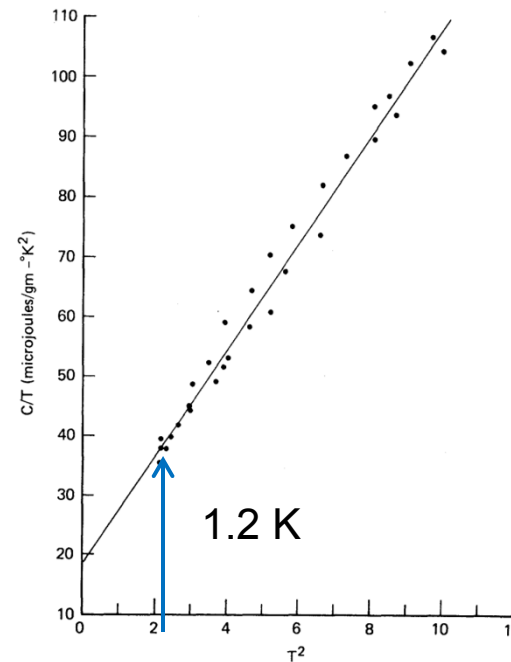
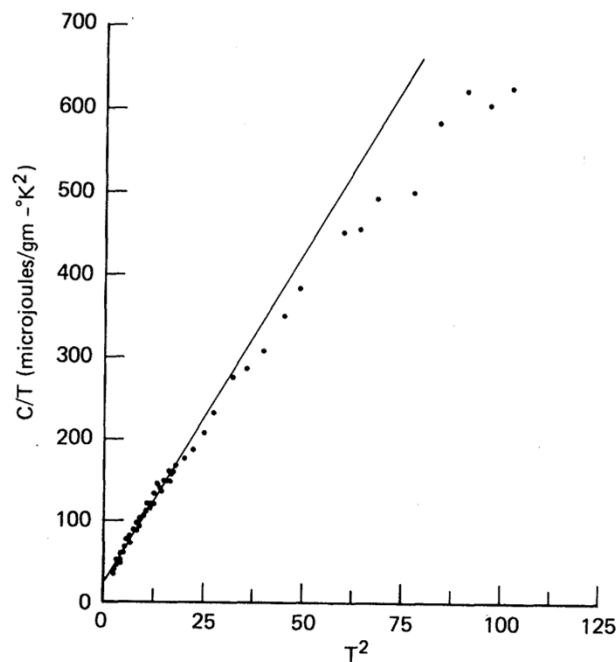
c

Low-Temperature Specific Heat of Polysulfur Nitride, $(\text{SN})_x$

PRL 34, 89 (1975)

R. L. Greene, P. M. Grant, and G. B. Street
IBM Research Laboratory, San Jose, California 95193
(Received 25 September 1974)

Measurements of the specific heat of crystalline $(\text{SN})_x$ in the region 1.5–10°K are reported. A linear temperature contribution to the specific heat is found and interpreted as arising from an electron state density of 0.18 state/(eV spin molecule) and a one-dimensional tight-binding conduction band of width ≥ 0.9 eV. Analysis of the lattice specific-heat contribution supports existing evidence that $(\text{SN})_x$ is a highly anisotropic crystalline polymer and suggests a possible explanation for the apparent absence of a Peierls transition.



Superconductivity in Polysulfur Nitride $(\text{SN})_x$

PRL 34, 577 (1975)

R. L. Greene and G. B. Street

IBM Research Laboratory, San Jose, California 95193

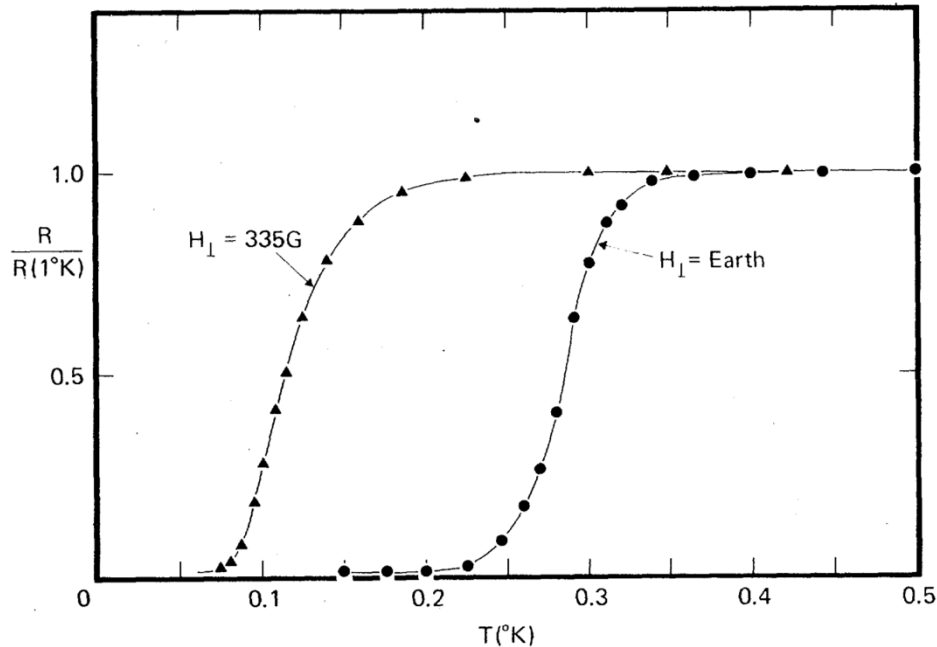
and

L. J. Suter*†

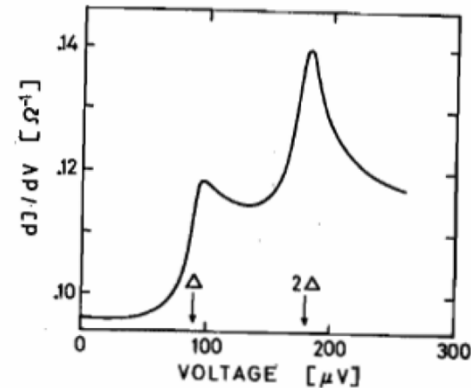
Department of Physics, Stanford University, Stanford, California 94305

(Received 27 January 1975)

The inorganic crystalline polymer polysulfur nitride has been found to become superconducting with a transition temperature of $(0.26 \pm 0.03)^\circ\text{K}$.



Precursor to a Nobel Prize



Tunneling Investigation of Superconducting $(\text{SN})_x$

G. Binnig and H.E. Hoenig

Physikalisches Institut der Universität Frankfurt, Germany

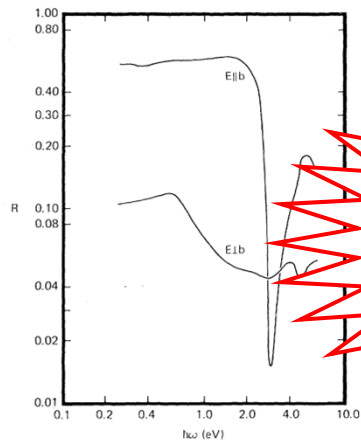
Z. Physik B 32, 23-26 (1978)

Optical Properties of Polymeric Sulfur Nitride, (SN)_x†

PRL 35, 1743 (1975)

P. M. Grant, R. L. Greene, and G. B. Street
IBM Research Laboratory, San Jose, California 95193
(Received 30 June 1975)

We report polarized reflectivity measurements on crystalline (SN)_x in the range of 0.25–6.0 eV. Our analysis of the data gives $\hbar\omega_p = 4.6$ eV and $m^* = 2m_e$, values considerably different from those previously reported by other workers. The data also suggest that (SN)_x has sufficient electronic dimensionality to suppress a Peierls distortion.



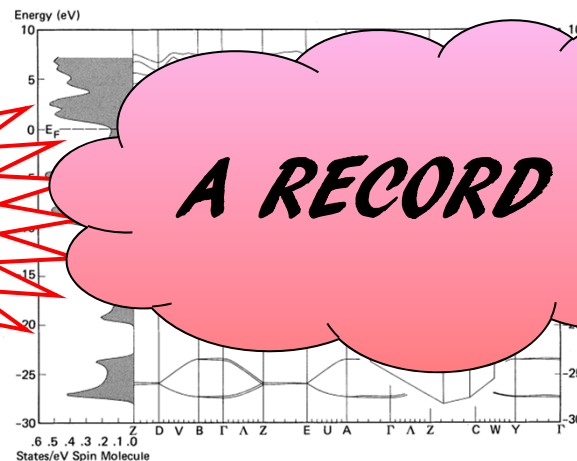
Three
PRLs
In One Month!

Orthogonalized-Plane-Wave Band Structure of Polymeric Sulfur Nitride, (SN)_x

PRL 35, 1799 (1975)

W. E. Rudge and P. M. Grant
IBM Research Laboratory, San Jose, California 95193
(Received 22 September 1975)

We present the first orthogonalized-plane-wave band structures and corresponding densities of states for two reported crystal structures of polymeric sulfur nitride, (SN)_x, and compare our results with experiment. We examine the band structures in light of the low-temperature stability of the metallic and superconducting states in (SN)_x and conclude that this stability derives from closed Fermi surfaces introduced by electronic interchain coupling.



A RECORD ?

X-Ray-Photoelectron-Spectroscopy Determination of the Valence Band Structure of Polymeric Sulfur Nitride, (SN)_x

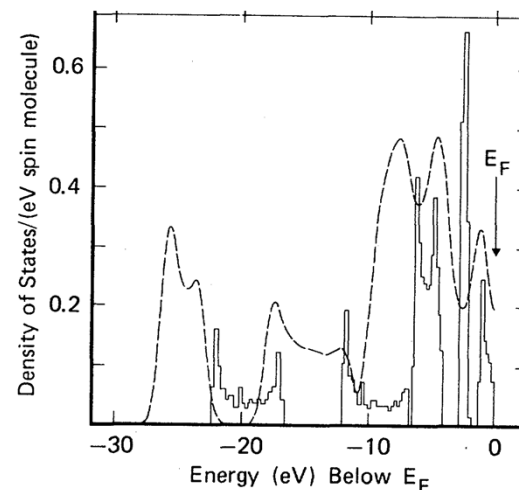
PRL 35, 1803 (1975)

P. Mengel,* P. M. Grant, W. E. Rudge, and B. H. Schechtman
IBM Research Laboratory, San Jose, California 95193

and

D. W. Rice
IBM General Products Division, San Jose, California 95193
(Received 22 September 1975)

We report x-ray photoemission (XPS) measurements on polymeric sulfur nitride, (SN)_x. Both valence-band states and core-level binding energies have been studied. The charge transfer δ in the S⁺ δ N⁻ δ bond is estimated to be 0.30–0.42 electrons. The XPS spectra are compared with densities of states derived from a single-chain tight-binding calculation and also with three-dimensional orthogonal-plane-wave (OPW) calculations based on the two reported (SN)_x crystal structures. Good quantitative agreement is found with the OPW density of states.



ELECTRONIC STRUCTURE AND OPTICAL PROPERTIES OF POLYSULFUR NITRIDE, $(\text{SN})_x$

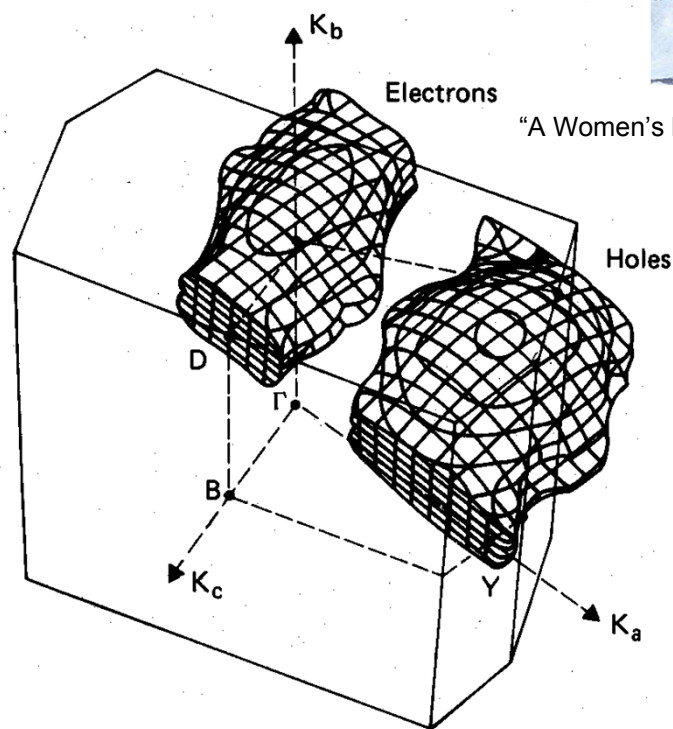
P.M. GRANT, W.E. RUDGE and I.B. ORTENBURGER

IBM Research Laboratory San Jose, California 95193, USA

Two-Band Semimetal

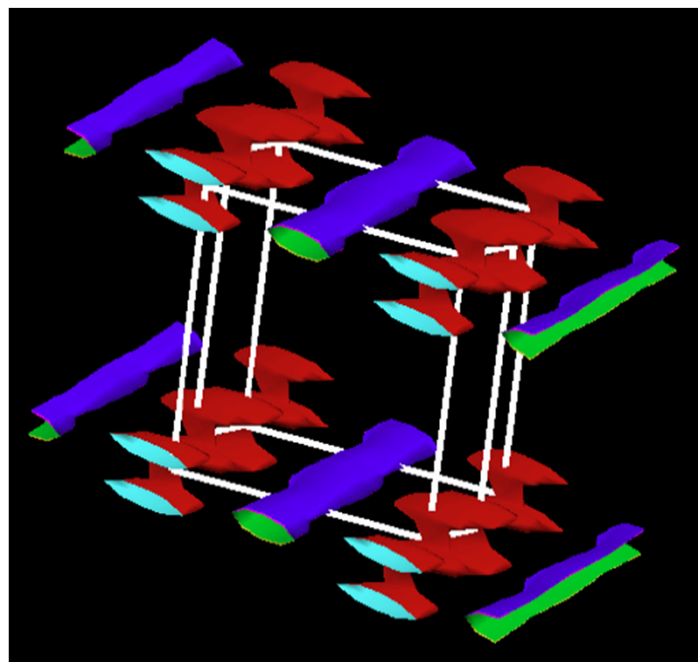
MgB_2 ?
Fe-Pnictides ?

OPW, 1975-6



"A Women's Place is on Top"

Quantum-Espresso, 2009





Solid State Communications, Vol. 29, pp. 225–229.
Pergamon Press Ltd. 1979. Printed in Great Britain.

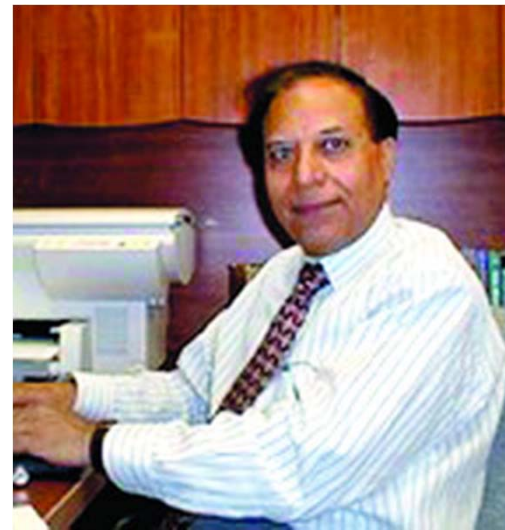
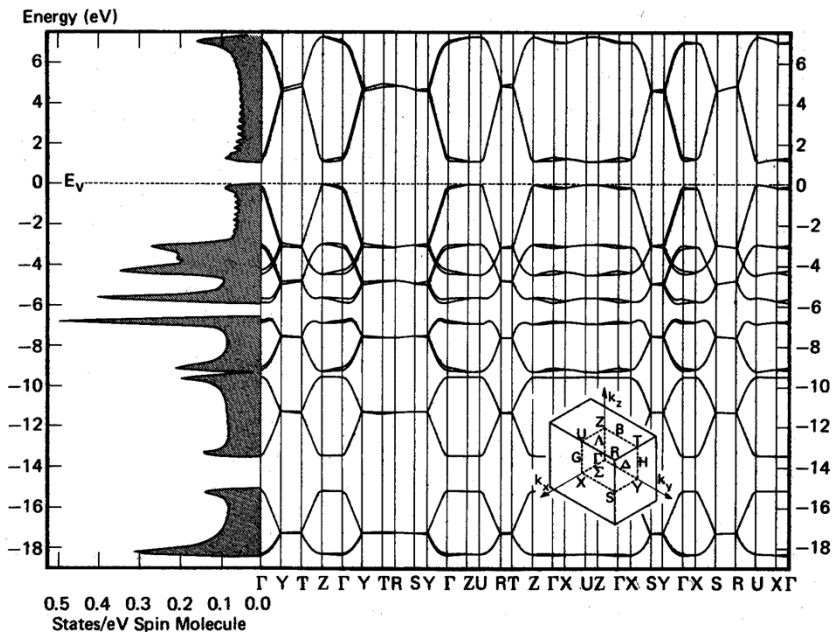
BAND STRUCTURE OF POLYACETYLENE, $(CH)_x$

P.M. Grant and I.P. Batra

IBM Research Laboratory, San Jose, CA 95193, U.S.A.

(Received 17 August 1978 by A.A. Maradudin)

The one-electron energy bands and densities of states of polyacetylene in both *cis*- and *trans*-conformations have been investigated. The principal issue addressed is whether the itinerant picture alone is sufficient to explain the experimental properties of this material. We conclude that the one-electron model provides an excellent zeroth-order explanation of current observations of optical and transport effects in both pure and doped forms of this unusual polymer.



JOURNAL DE PHYSIQUE

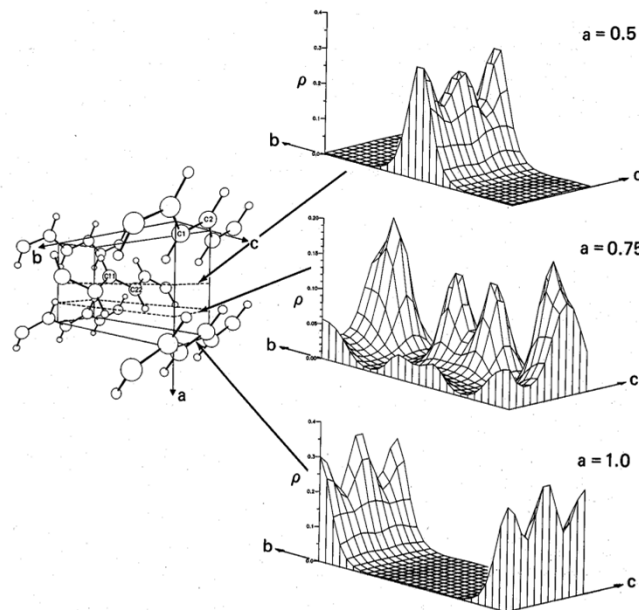
Colloque C3, supplément au n°6, Tome 44, juin 1983

SELF-CONSISTENT CRYSTAL POTENTIAL AND BAND STRUCTURE OF THREE-DIMENSIONAL TRANS-POLYACETYLENE

P.M. Grant and Inder P. Batra

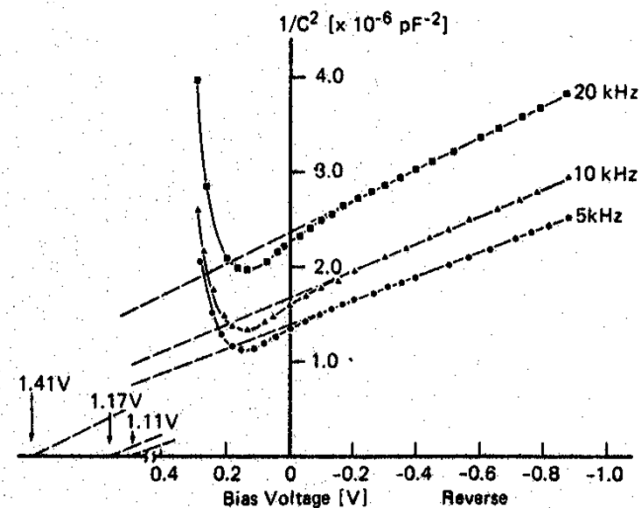
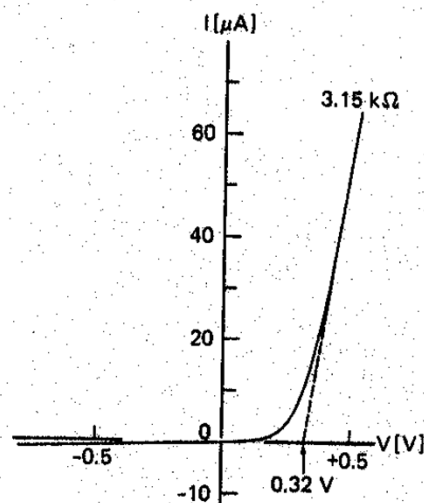
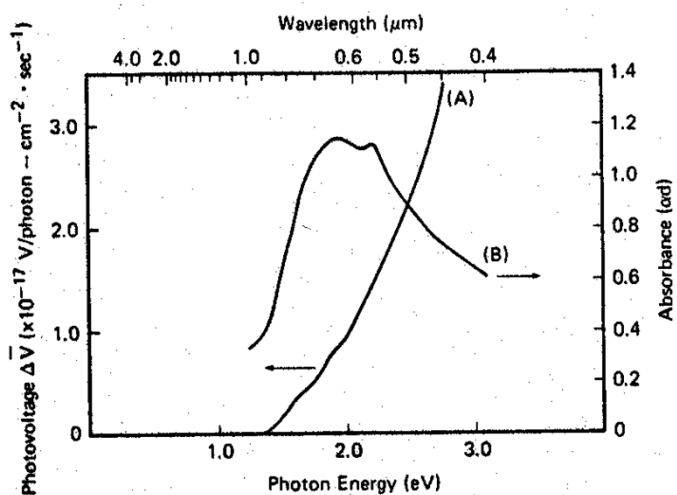
IBM Research Laboratory, 5600 Cottle Road, San Jose, California 95193, U.S.A.

Résumé — Nous avons calculé la structure des bandes à trois dimensions d'un cristal parfait de *trans*-polyacétylène en utilisant une technique self-consistante de pseudopotentiél. Nous avons obtenu la distribution de la densité de charge dans la cellule élémentaire. Nous trouvons que les propriétés à un électron sont extrêmement anisotropes dans le *trans*-polyacétylène. Nous suggérons que les interactions des solitons (ou <<kink>>) entre chaînes pourraient être assez faibles.



PHOTOCONDUCTIVITY AND JUNCTION PROPERTIES OF POLY-ACETYLENE FILMS*·**

T. TANI,[†] W. D. GILL, P. M. GRANT, T. C. CLARKE and G. B. STREET
IBM Research Laboratory, San Jose, Cal. 95193 (U.S.A.)



First paper on polymer electronic and solar devices

Broken-Symmetry Band Structure of Ditetramethyltetraselenafulvalene-X [(TMTSF)₂X]

P. M. Grant

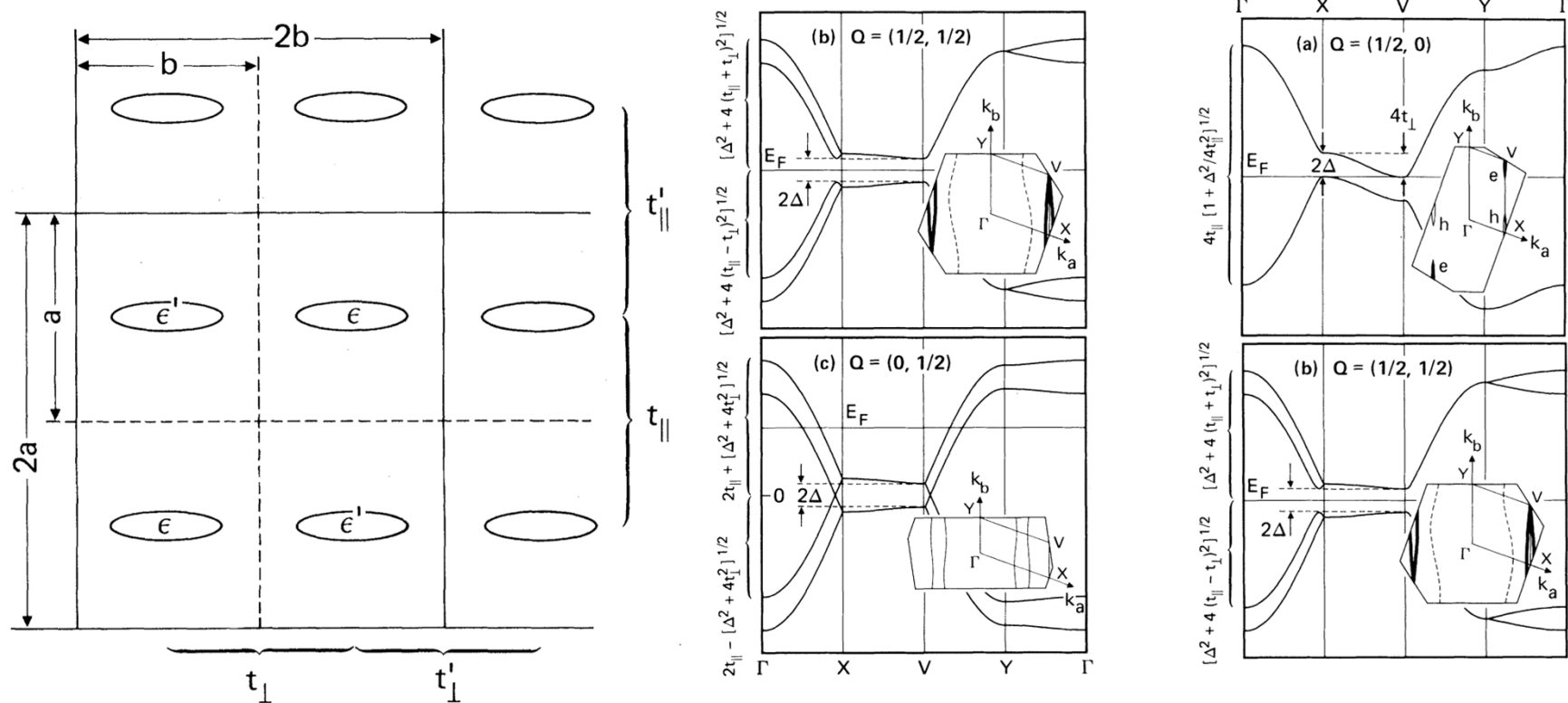
IBM Research Laboratory, San Jose, California 95193

(Received 19 November 1982)

The author derives a set of two-dimensional band structures arising from spin- and/or lattice-induced commensurate symmetry breaking of the high-temperature, ambient-pressure phase of ditetramethyltetraselenafulvalene-X. These band structures are proposed as the framework for many of the low-temperature transport properties of these compounds and are shown to be consistent with experiment in those cases where the broken symmetry condition

Relevant to today's T* - T_C conundrum?

- X =
- PF₆
- AsF₆
- SbF₆
- TaF₆
- ClO₄
- ReO₄
- NO₃



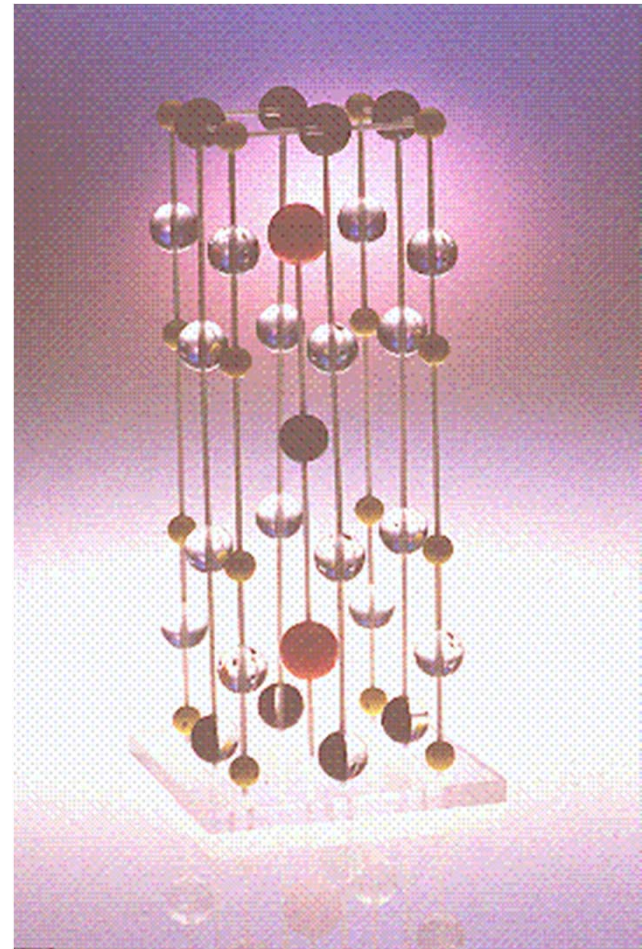
26 February 1987
Back from UCSB



The Almaden 1-2-3 Story: 1986-89



2 March 1987
"1-2-3"



2 March 1987

“1-2-3”



Superconductivity above Liquid Nitrogen Temperature: Preparation and Properties of a Family of Perovskite-Based Superconductors

JACS 109, 2848 (1987)

E. M. Engler,* V. Y. Lee, A. I. Nazzari, R. B. Beyers,
G. Lim, P. M. Grant, S. S. P. Parkin, M. L. Ramirez,
J. E. Vazquez, and R. J. Savoy

IBM Almaden Research Center
San Jose, California 95120

Received March 25, 1987

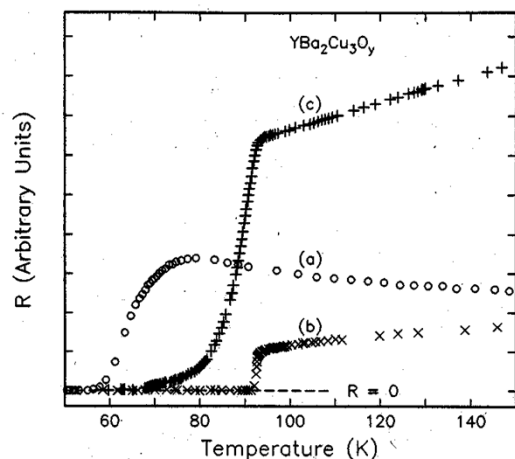


Figure 2. Plot of four-probe electrical resistivity vs. temperature for $Y_1Ba_2Cu_3O_y$ under various preparative conditions: (a) fast removal of pellets from oxygen anneal at 900 °C; (b) slow cooling of oxygen annealed sample from 900 to 200 °C over 5 h; (c) same as (b) except air anneal.

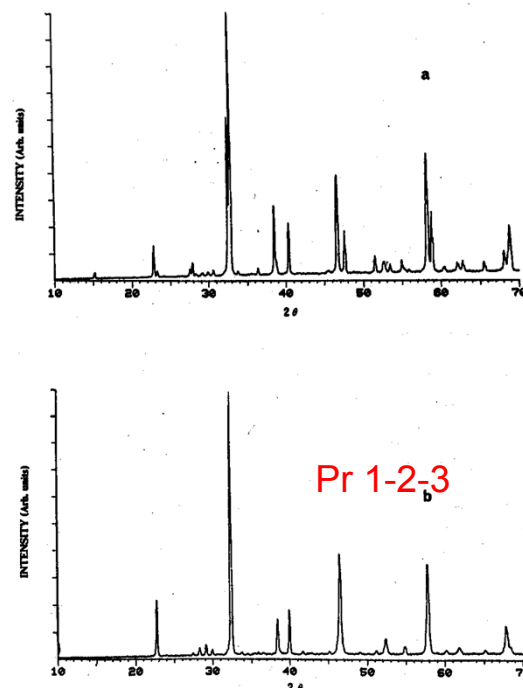


Figure 1. X-ray powder diffraction patterns for (a) $Y_1Ba_2Cu_3O_y$ and (b) $Pr_{1-2-3}Ba_2Cu_3O_y$.

Table I. Superconducting Properties of $Y_1Ba_2Cu_3O_y$ Derivatives

| compd | T onset | T _c (midpoint), K | ΔT _c (90–10% value), K |
|------------------------------|---------|------------------------------|-----------------------------------|
| $YBa_2Cu_3O_y$ | 98 | 94 | 2 |
| $NdBa_2Cu_3O_y$ | 80 | ~45 | ~50 |
| $SmBa_2Cu_3O_y$ | 90 | 85 | 8 |
| $EuBa_2Cu_3O_y$ | 98 | 92 | 1 |
| $GdBa_2Cu_3O_y$ | 92 | 86 | 8 |
| $DyBa_2Cu_3O_y$ | 95 | 91 | 2 |
| $HoBa_2Cu_3O_y$ | 96 | 92 | 1 |
| $YbBa_2Cu_3O_y$ | 93 | 90 | 2 |
| $LuBa_2Cu_3O_y$ | 45 | 32 | ~20 |
| $Y_{0.5}Sc_{0.5}Ba_2Cu_3O_y$ | 94 | 90 | 4 |
| $Y_{0.5}La_{0.5}Ba_2Cu_3O_y$ | 90 | 80 | 10 |
| $Y_{0.5}Lu_{0.5}Ba_2Cu_3O_y$ | 96 | 92 | 1 |
| $YSrCaCu_3O_y$ | 85 | 82 | 3 |
| $YBaSrCu_3O_y$ | 89 | 85 | 1 |
| $YBaCaCu_3O_y$ | 87 | 82 | 1 |
| $YbBaSrCu_3O_y$ | 85 | 81 | 2 |
| $YbBaCaCu_3O_y$ | 85 | 81 | 2 |

17 - 19 March 1987
The Woodstock of Physics



Evidence for Superconductivity in La_2CuO_4

P. M. Grant, S. S. P. Parkin, V. Y. Lee, E. M. Engler, M. L. Ramirez, J. E. Vazquez, G. Lim,
and R. D. Jacowitz

IBM Almaden Research Center, San Jose, California 95120

and

R. L. Greene

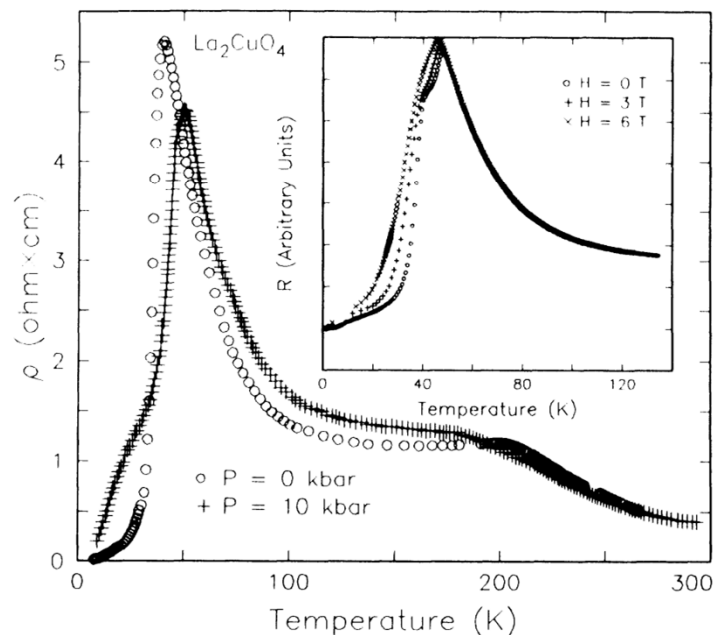
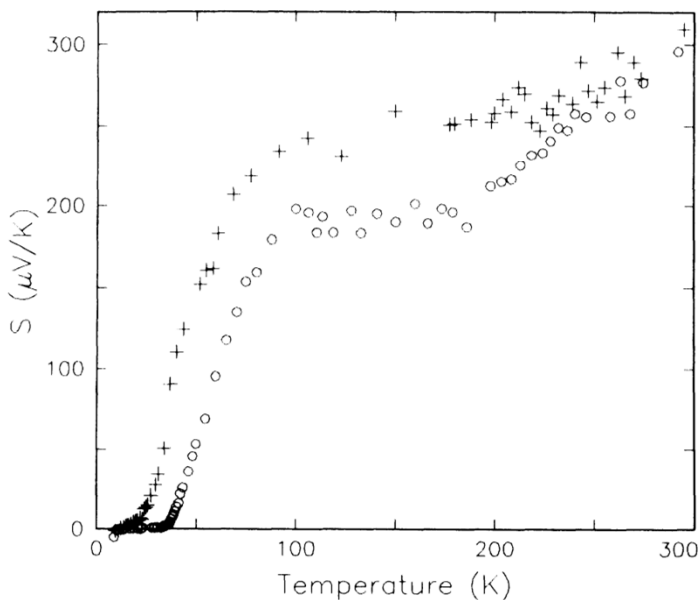
IBM Thomas J. Watson Research Center, Yorktown Heights, New York 10598

(Received 28 April 1987; revised manuscript received 15 May 1987)

We report evidence for superconductivity in undoped La_2CuO_4 obtained from resistivity, thermoelectric power, and susceptibility measurements. The onset temperature is near 40 K and we have deter-

High-Tc could have been discovered in the 1960s !

and can be controlled by oxygen pressure. We discuss several likely sources for the superconducting activity.

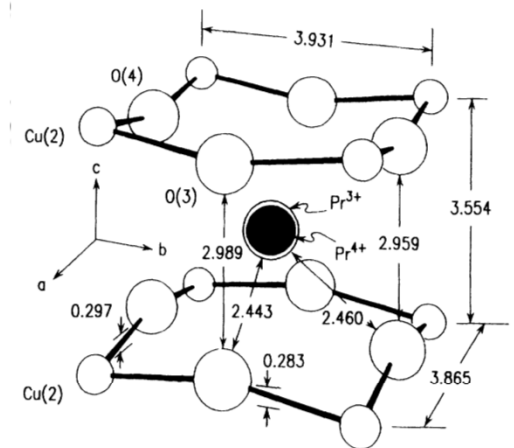
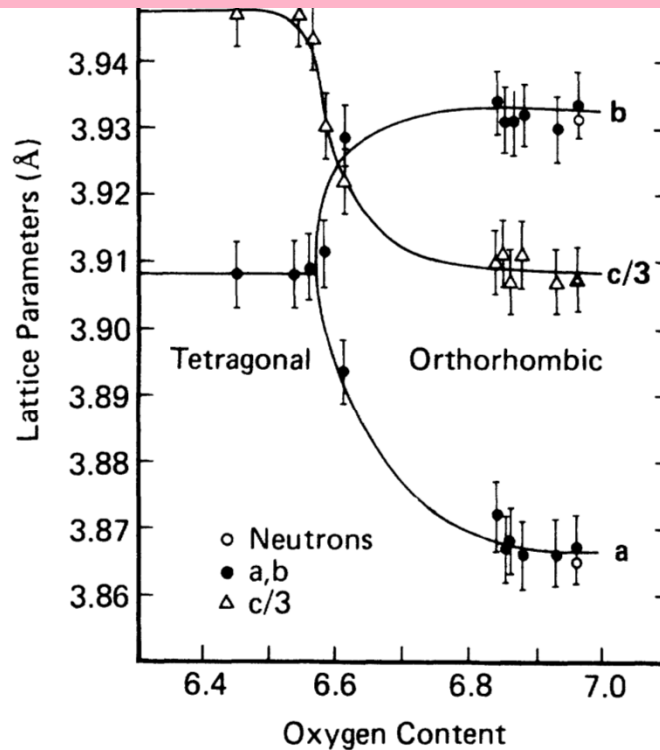
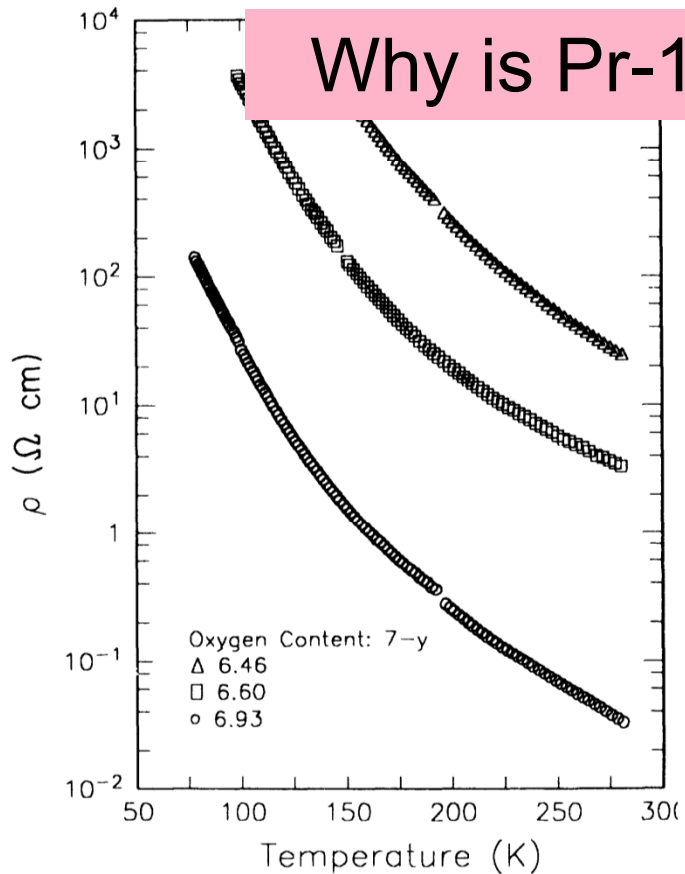


The Praseodymium Paradox

Role of oxygen in $\text{PrBa}_2\text{Cu}_3\text{O}_{7-y}$: Effect on structural and physical properties

M. E. López-Morales,* D. Ríos-Jara, J. Tagüeña, and R. Escudero
Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México,

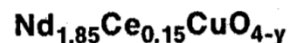
Why is Pr-123 not even a conductor?



A Clue to the mystery of HTSC?

1989: World Record T_C in n-Type T' Copper Oxide Perovskites

THE EFFECTS OF SYNTHESIS AND REDUCTION PROCESSING ON THE PHYSICAL PROPERTIES OF CERAMIC



M. E. López-Morales*, B. T. Ahn,
R. B. Beyers,
and P. M. Grant

IBM Research Division
Almaden Research Center
650 Harry Road
San Jose, California 95120-6099

"Effects of Synthetic Conditions and Reduction Processing on the Physical Properties of Ceramic $\text{Nd}_{2-x}\text{CexCuO}_{4-y}$." M. E. López-Morales, B. T. Ahn, R. B. Beyers and P. M. Grant, *Proceedings of the XI Winter Meeting on Low Temperature Physics (14-17 January 1990, Cocoyoc, Morelos, México): Progress in High Temperature Superconductivity, Vol. 26*, ed. by J. A. Cogordan, E. Sansores, T. Akachi and A. A. Valladares (World Scientific, Singapore, 1991), p. 93.

- Why is T_C so low in the n-types?
- Well?
- Maybe that's another clue to the mystery of High- T_C

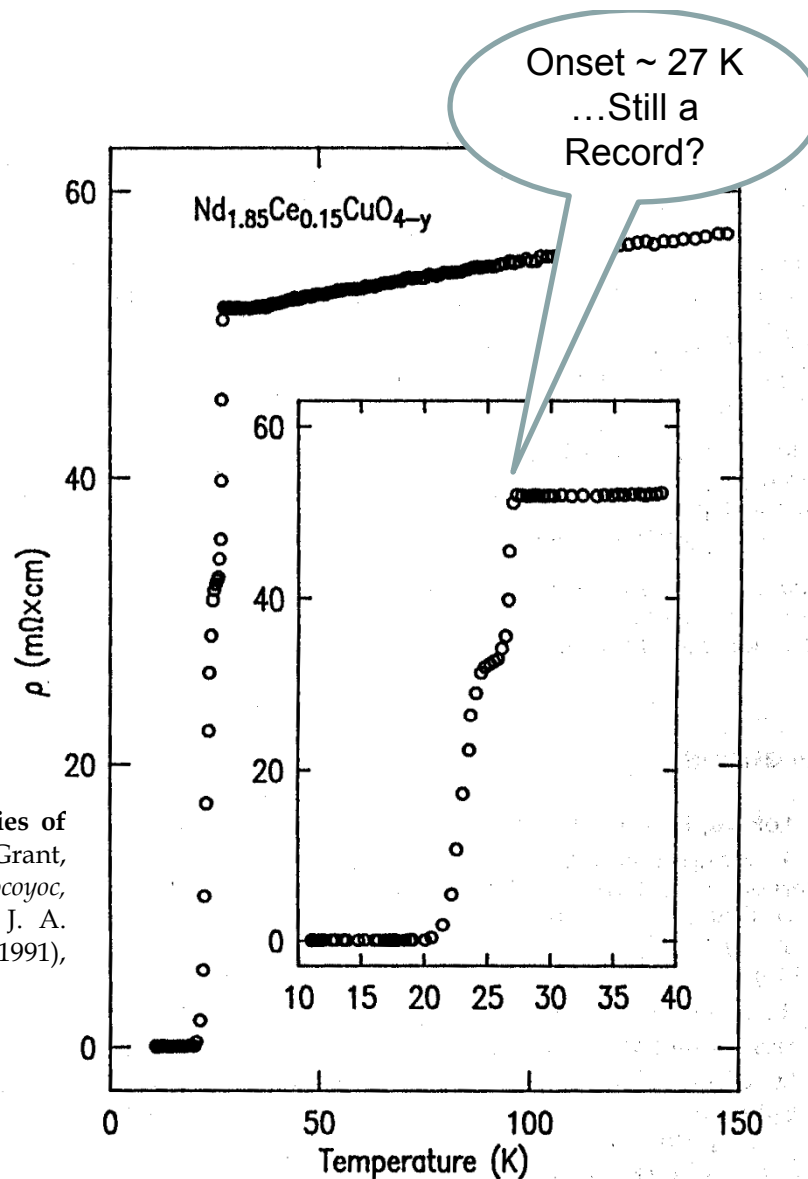


Fig. 2. Temperature dependence of the resistivity of $\text{Nd}_{1.85}\text{Ce}_{0.15}\text{CuO}_{4-y}$

Field Dependence of Diamagnetic Shielding Fraction with Carrier Concentration in HTSCs

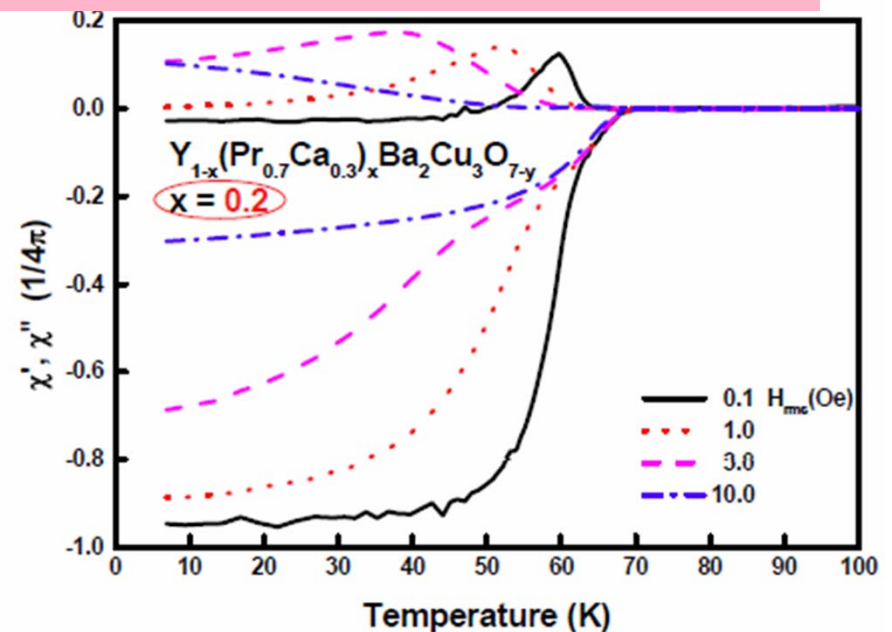
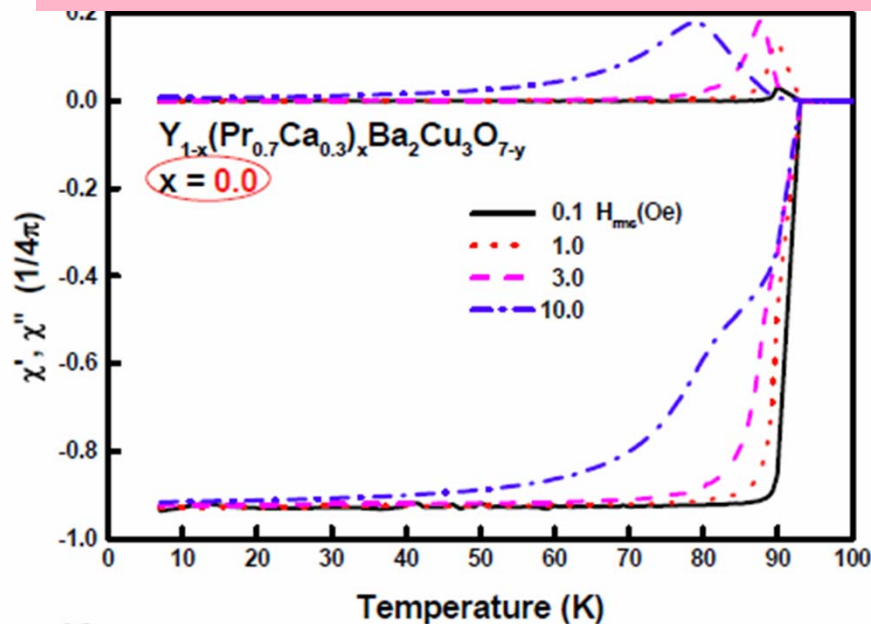
100th Anniversary of APS, Atlanta, GA

*P.M. Grant, W.Y. Lee, A. Nazzari (IBM Almaden Research Center),
M.E. López-Morales (IIM-UNAM)*

Work performed at IBM ARC and IIM-UNAM, May 1992-January 1993

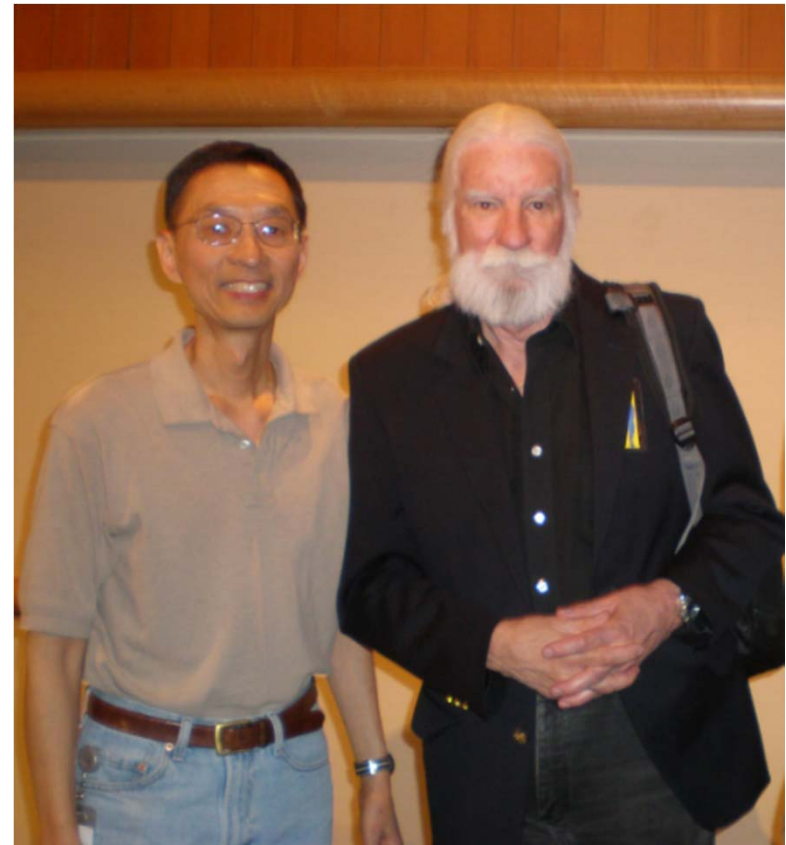
WC25.03: 14:24 24 March 1999

Is this evidence of “electronically granular” superconductivity?
Stripes, perhaps?



Band of Brothers (and a Sister!)

<http://www.w2agz.com/The%20Picture%20Story.htm>



Almaden Superconductivity Scoreboard

- Polysulfur Nitride
 - January, 1976
 - $T_C = 0.3$ K
- “ET” $(\text{BEDT-TTF})_4(\text{ReO}_4)_2$
 - 1982
 - $T_C \sim 2$ K
- Undoped $\text{La}_2\text{CuO}_{4+x}$
 - January, 1987
 - $T_C = 40$ K
- TI-2223 $(\text{Tl}_2\text{Ba}_2\text{Ca}_2\text{Cu}_3\text{O}_z)$
 - February, 1988
 - $T_C = 125$ K
- TI-1223 $(\text{TlBa}_2\text{Ca}_2\text{Cu}_3\text{O}_z)$
 - March, 1988
 - $T_C = 110$ K

IBM RD Scoreboard

| | |
|----------|---|
| Almaden | 5 |
| Zurich | 2 |
| Yorktown | 0 |

Do-it-yourself superconductors

It is extremely easy to make high-temperature superconductors. Schools in the United States and Britain have already produced their own samples. Here is the recipe

Paul Grant



“Shake ‘n’ bake” recipe for 1-2-3 ($\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$)

Mix 1.13 grams yttrium
oxide, 3.95 grams barium
carbonate, 2.39 grams
copper oxide

Compact

Grind in mortar and pestle

Bake in air at 950°C

(1650°F)

Regrind in mortar and
pestle

Press into pellets

Rebake pellets in flowing
oxygen at 950°C (1650°F)

Allow to cool very slowly

Recipe by Heidi Grant

Left: Heidi Grant
demonstrates superconductivity
at the US National Science
Foundation

- Distributed to members of US Congress (at their request)
- 35,000 copies distributed to high schools worldwide by ICTP-Trieste

Rio de Janeiro 4-6 May 1988



Nova 1988

PMG Questioned on Demise of IBM's Josephson
Computer Effort



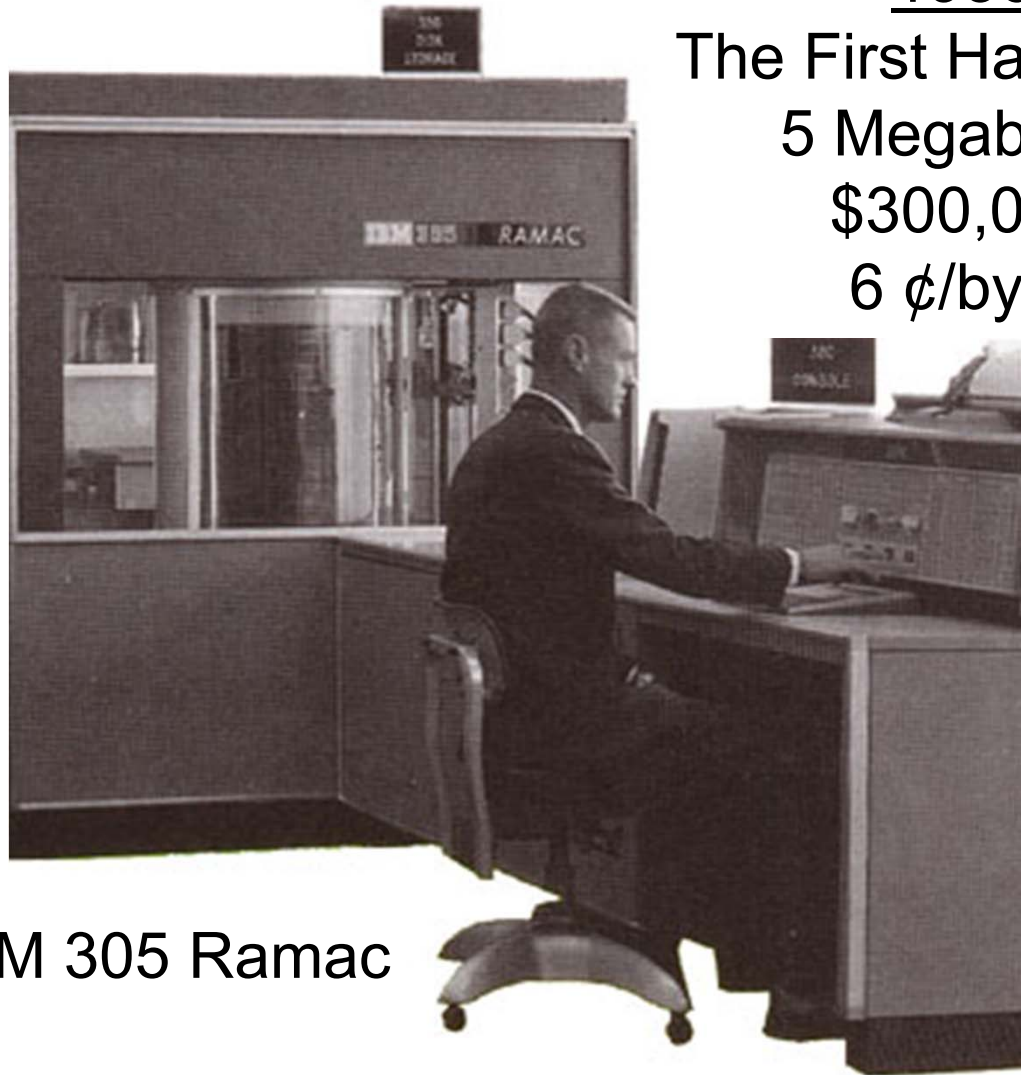
EPRI

...in their shoes...



- Paul Archibald Grant
 - W2AGZ
 - US Navy, WWII
 - IBM, 1948-1974
 - Ski Patrol, 1948-1970
- Mary Ann Whalen Grant
 - CYO BB Champ, 1921
 - NYS Bowling Champ, 1939
 - Women's Baseball, '33-'47
 - CHG&E, 1927-1965

From this...faster, smaller, cooler...and cheaper!



IBM 305 Ramac

1956

The First Hard Drive

5 Megabytes

\$300,000

6 ¢/byte

2011 (+55)

HP Personal Media

2 Terabytes

\$100

5 nano-¢/byte



I got two of 'em!

To this...



...and this...

Texas '03

New York '99

Detroit '00

Chicago '99

Northern California '01

West Coast '96

San Francisco '00

Atlanta '99

Delaware '99

New Orleans '99

...and this!

PUC orders PG&E to let customers opt out of SmartMeter program



The PUC order is a stunning turnabout on a technology that many consider a key to managing energy use in the future. Utilities around the country have installed the electronic meters -- which can be monitored and adjusted wirelessly -- with little incident. But in Northern California, angry residents have expressed concerns that the meters can lead to overbilling and **cause health problems**, and PG&E has struggled to counter the bad publicity.

Bob Park!
Where are you when we need you!

...and...Finally This!

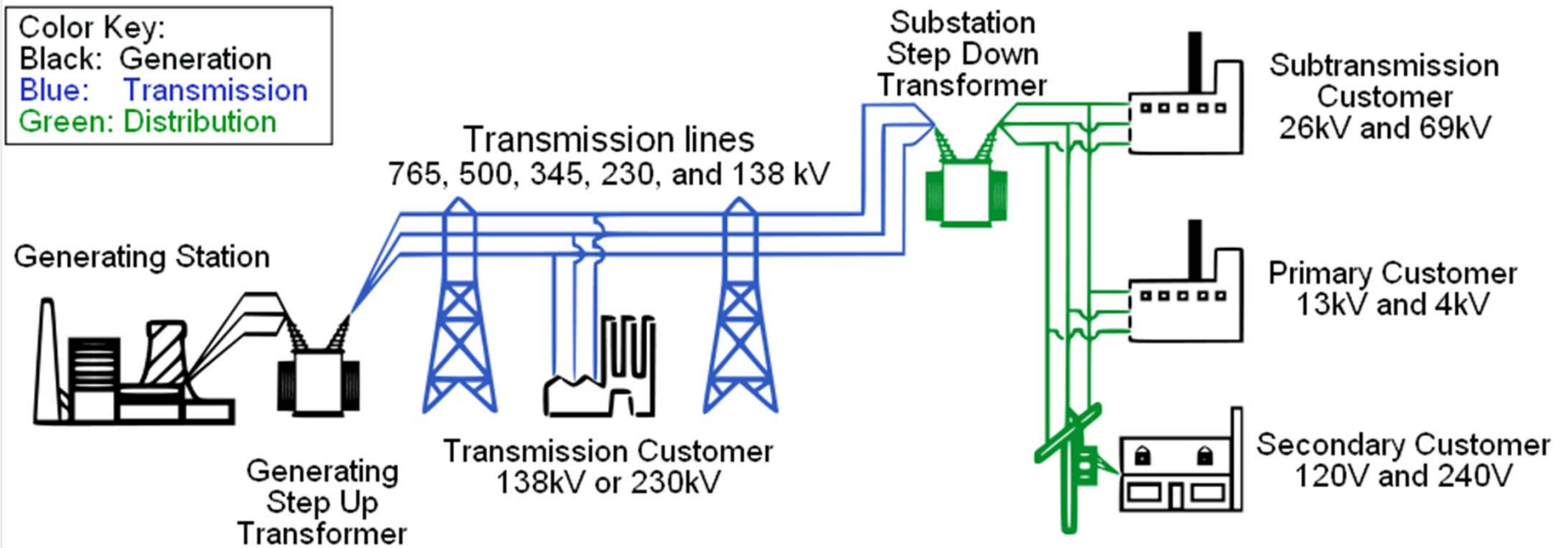


AP/Kyodo News

Blast at Japan nuke plant; thousands missing

Spraying water to cool stressed reactor...Sure. Duh! It's a gas/petrol storage port!

Where Can We Apply Superconductivity to Electric Power?



Potentially Everywhere

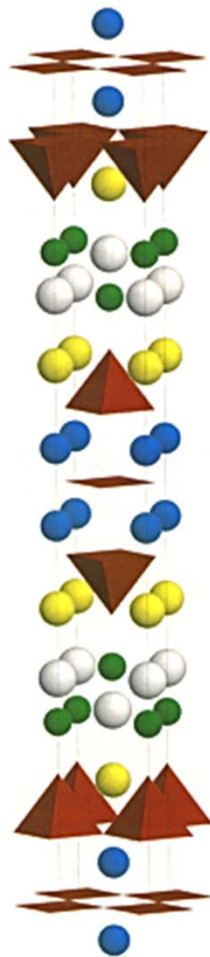
EPRI & Superconductivity

1993-2003 (\$18M)

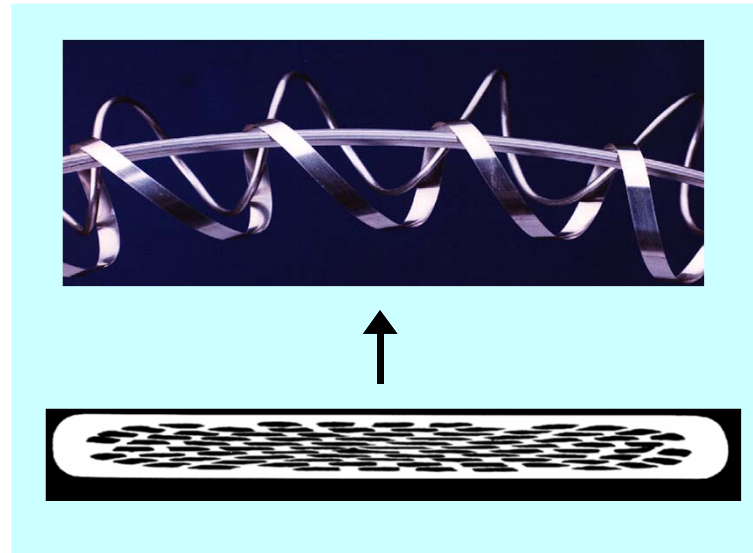
| <u>Universities</u> | <u>Industry</u> | <u>Institutions</u> |
|---------------------|-----------------|---------------------|
| Wisconsin | AMSC* | LANL |
| Stanford | Superpower | LBNL |
| MIT | IBM | ORNL |
| Houston | Pirelli | DOE (Partner) |
| Maryland | Westinghouse | CCAS |
| | Detroit Edison | |
| | | |

*Coated Conductor Alliance (\$4M(EPRI)+\$6M(AMSC))

First HTSC "Wire"



2223



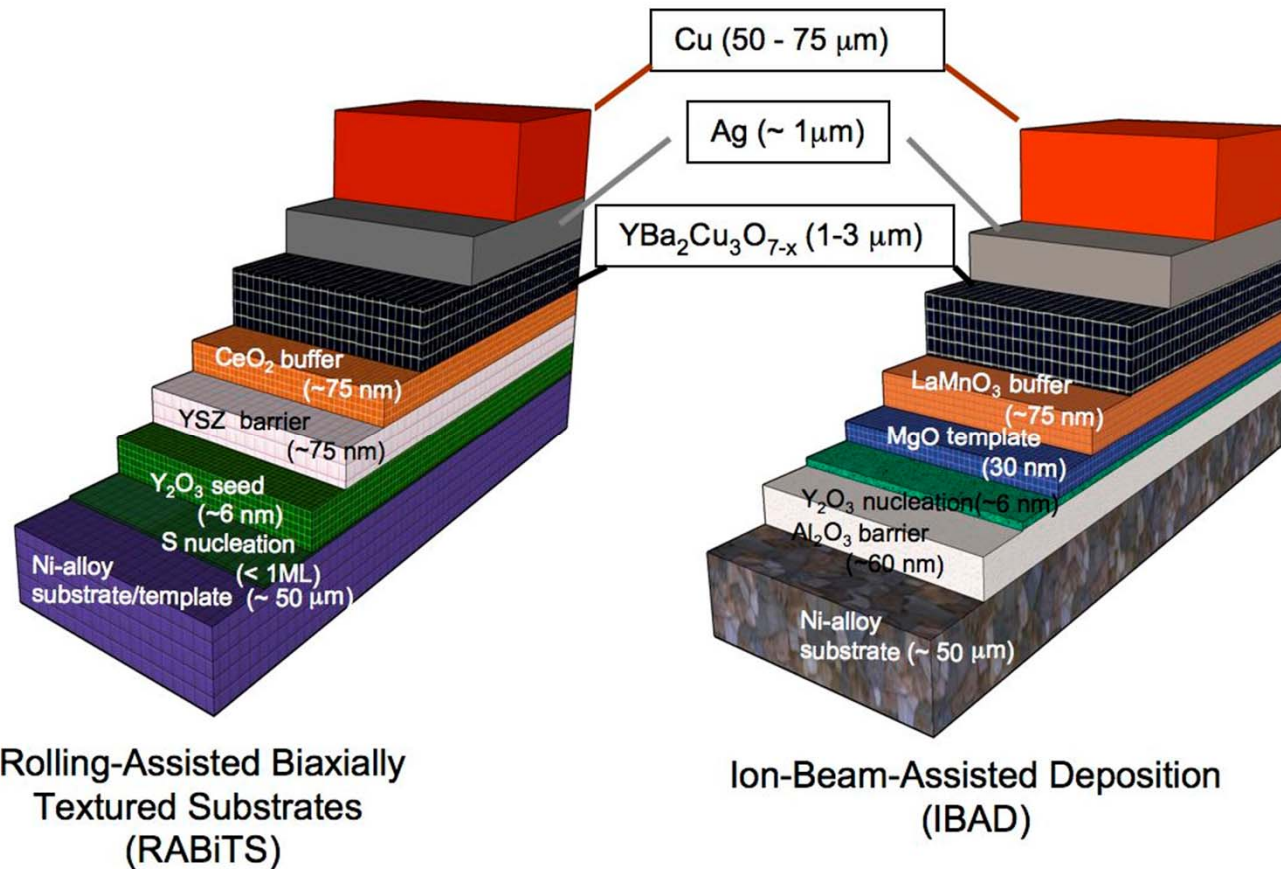
Gen 1



Pirelli



Gen II Coated Conductor



American Superconductor

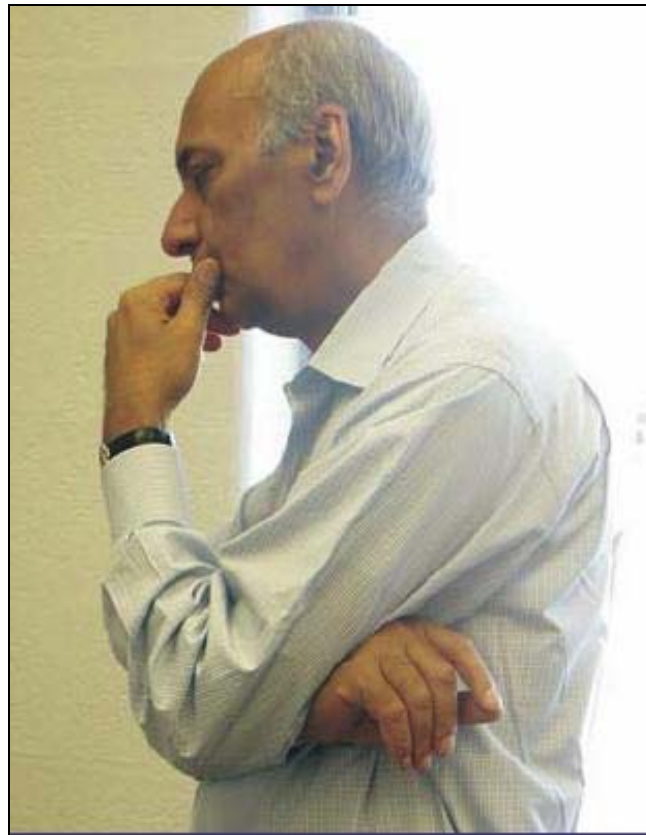
SuperPower

Orientation Dependence of Grain-Boundary Critical Currents in $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ Bicrystals

D. Dimos, P. Chaudhari, J. Mannhart, and F. K. LeGoues

*Thomas J. Watson Research Center, IBM Research Division,
Yorktown Heights, New York, 10598*

(Received 4 May 1988)



Praveen Chaudhari, 1937 - 2010

Physics Today, p.64, April 2010

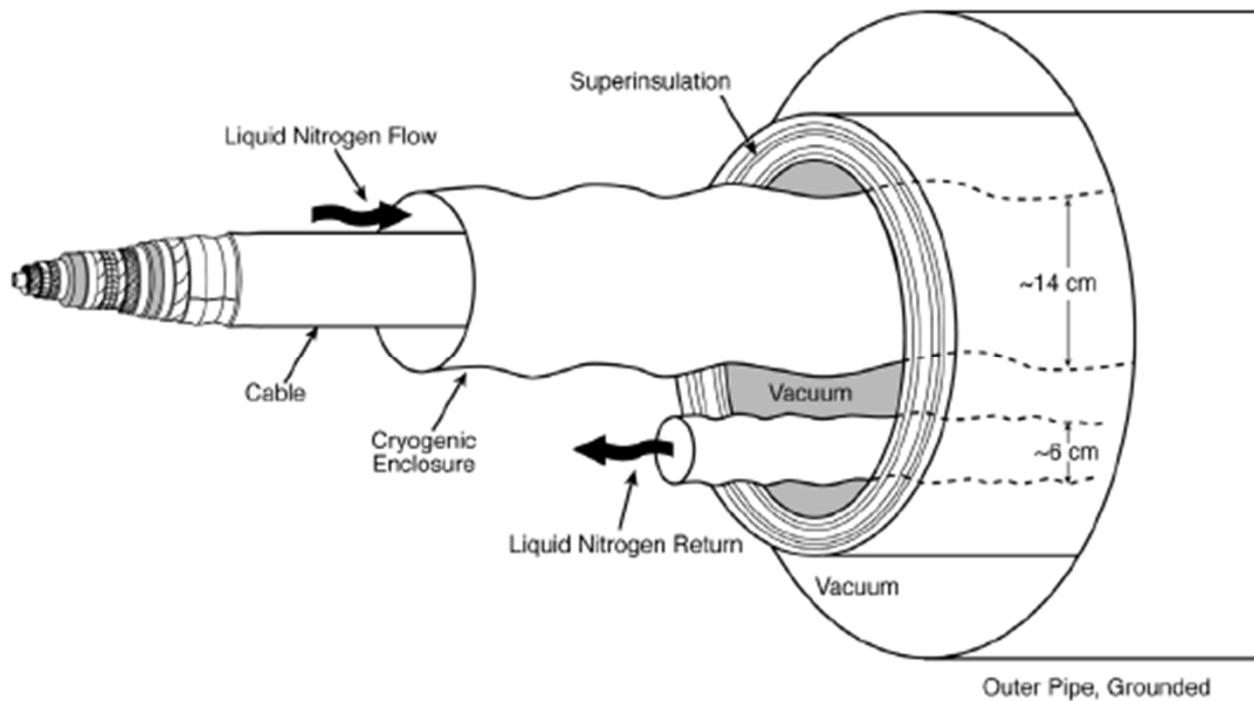
AMSC/Nexans Long Island Power Authority



A Superconducting dc Cable

EPRI Report 1020458 (2009)

Hassenzahl, Gregory, Eckroad, Nilsson, Daneshpooy, Grant



Monopole Specs

100-kV, 100-kA, 10-GW

66 K < T < 69 K

The Tres Amigas SuperStation



Transmission Lines from Western Interconnection

Transmission Lines from Eastern Interconnection

- Will TA go forward using superconducting cables?
- Uncertainties:
 - ERCOT?
 - Renewables?
 - Silicon City?

Filled up with VSC's

4 Miles

5 Miles

Transmission Lines from ERCOT
One or more transmission lines from the Texas Interconnection (see the U.S. Grid Interconnections box) connect to this HVDC terminal.



US Department of Energy

Budget of the Office of Electricity Delivery and Energy Reliability: FY 2010-11 (10³ USD)

| | FY 2009 | | FY 2010 | FY 2011 |
|--|-----------------------|--------------------|-----------------------|-----------------------|
| | Current Appropriation | ARRA Appropriation | Current Appropriation | Congressional Request |
| Research and Development | | | | |
| High Temperature Superconductivity | 23,130 | | ? | ? |
| Visualization and Controls | 24,461 | | | |
| Energy Storage and Power Electronics | 6,368 | | | |
| Renewable and Distributed Systems Integration | 29,160 | | | |
| Clean Energy Transmission and Reliability | | | 38,450 | 35,000 |
| Smart Grid Research and Development | | | 32,450 | 39,293 |
| Energy Storage | | | 14,000 | 40,000 |
| Cyber Security for Energy Delivery Systems | | | 40,000 | 30,000 |
| SUBTOTAL Research and Development | 83,119 | | 124,900 | 144,293 |
| Permitting, Siting, and Analysis | 5,271 | | 6,400 | 6,400 |
| Infrastructure Security and Energy Restoration | 6,180 | | 6,187 | 6,188 |
| Program Direction | 21,180 | | 21,420 | 29,049 |
| Congressionally Directed Activities | 19,648 | | 13,075 | |
| American Recovery and Reinvestment Act, 2009 | | 4,495,712 | | |
| Use of prior year balances | -769 | | | |
| TOTAL | 134,629 | 4,495,712 | 171,982 | 185,930 |

WOW ! "Obama Cash"

A Modest Proposal

-Upbraiding the Utilities-

- More than a half-century of successful demonstrations/prototyping power applications of superconductivity (1950s - >2000, in Japan and US)...low- and high-T_c...now sitting “on the shelf.”
- Why aren't they “in the field” today?
- Is their absence due to...
 - Cost?
 - Hassle?
 - or “lack of compelling” need?
 - or “all of the above?”

- US utilities have long claimed to “want” ...
 - Efficient long-length cables
 - Oil-free transformers
 - Energy Storage
 - Fast fault current limiters at high voltage (FCLs)
 - Efficient rotating machinery (aka, motors and generators)
- Well, we got ‘em. Utilities claim:
 - They’re too high-cost, because,
 - The wire is too expensive.
 - They have to be kept too cold.
 - Electricity is cheap, and “in field” energy efficiency is not a “compelling” driver
 - Anyway, we can solve our needs by incrementally improving the “old” ways (don’t ever underestimate the ingenuity of a utility engineer to improvise, adopt and adapt)

“Then...a modest proposal...”

- If the “cost” of the wire in any given application were to be “zero,” ...
- Would the utilities then “buy them?” And sign a “letter of intent” to purchase “x” number?
 - e.g., Fault Current Limiters, for which US utilities have long claimed a need
- “Zero cost” would be obtained as a Federal or State “tax credit” for the wire cost of the quantity purchased by the utility equipment vendor or the utility itself...
- Well?

Questions for US HTSC Wire Manufacturers

- AMSC
 - Estimated gross revenue from wire sales (and actual delivery) for FY2011?
 - Note: 3Q10 gross revenue from wire sales was 1.8% of total quarter
- SuperPower
 - Same as AMSC #1 above
 - Estimated employee/manpower growth in CY2011
- Ultera/Southwire
 - Is Carrolton plant cable (Gen 1) still in operation?
 - Plans to replace/extend?
- Nexans/AMSC/LIPA
 - Status of Gen II wire/cable upgrade
- AMSC/ConEd/DHS
 - Status/funding of Project Hydra

My Virtual Grandfather (@ 94)



W2AGZ & Beyond

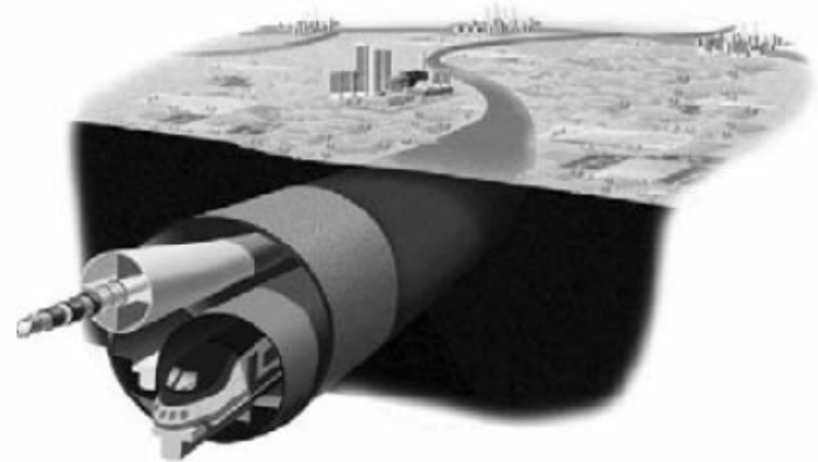
Superconductivity: 100 Years and Counting



First in a year-long series of editorial pieces celebrating the history and progress of superconductivity

by Dr. Paul Michael Grant, W2AGZ Technologies, w2agz@w2agz.com, www.w2agz.com

The following invited article is based on a presentation by Dr. Paul Grant at the July 2010 ICEC/ICMC in Wroclaw, Poland. It is the first in a year-long series of articles in which Cold Facts will be celebrating the 100th anniversary of the discovery of superconductivity.



Down the path of least resistance

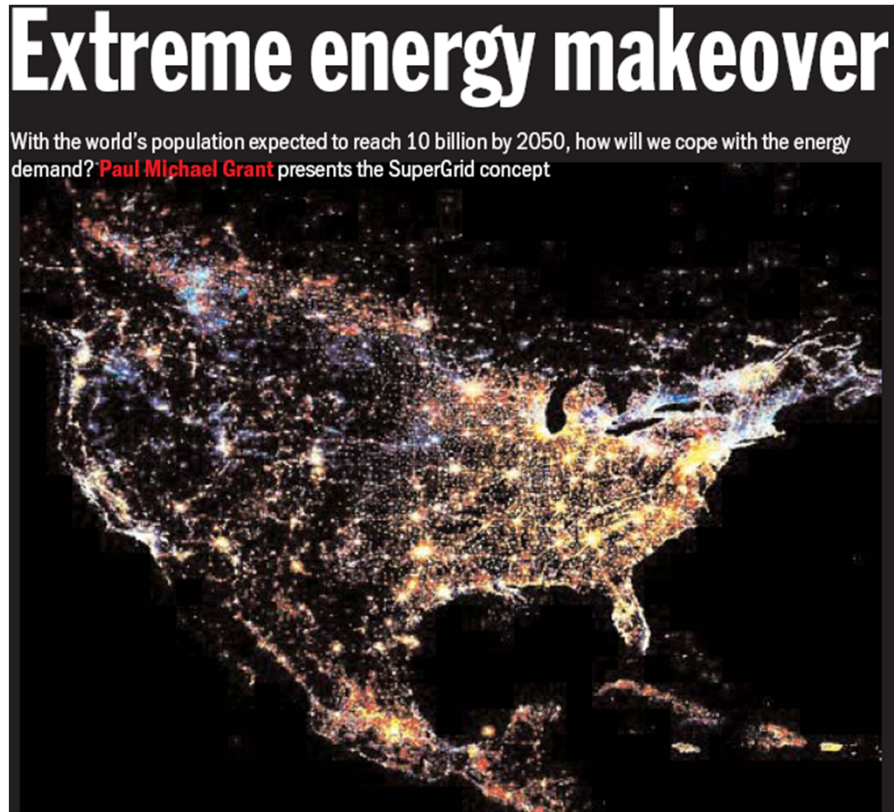
Since its discovery 100 years ago, our understanding of superconductivity has developed in a far from smooth fashion. **Paul Michael Grant** explains exactly why this beautiful, elegant and profound phenomenon continues to confound and baffle condensed-matter physicists today

Five of the best

Superconductivity may be a beautiful phenomenon, but materials that can conduct with zero resistance have not quite transformed the world in the way that many might have imagined. Presented here are the top five applications, ranked in terms of their impact on society today

1. Wires & Films
2. Medical Imaging
3. High Energy Physics
4. Rotating Machinery
5. Dark Matter

Physics World, October 2009



From [The Times](#)

October 3, 2009

Science: Stand by for the Supergrid

Why the world needs an 'extreme energy makeover'

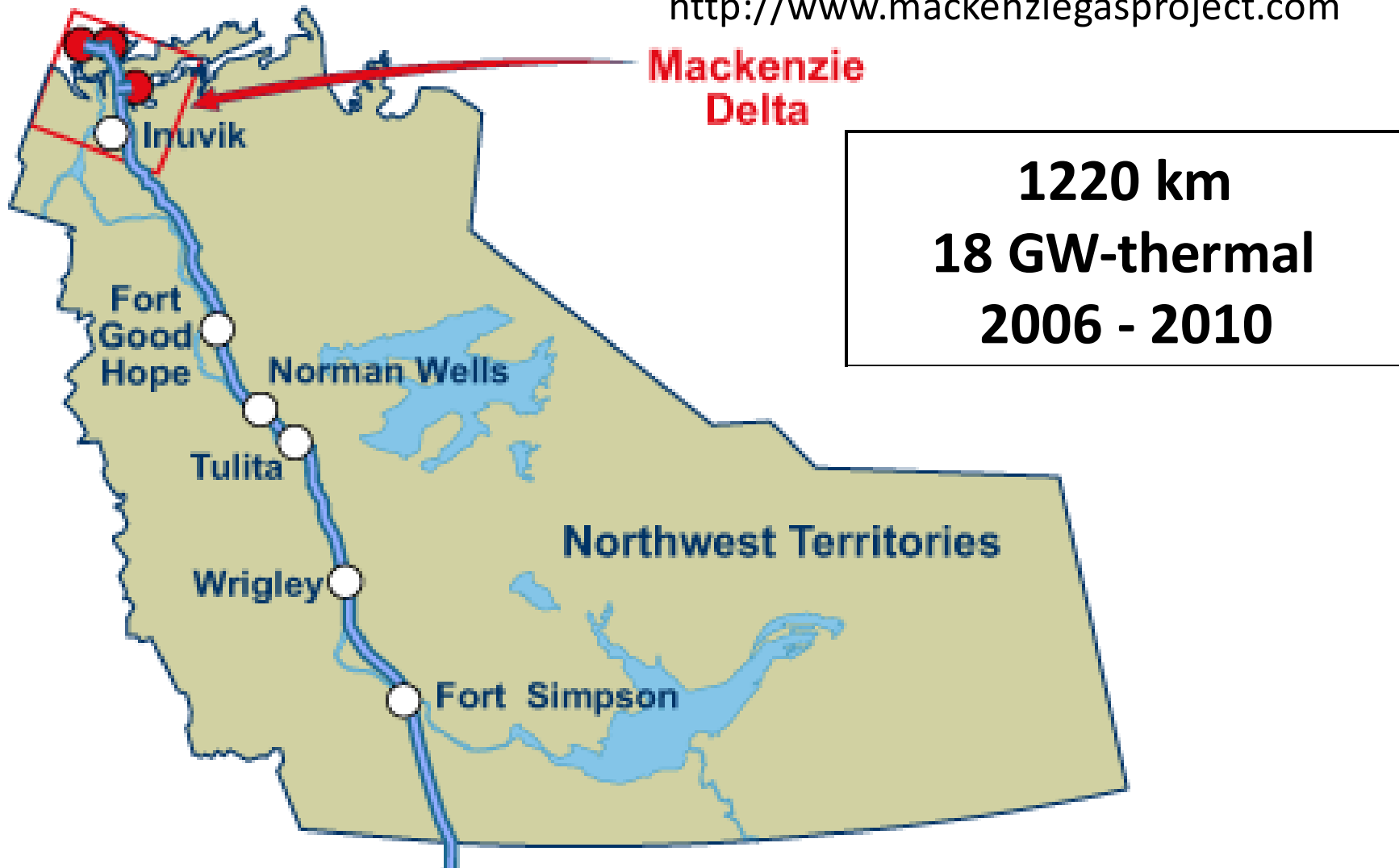
[Anjana Ahuja](#)



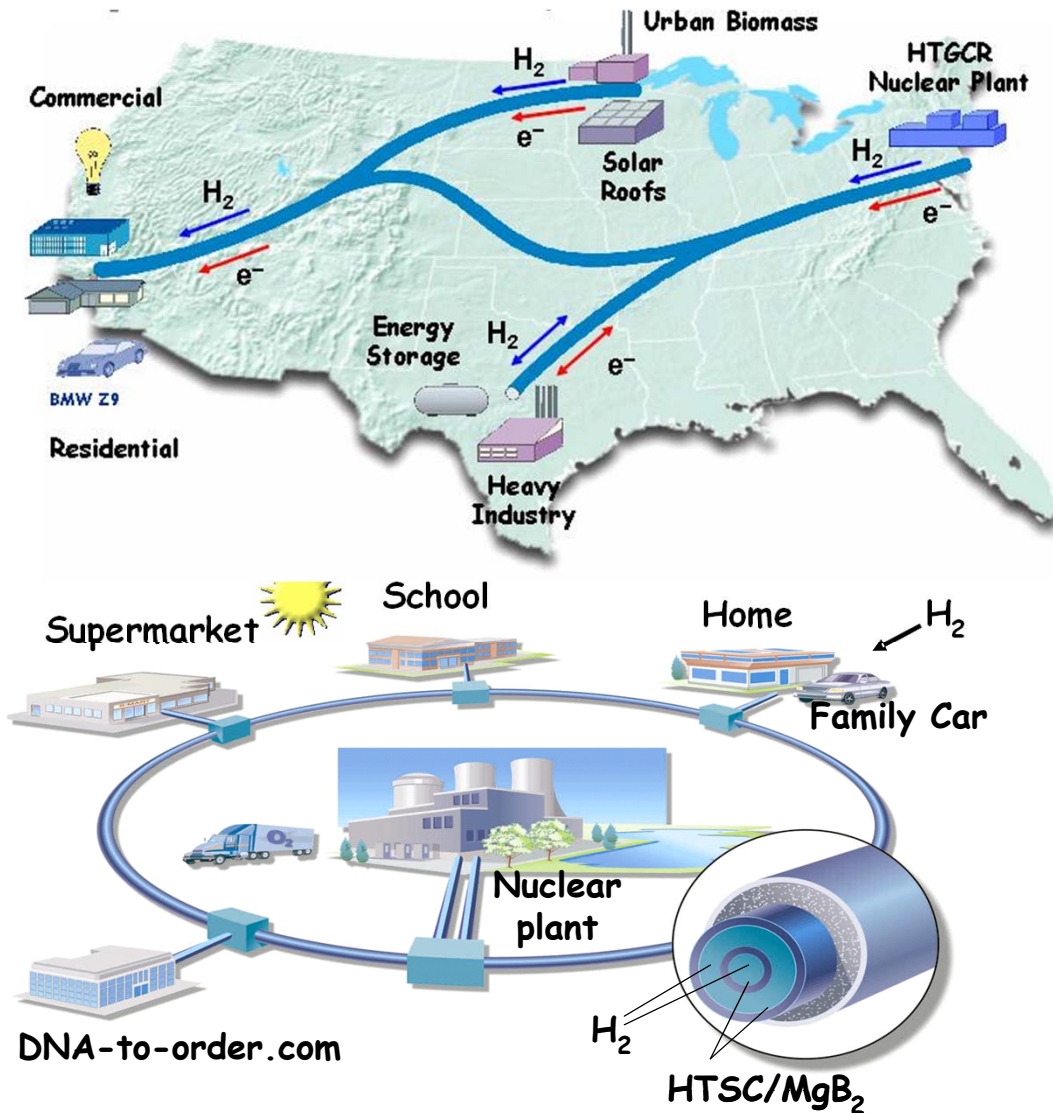
...a future editor of
Nature...?

The Mackenzie Valley Pipeline

<http://www.mackenziegasproject.com>



SuperCities & SuperGrids



- Nuclear Power can generate both electricity and hydrogen – “Hydricity”
- Hydricity can be distributed in underground pipelines like natural gas
- The infrastructure can take the form of a **SuperGrid**
- ...or a **SuperCity**

SuperSuburb

SuperSuburb

Households: 300,000
Electricity: 1800 MW
Hydrogen: 800 MW



SuperNuke

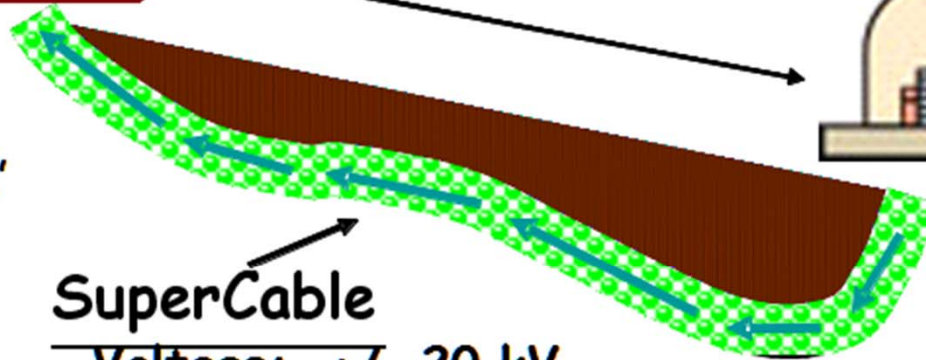
electrons + protons
=> 2600 MW



250 km

SuperCable

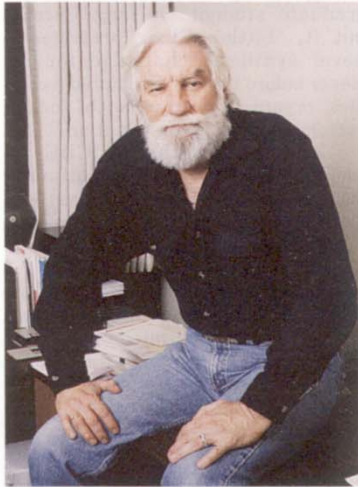
Voltage: +/- 20 kV
Current: 45 kA
H₂ Storage: 28 GWh
H₂ Flow: 2 m/s => 6.8 kg/s



The Future?

Physics Today, November 1998

PHYSICS TOMORROW: ESSAY CONTEST WINNER



RESEARCHERS FIND
EXTRAORDINARILY HIGH
TEMPERATURE
SUPERCONDUCTIVITY IN
BIO-INSPIRED NANOPOLYMER

Paul M. Grant
May 2028


700 K !

May, 2028

So Now We Have a Room Temperature Superconductor... So What? (Will We Be Able to Use It?)

Paul M. Grant

Visiting Scholar, Stanford
IBM Research Staff Member Emeritus
EPRI Science Fellow (Retired)
Principal, W2AGZ Technologies



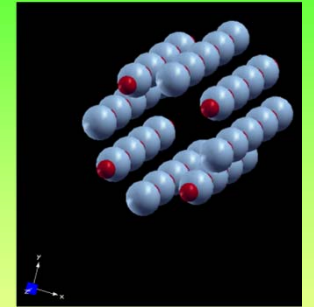
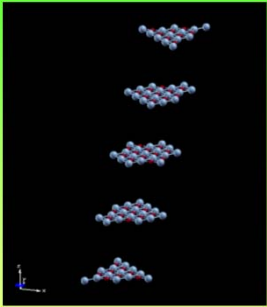
Finally
Enable the
Hydrogen
Economy ?

The Road to Room Temperature Superconductivity
Loen, Norway
17-22 June 2007

<http://www.w2agz.com/rtsc06.htm>

Road2RTS

A DFT (LDA+U) Study of the Electronic Properties of Square-Planar Coordinated Copper Monoxide Structures

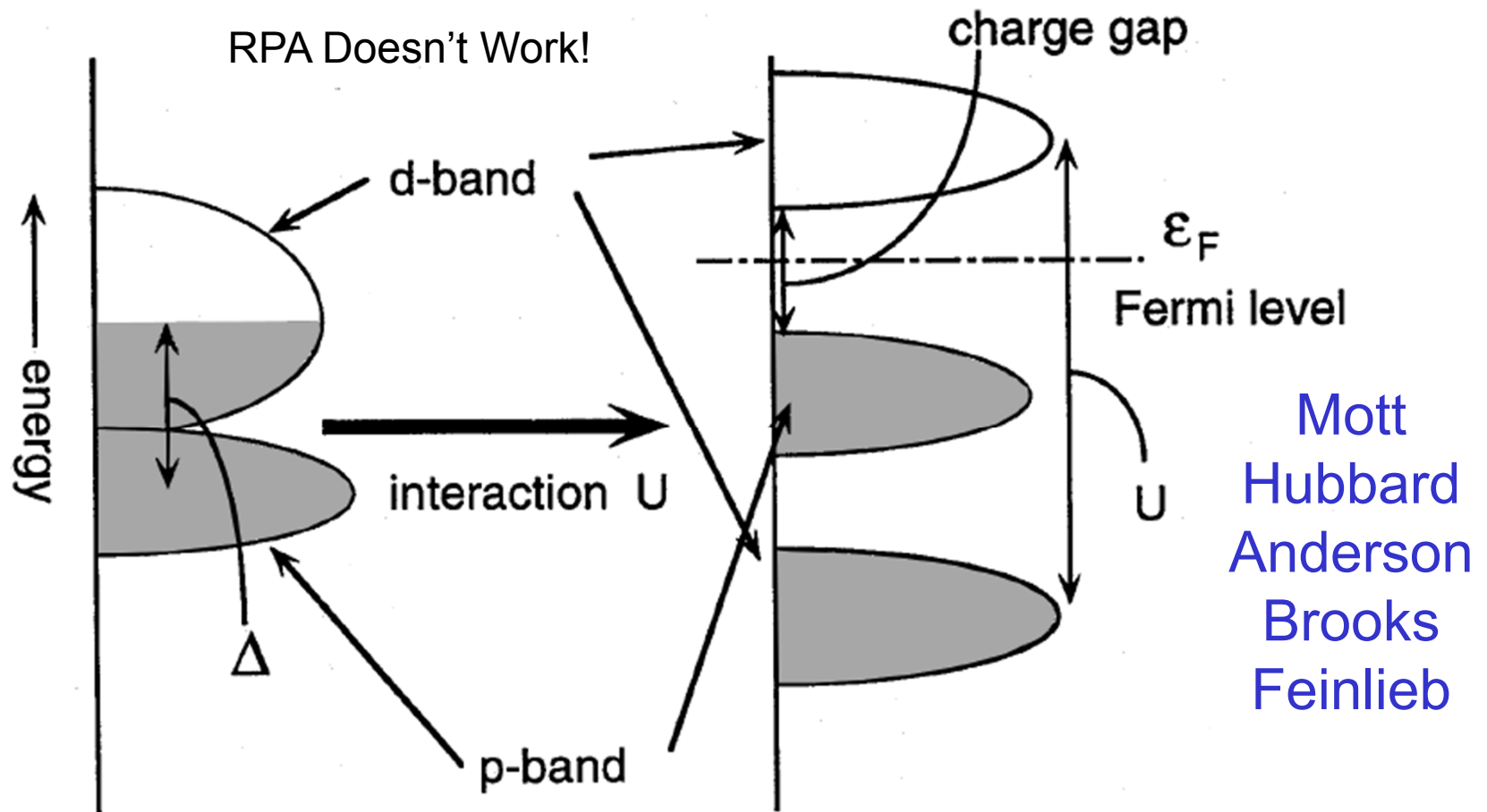


**... And Now for
Something Completely
Different ...**

**Back to the Future...
My SJRL Day Job of the 60s and 70s...
Electronic Structure Calculations**

Transition Metal Oxides

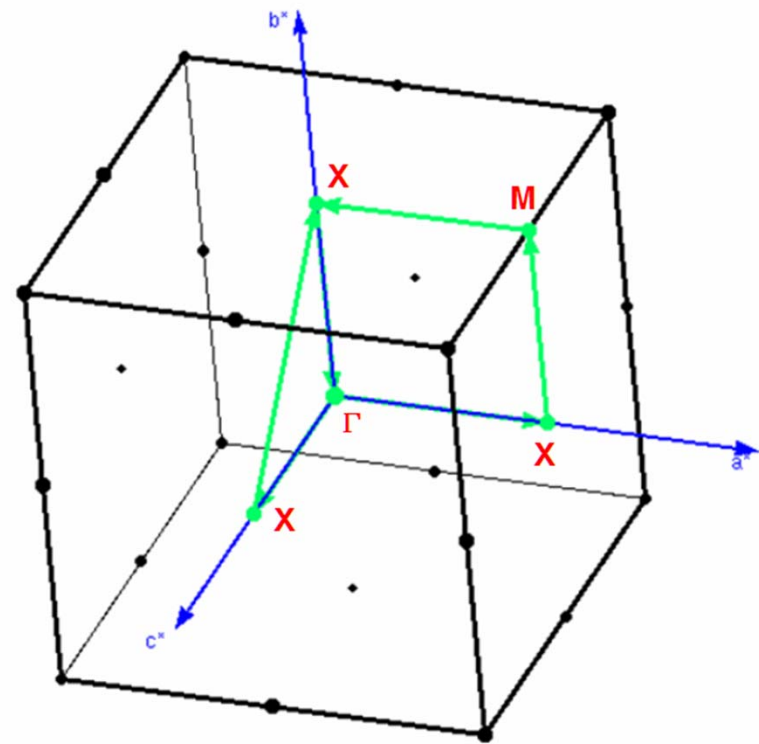
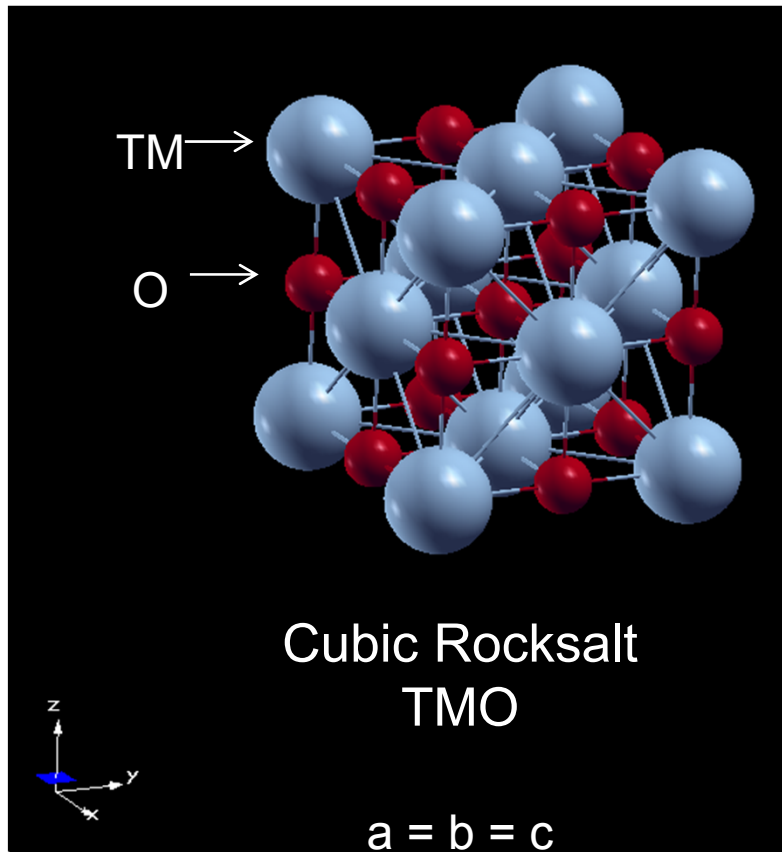
“Should be Metals, But Aren’t”
(Charge Transfer Insulators, Instead)



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

Cubic Rocksalt TMOs

Direct and Reciprocal Lattices



Cubic Rocksalt Divalent TMOs

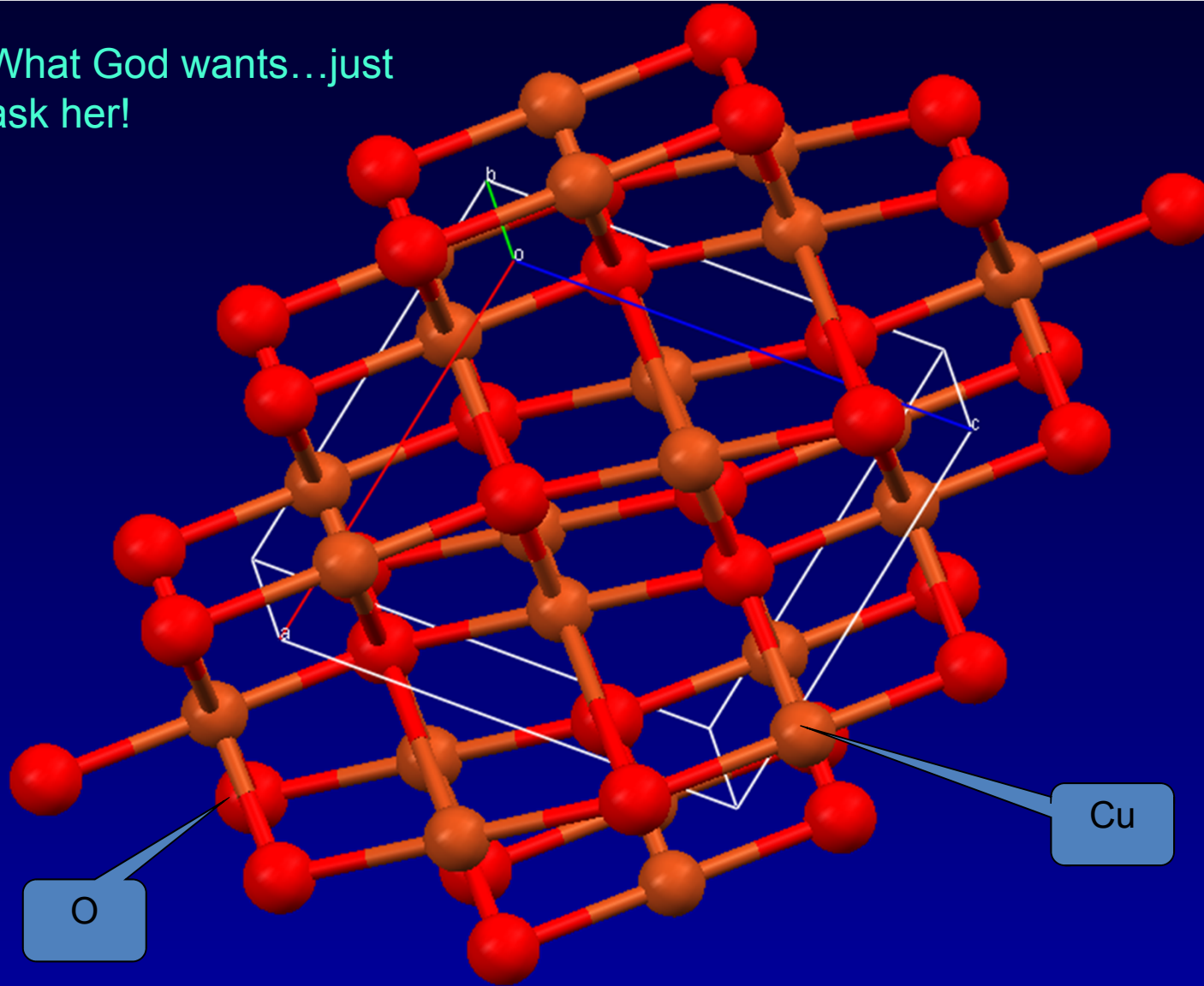
| <u>TMO</u> | <u>3d Config</u> | <u>Properties</u> |
|------------|------------------|---------------------------------|
| MnO | 5 | MH-CTI (5.6) |
| FeO | 6 | MH-CTI (5.9) |
| CoO | 7 | MH-CTI (6.3) |
| NiO | 8 | MH-CTI (6.5) |
| CuO | 9 | <i>XX Doesn't Exist!</i> |

See Imada, Fujimore,
Tokura, RPM 70 (1988)

Why Not?

Tenorite (Monoclinic CuO)

What God wants...just ask her!



Can Application of DFT (LDA+U) Help Unravel the Cubic Rocksalt CuO Enigma?

...Let's see...

DFT & (LDA + U)

$$E_{\text{LDA+U}}[n(\mathbf{r})] = E_{\text{LDA}}[n(\mathbf{r})] + E_{\text{HUB}}\left[\left\{n_m^{l\sigma}\right\}\right] - E_{\text{DC}}\left[\left\{n^{l\sigma}\right\}\right]$$

- Implemented in LMTO by Anisimov, et al, JPCM 2, 3973 (1990)
 - Applied to NiO, MnO, FeO, CoO and La₂CuO₄
- Plane-Wave Pseudopotential Implementation by Cococcioni and de Gironcoli, PRB 71, 035105 (2005)
 - Applied to FeO and NiO
 - Download open-source package from <http://www.pwscf.org>

Proxy Structures

A New Materials Science Discipline

- You want to understand the basic physics of some given system...(e.g., HTSCs)
- So try to synthesize a simple proxy...(e.g., rocksalt CuO)
- But “Mother Nature” won’t “agree.” (She’s a woman!)
- However, you can build it in a computer and perform various “ab initio” experiments.
- And from such, numerically calculate “observables,” e.g., “response functions.”
- Try it out...it’s lots of fun! And perhaps you’ll discover something as well!

Tools

QUANTUM-ESPRESSO Suite of Codes

DFT (LDA+U) plus electron-phonon

Graphics by Tone Kolalj (XCrysDen)

www.quantum-espresso.org

“Dial-in” Parameters

$G^2 = 40 \text{ Ry}$ $\rho = 320 \text{ Ry}$

Convergence $\leq 10^{-6} \text{ Ry}$

“Smearing” = Methfessel-Paxton

Pseudopotentials: Ultrasoft, XC = Perdew-Zunger

Cu: $3d^9 4s^2$ O: $2s^2 2p^4$



Viva Italia!

Hardware

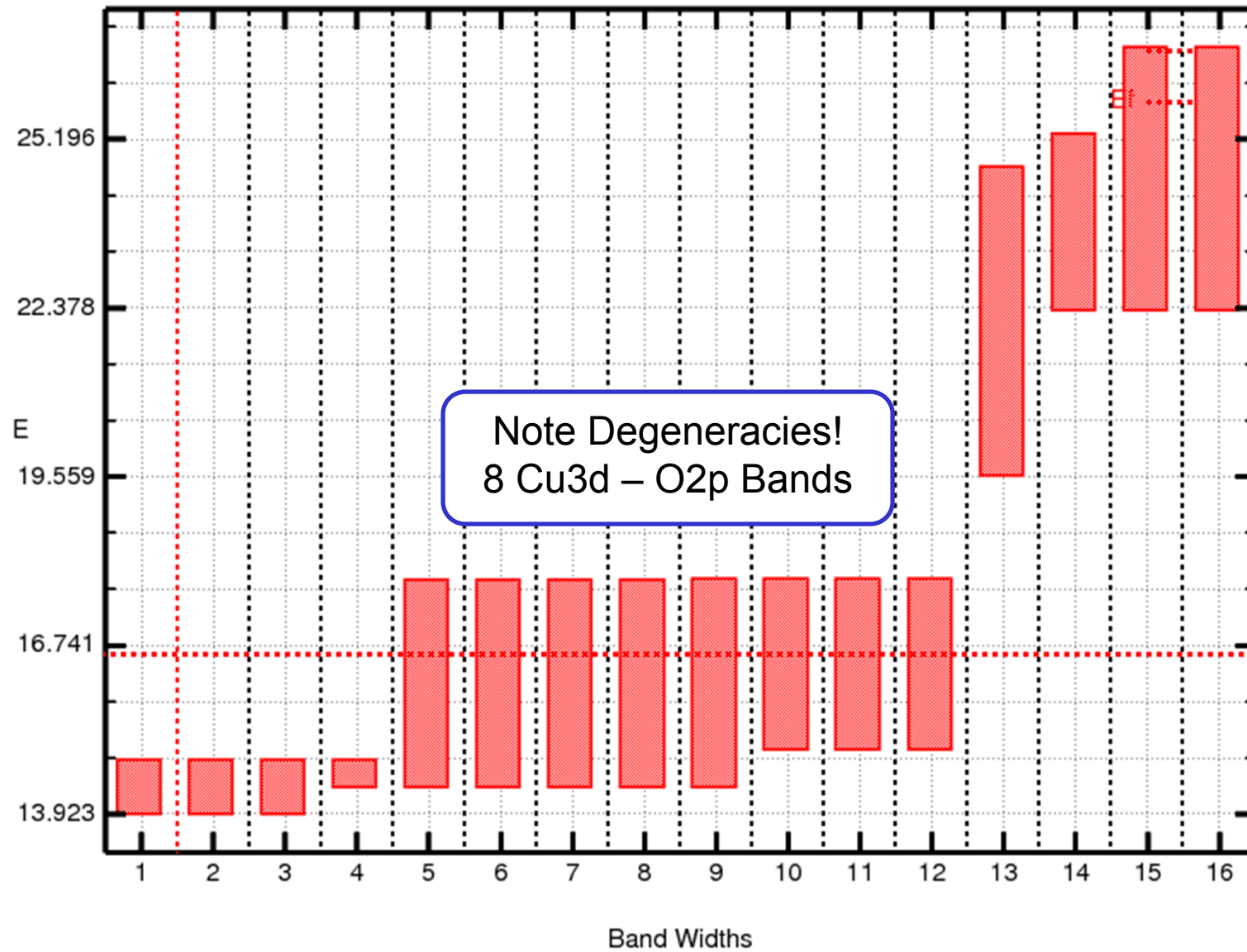
3.33 GHz Intel Core i7 – 12 GB+ (Gaming Box – Home Built)

Software

Linux Kubuntu

Rocksalt CuO Band Widths

$U = 0 \text{ eV}$

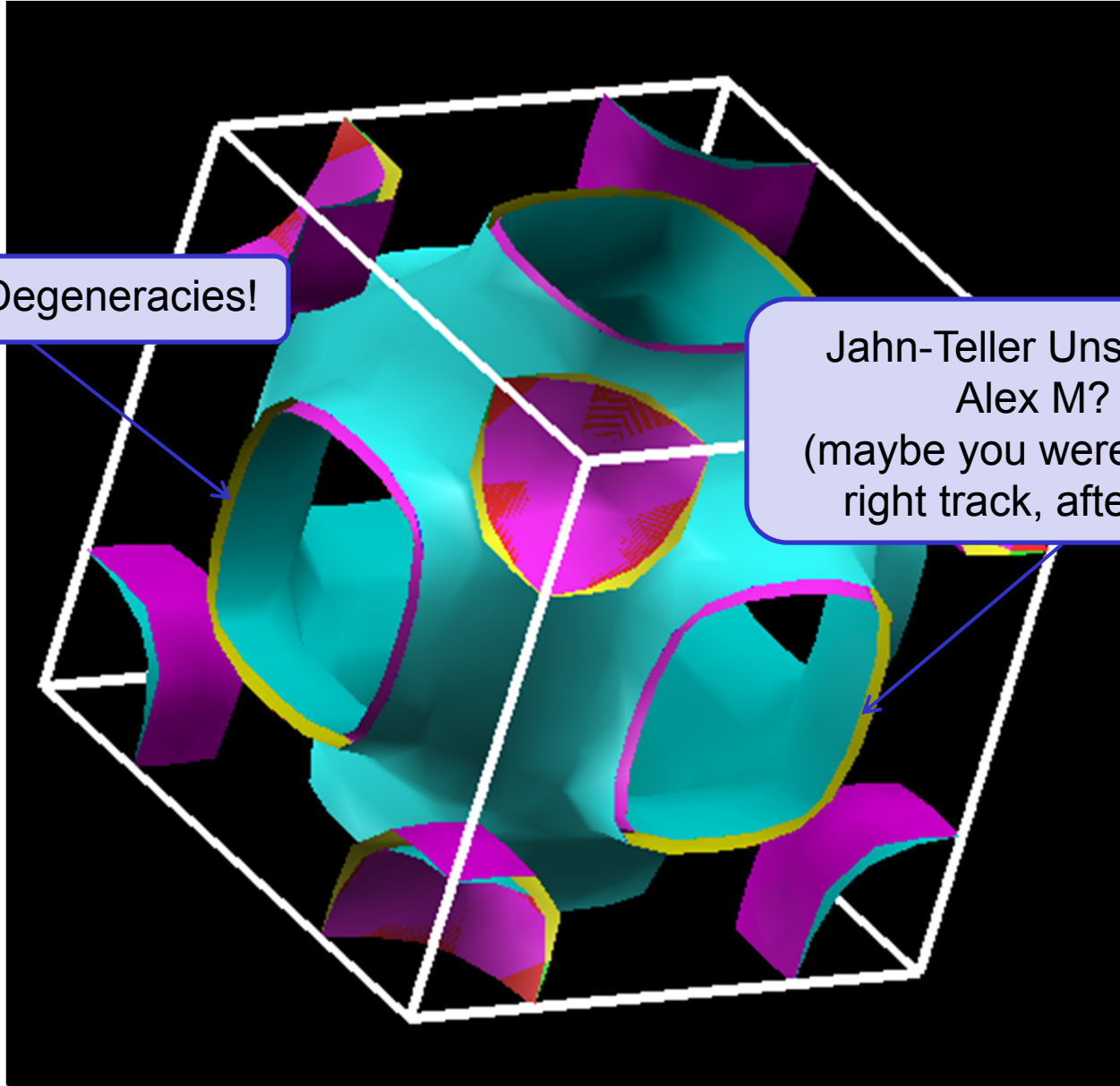


Rocksalt CuO Fermiology ($U = 0$ eV)

(8 Bands Combined)

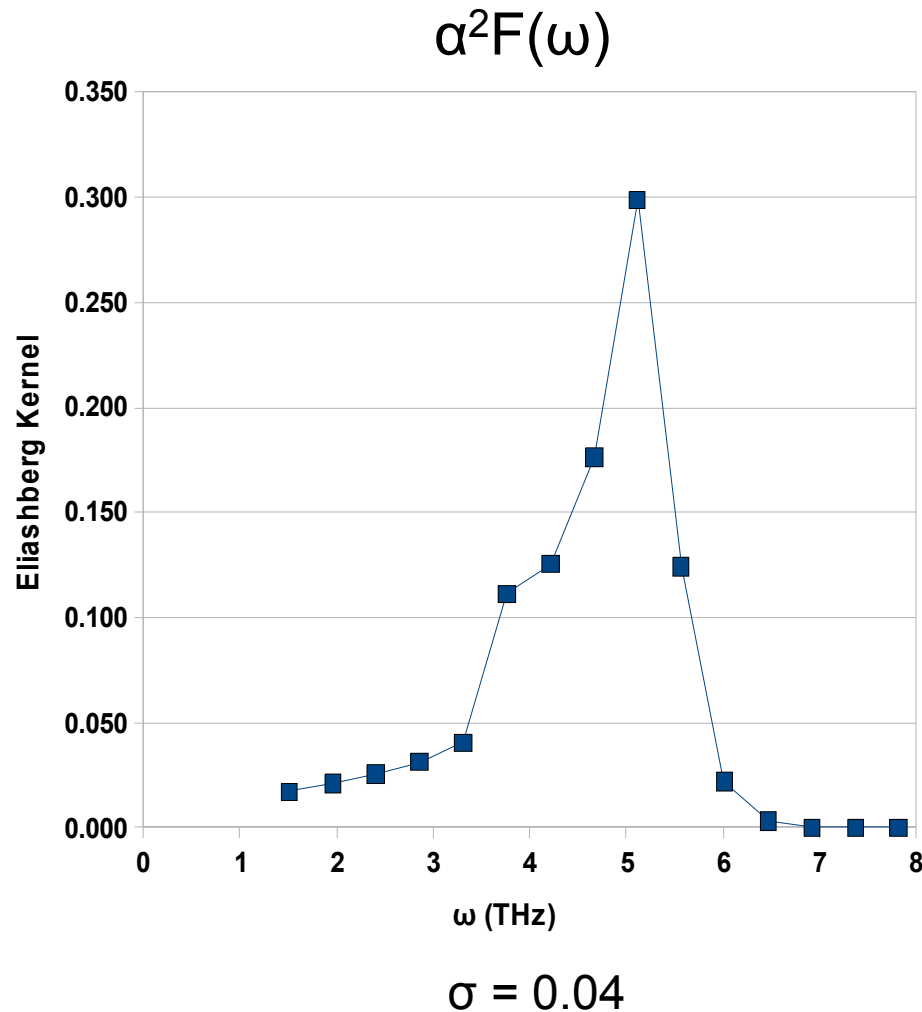
Note (Near) Degeneracies!

Jahn-Teller Unstable?
Alex M?
(maybe you were on the right track, after all!)



Non-Magnetic ($U = 0$) Cubic Rocksalt CuO

-- Electron-Phonon Properties --



- $\lambda \sim 0.6 - 0.7$
- Consistent with other non-magnetic "HTSCs"

$$T_C = a\Theta e^{\frac{1}{\lambda - \mu^*}} \quad \lambda k\Theta \ll E_F$$

| | T_C (K) | λ | μ^* |
|--------------|--------------|-----------|---------|
| K_3C_{60} | 16.3 | 0.51 | - |
| Rb_3C_{60} | 30.5 | 0.61 | - |
| Cs_3C_{60} | 47.4 | 0.72 | - |

Are There Phonons w/ High-Tc in YBCO?

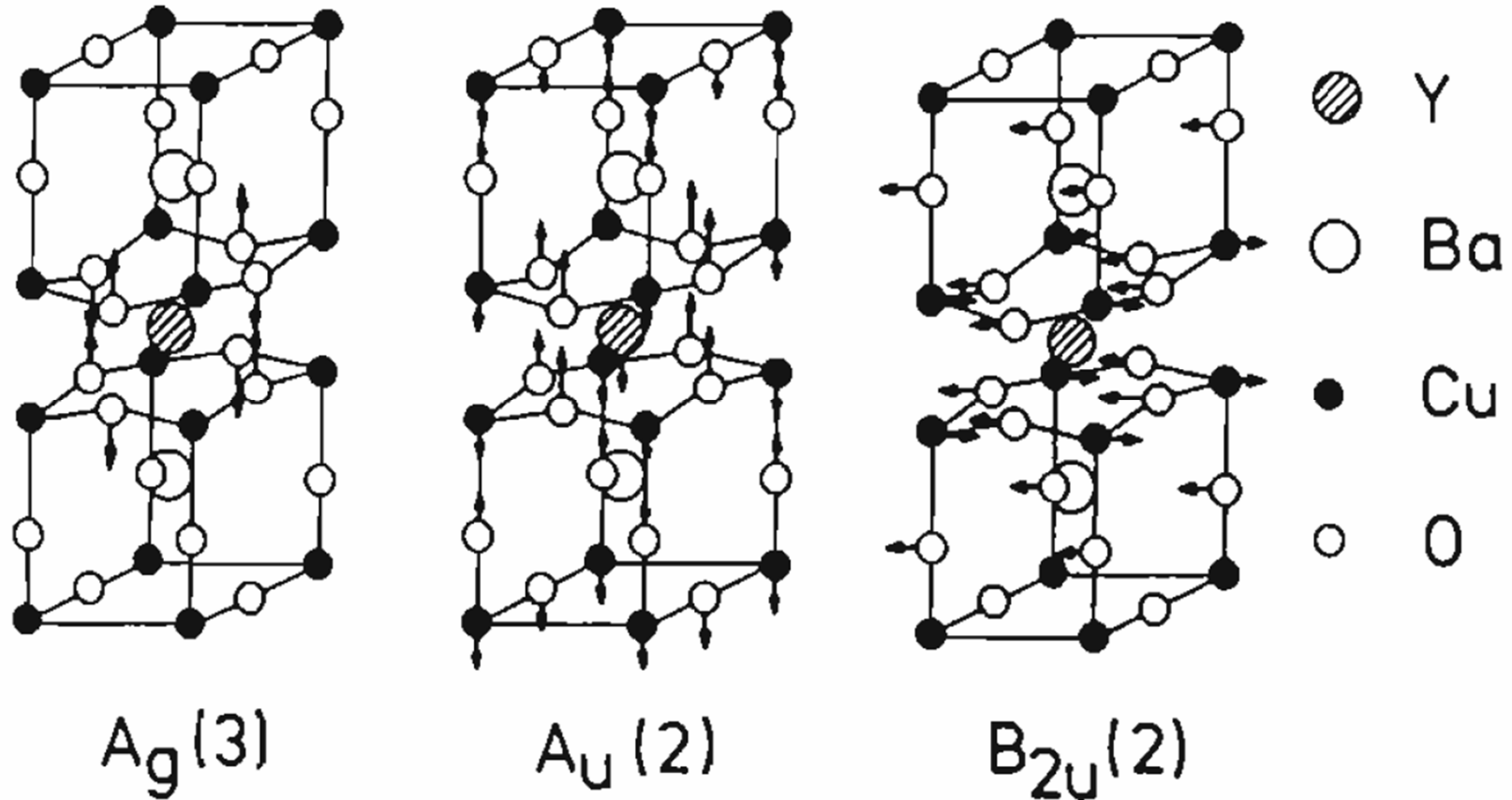
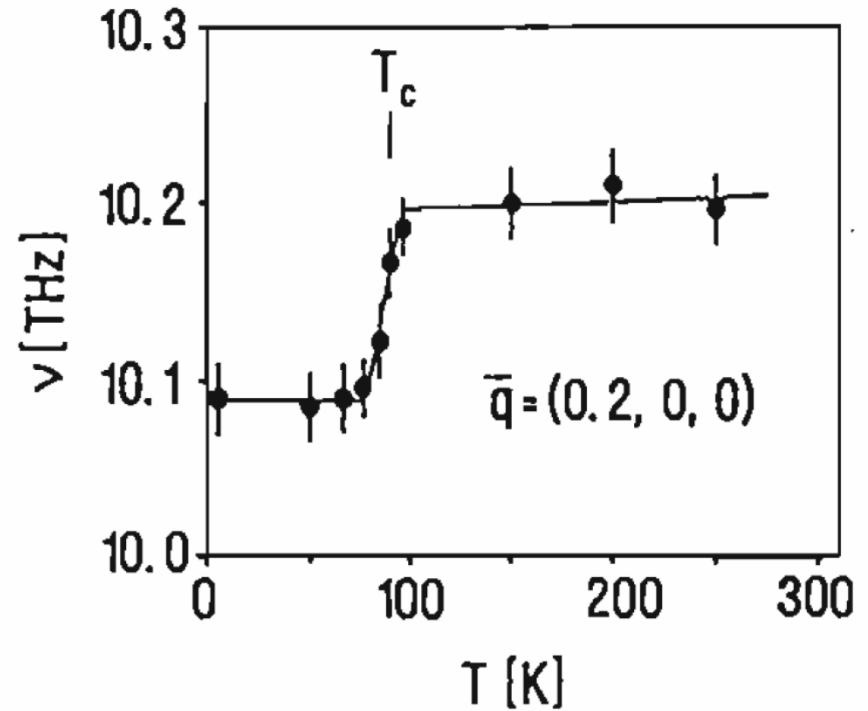
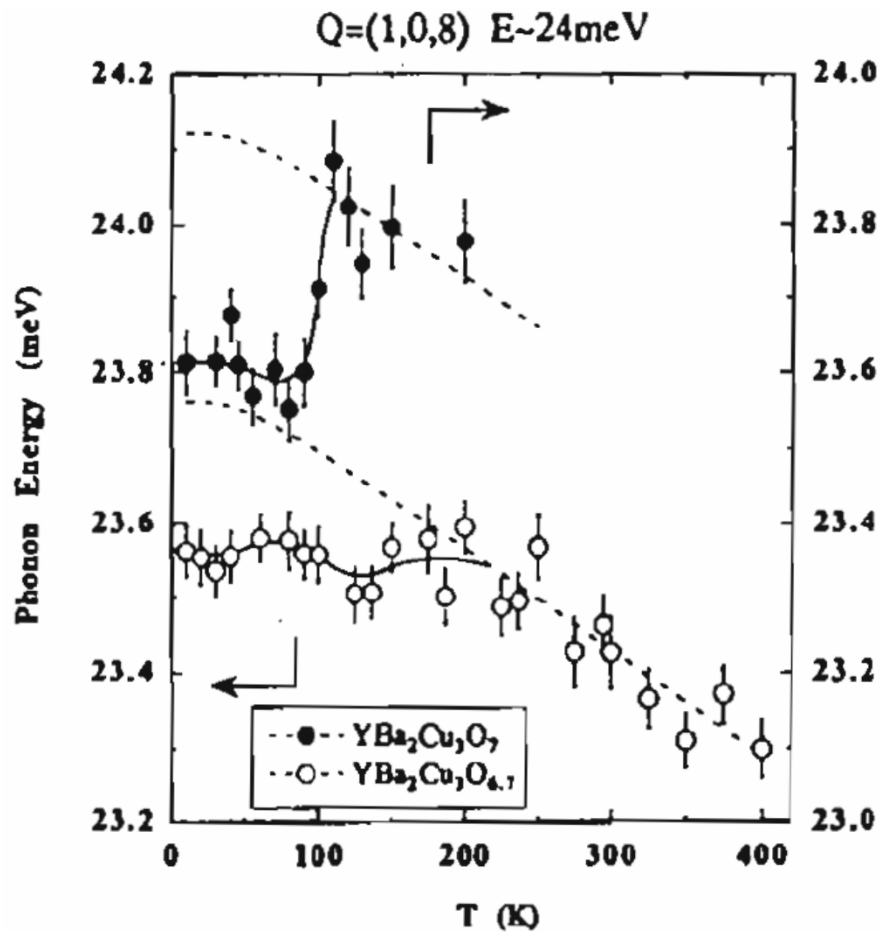


Fig. 38: Pintschovius and Reichardt, in Furrer, ISBN 0-7923-5226-2

Yes -- They're There!

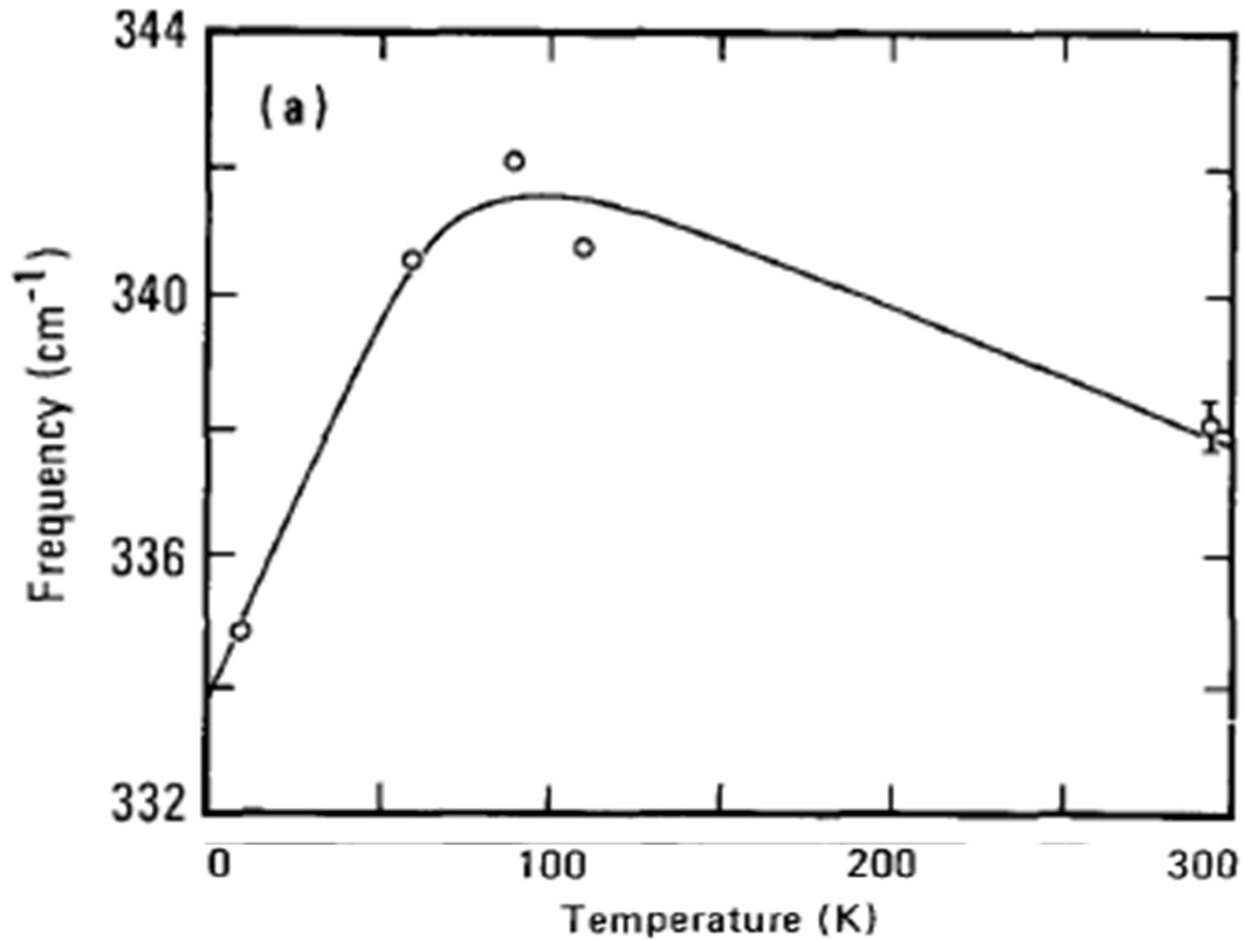


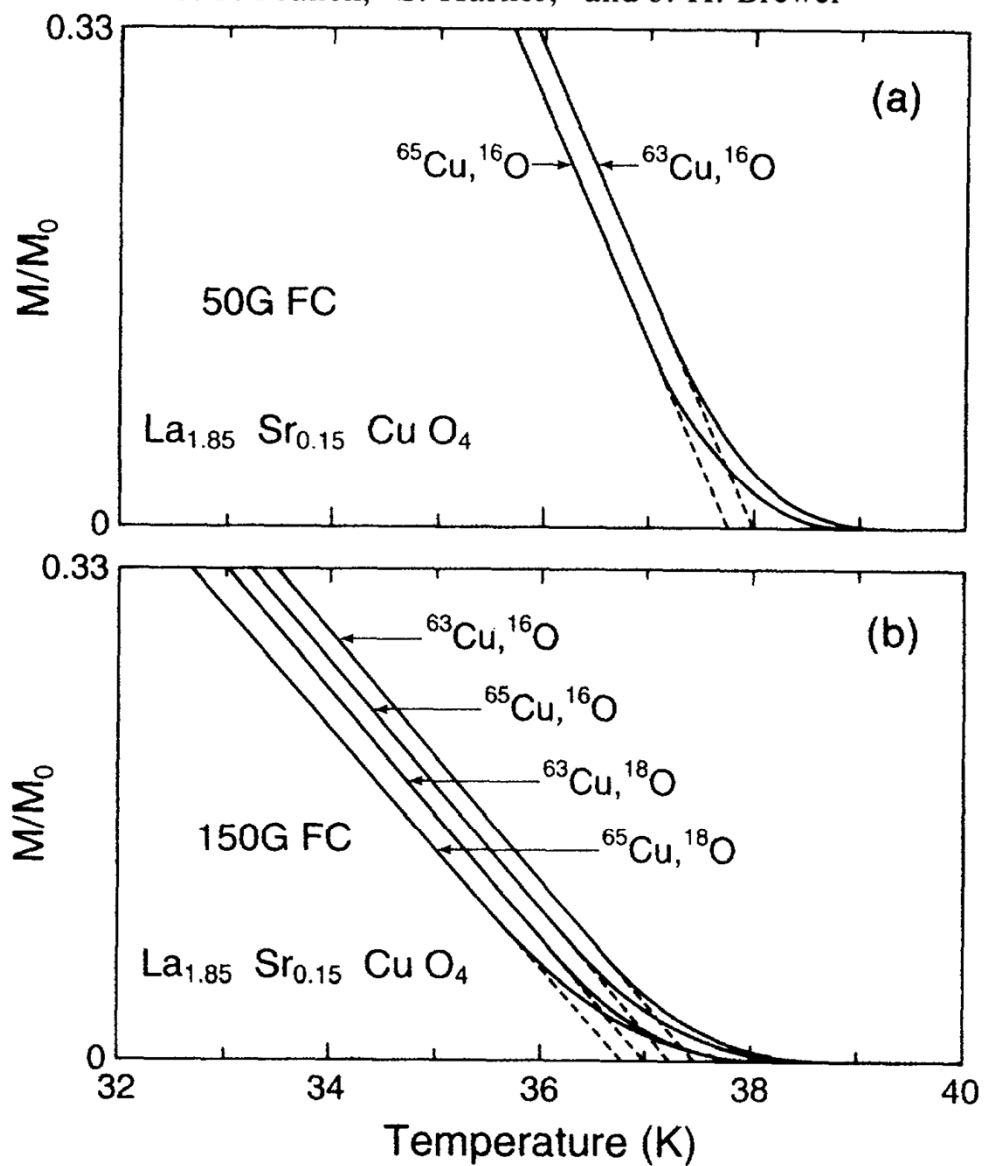
Pyka, et al., PRL 70, 1457, (1993)

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

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

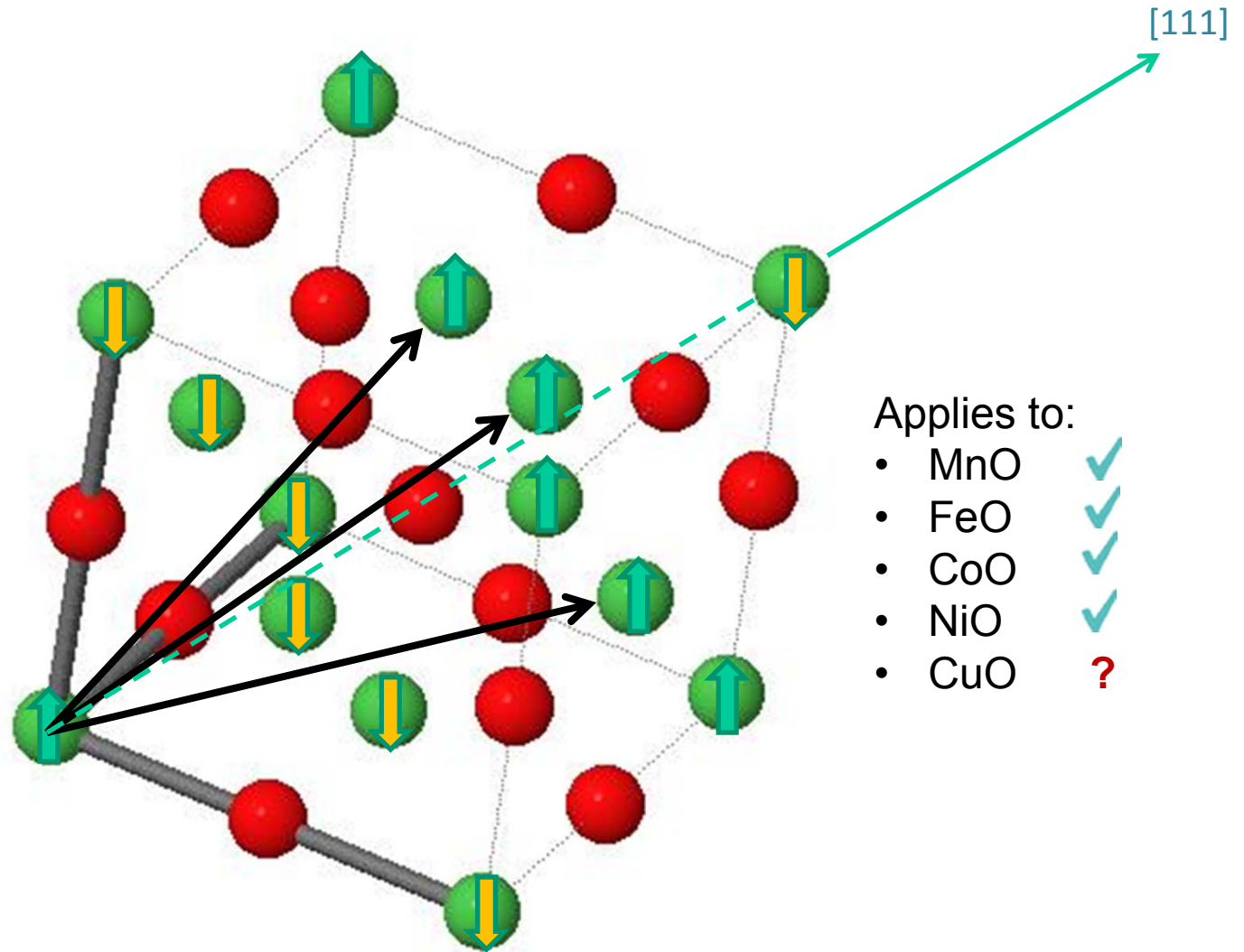
Raman Spectroscopy of YBCO



Copper and Oxygen Isotope Effects in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ J. P. Franck,¹ S. Harker,¹ and J. H. Brewer²

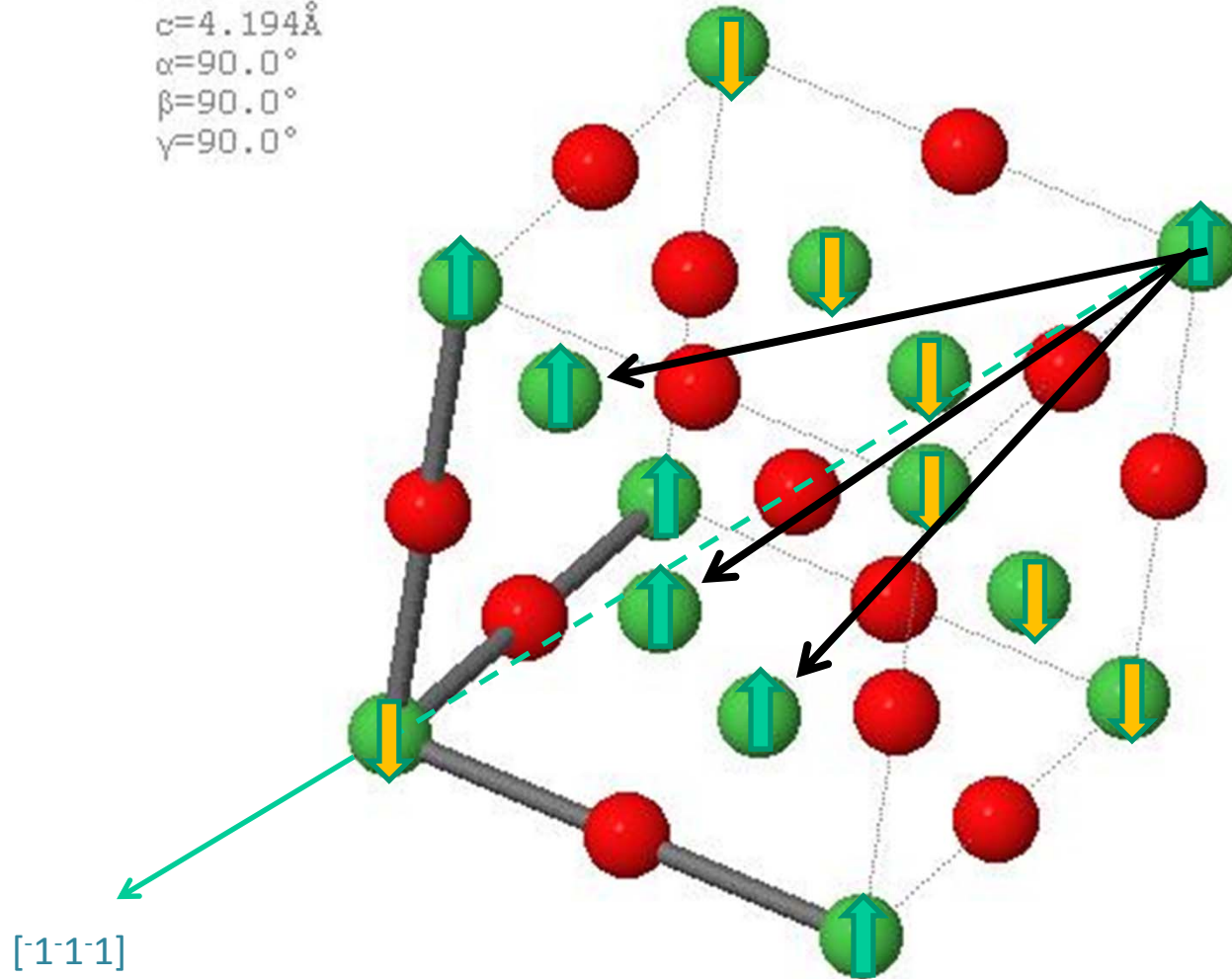
Proto-TMO AF-II Rocksalt Unit Cell

Fm-3m
a=4.194Å
b=4.194Å
c=4.194Å
α=90.0°
β=90.0°
γ=90.0°

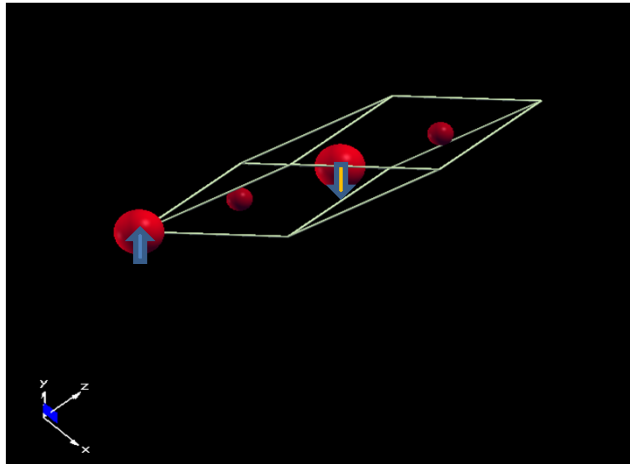


Proto-TMO AF-II Rocksalt

Fm-3m
a=4.194Å
b=4.194Å
c=4.194Å
α=90.0°
β=90.0°
γ=90.0°



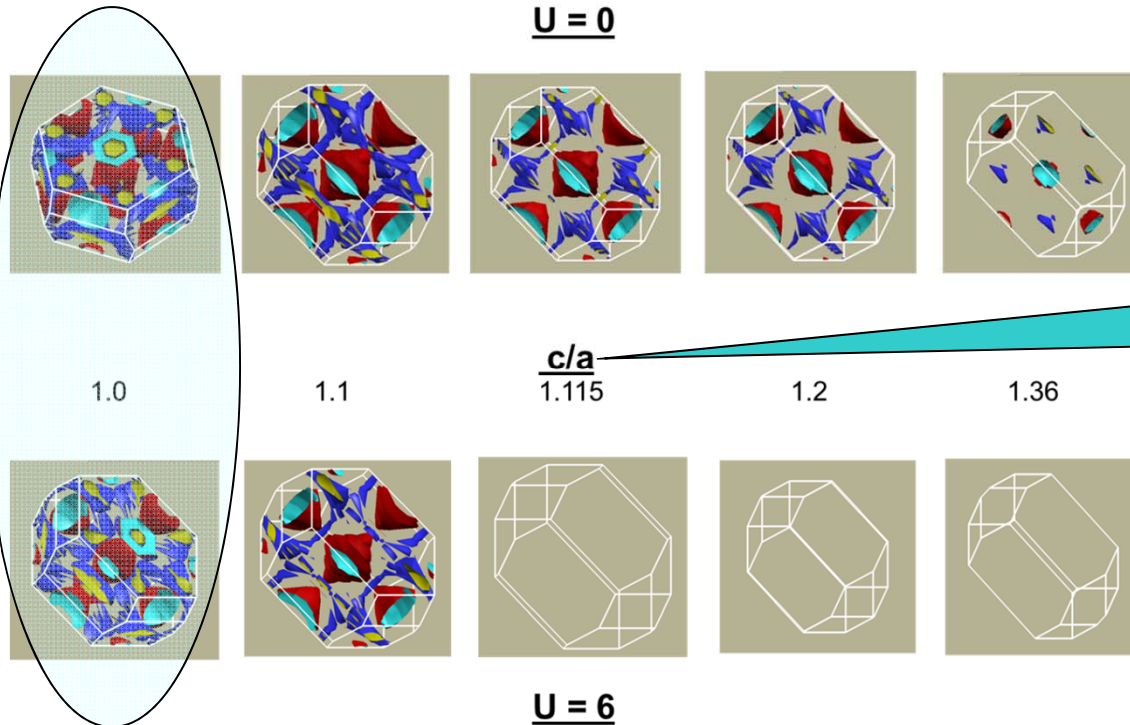
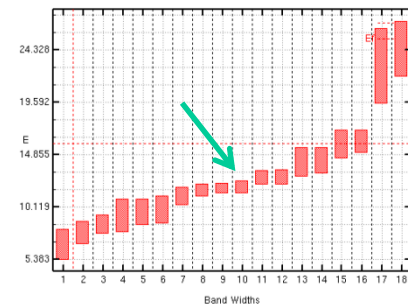
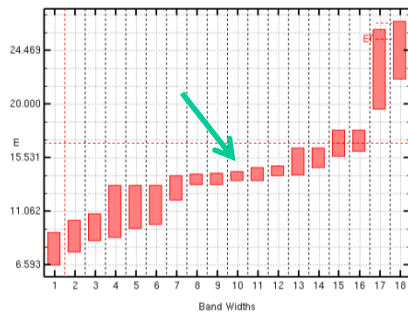
The Answer(s) !



TMO Asymmetric Type II
af-CuO Cell

LDA+U Calcs

Grant, IOP-CS 129 (2008) 102042
(Click [Here](#))



U = 0

c/a
1.115

U = 6

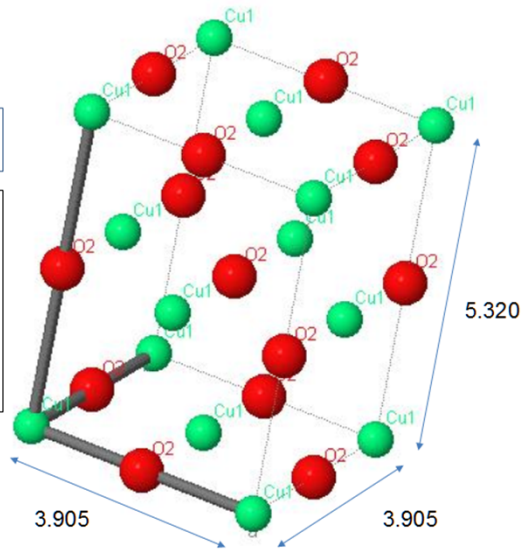
Tetragonal
Distortion

Siemons, et al,
PRB 79 (2009)
195122
(Click [Here](#))

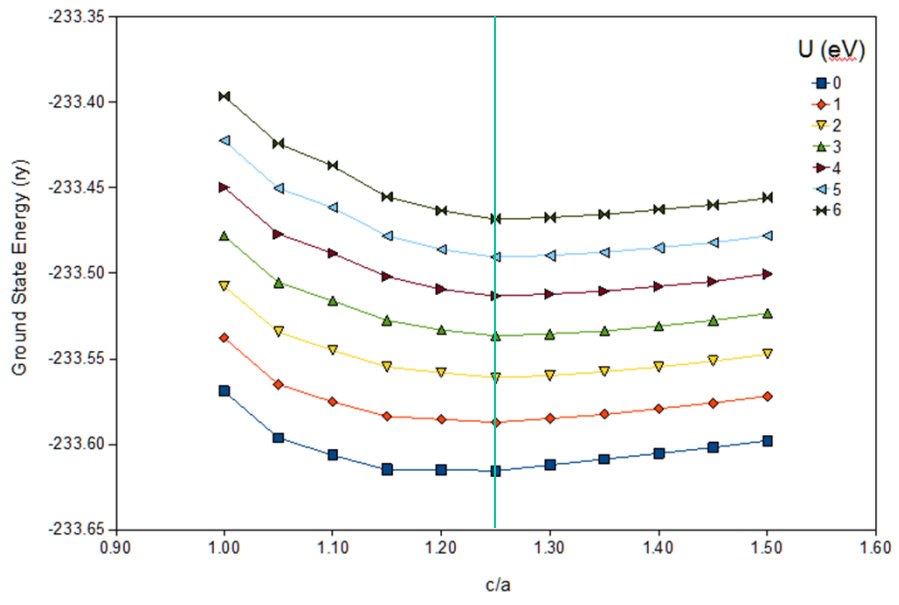
Tetragonal Rocksalt CuO

$Fm\bar{3}m$
 $a=3.905\text{\AA}$
 $b=3.905\text{\AA}$
 $c=5.320\text{\AA}$
 $\alpha=90.0^\circ$
 $\beta=90.0^\circ$
 $\gamma=90.0^\circ$
 $c/a = 1.36$

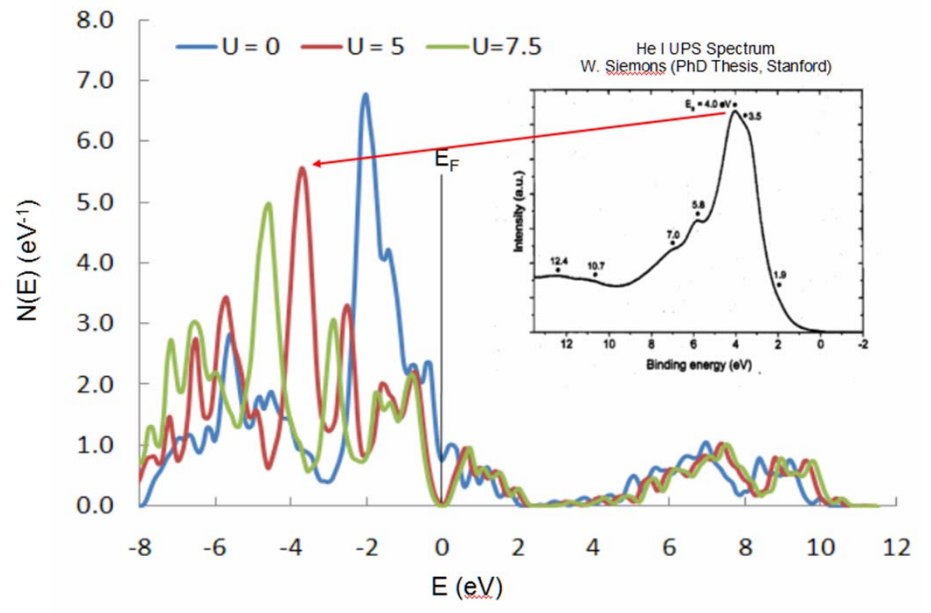
Measurements
 (Wolter Siemons)
 • 2-4 ML epi on STO
 • No Fermi Edge
 • No Exchange Bias on ferro-SRO ($T_c \sim 100-150\text{ K}$)



Ground State Energy vs c/a & U(eV)



t-CuO Density-of-States



References

The International Conference on Theoretical Physics 'Dubna-Nano2008'

IOP Publishing

Journal of Physics: Conference Series **129** (2008) 012042

doi:10.1088/1742-6596/129/1/012042

Electronic properties of rocksalt copper monoxide: A proxy structure for high temperature superconductivity

Paul M. Grant*

W2AGZ Technologies

“Electronic Properties of Rocksalt Copper Monoxide,”

APS MAR09-2008-006217, P. M. Grant, Pittsburgh (2009)

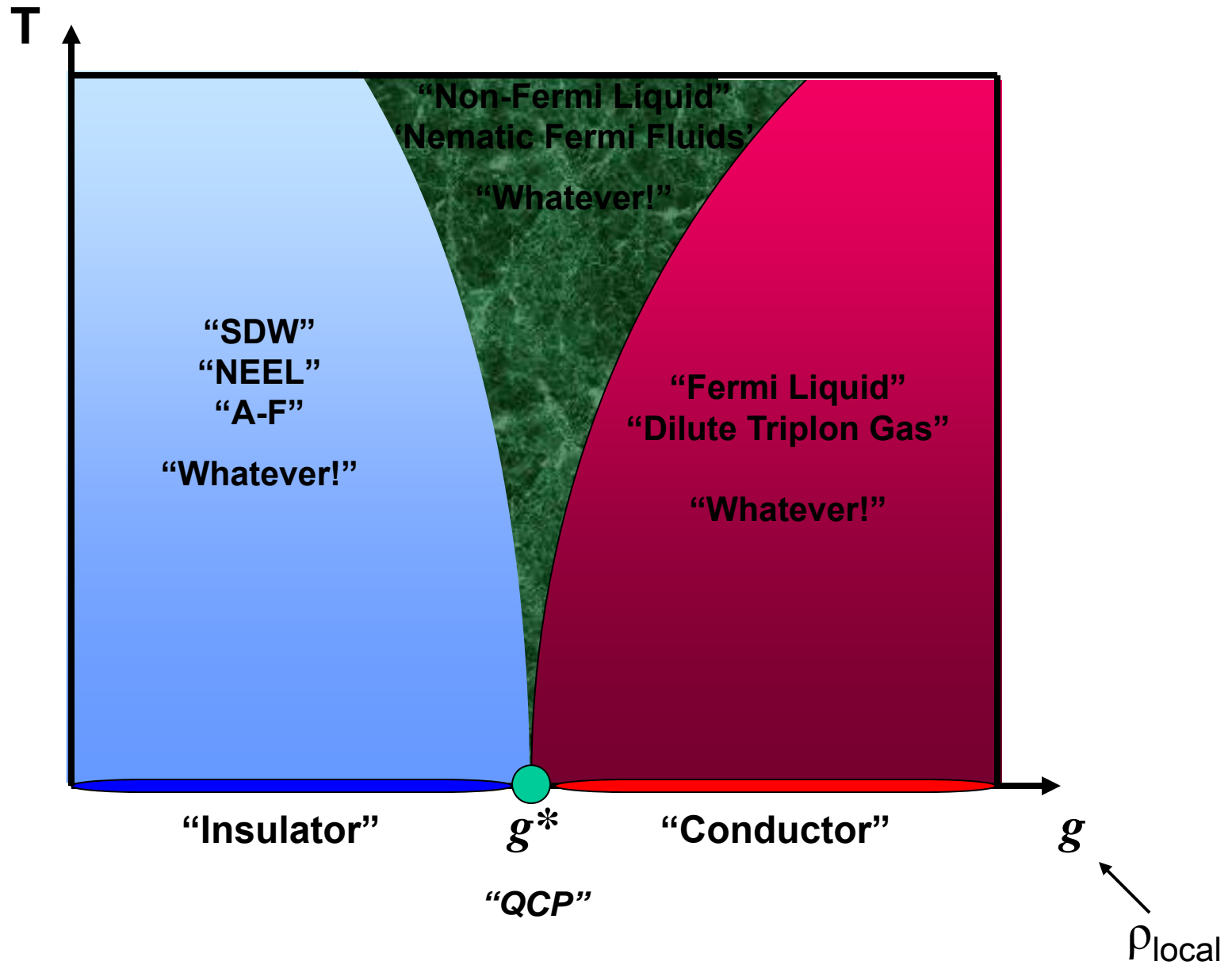
PHYSICAL REVIEW B **79**, 195122 (2009)



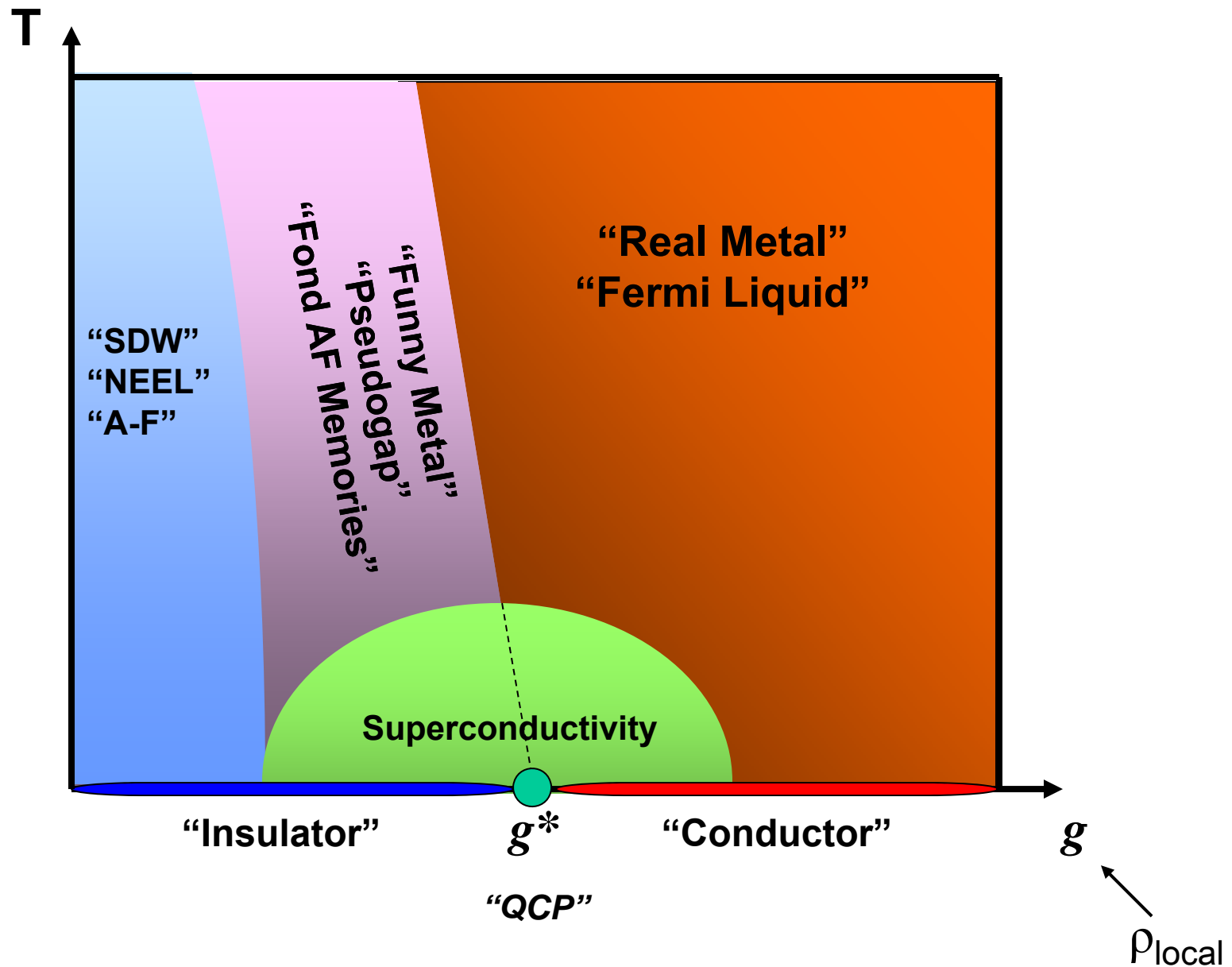
Tetragonal CuO: End member of the 3d transition metal monoxides

Wolter Siemons,^{1,2} Gertjan Koster,^{1,2,*} Dave H. A. Blank,¹ Robert H. Hammond,²
Theodore H. Geballe,² and Malcolm R. Beasley²

The Great Quantum Conundrum

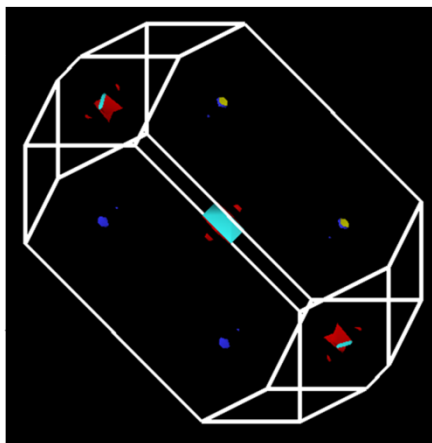
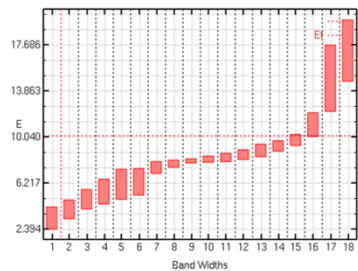


The Colossal Quantum Conundrum



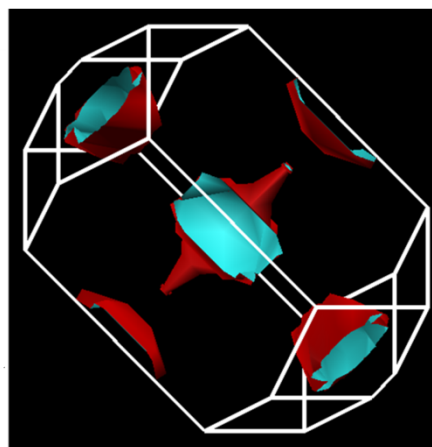
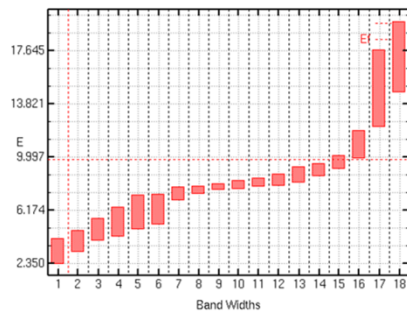
Hubbard (eV)

$U = 0$

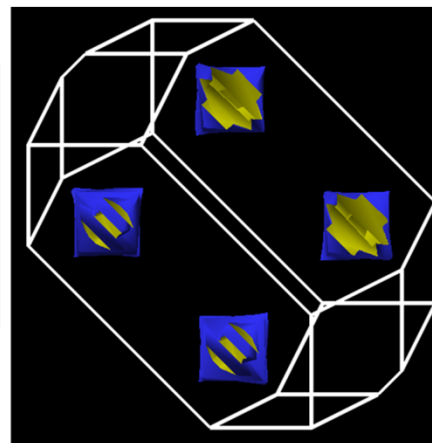
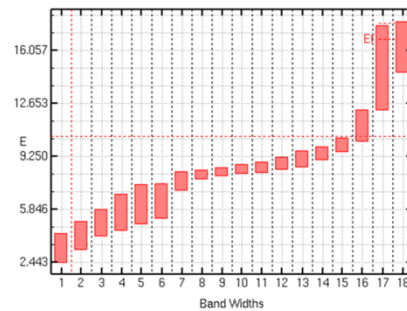


“Doping” (-e/CuO)

$n = 0.00$



$n = +0.15$

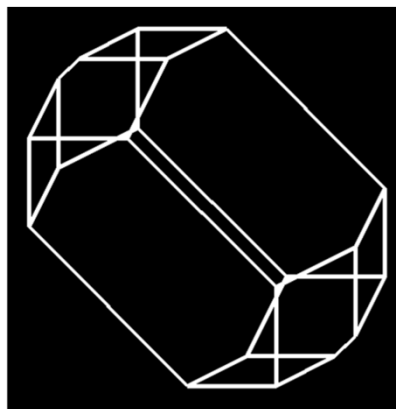
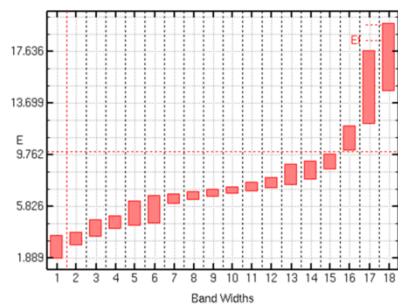


$n = -0.15$

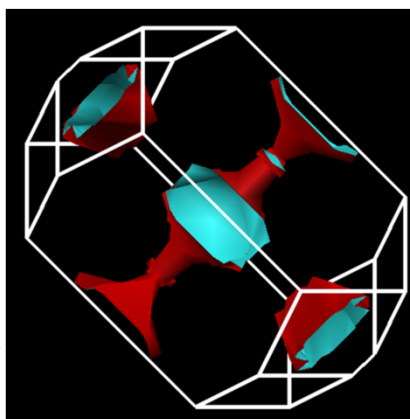
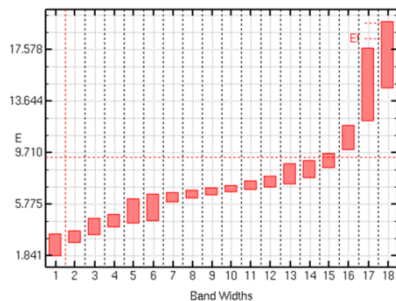
Hubbard (eV)

$U = 3$

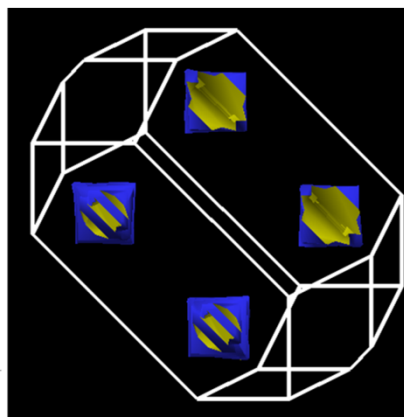
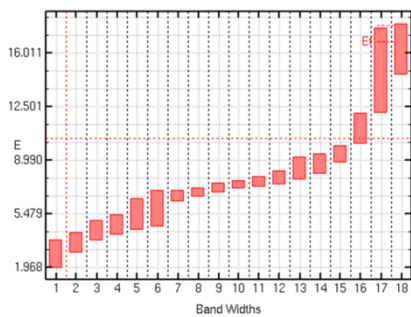
“Doping” ($-e/\text{CuO}$)



$n = 0.00$



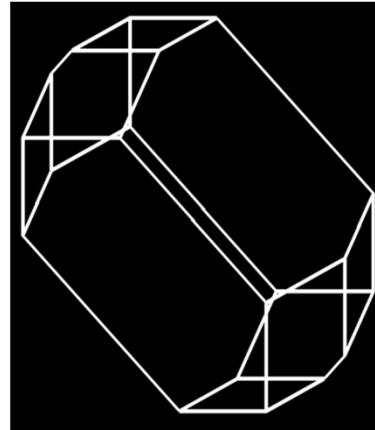
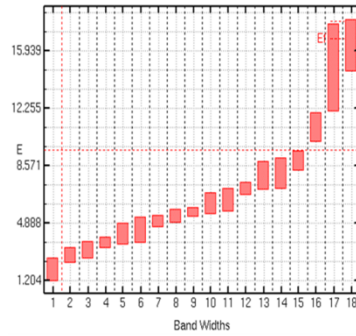
$n = +0.15$



$n = -0.15$

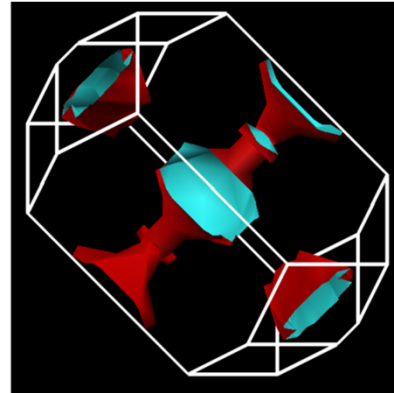
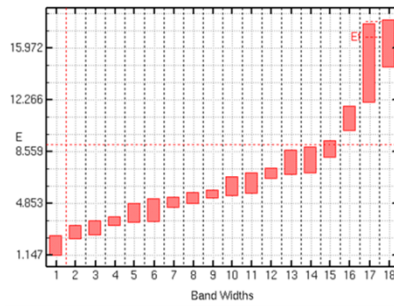
Hubbard (eV)

$U = 6$

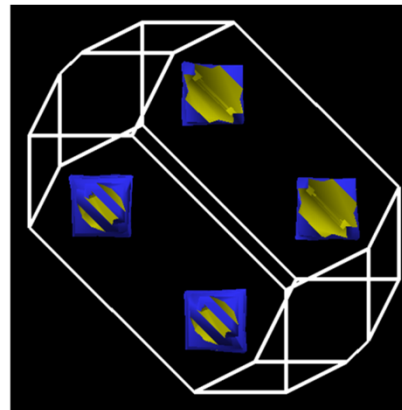
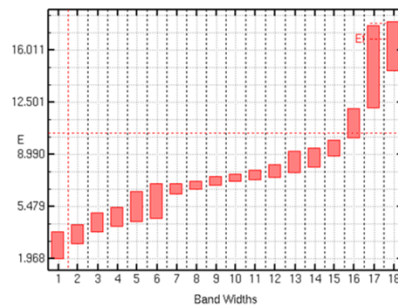


“Doping” (-e/CuO)

$n = 0.00$



$n = +0.15$



$n = -0.15$

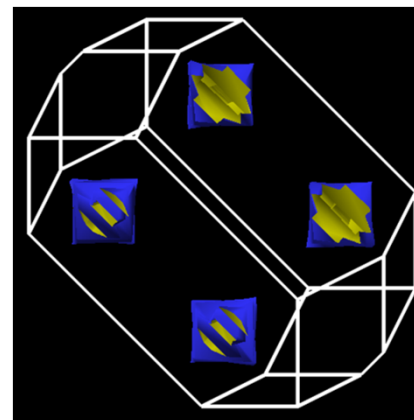
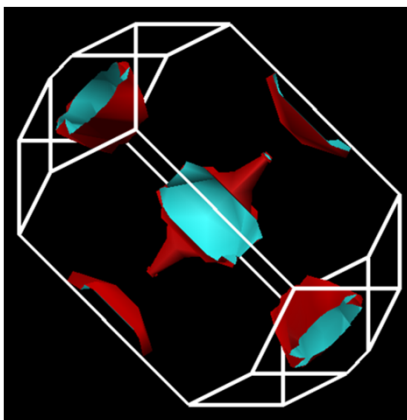
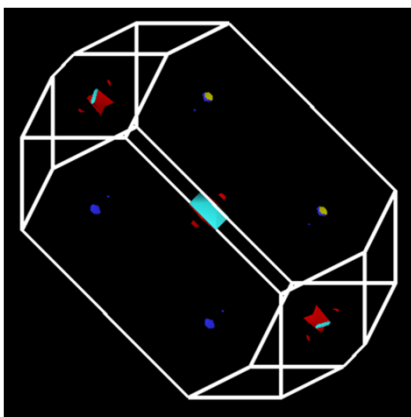
$\frac{U}{n}$

0.00

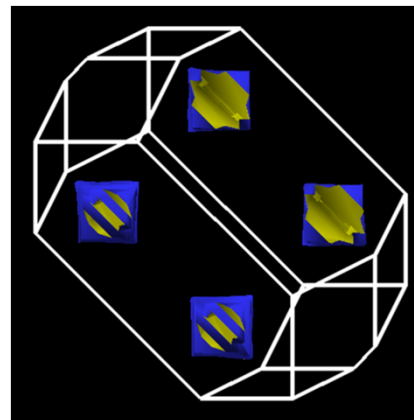
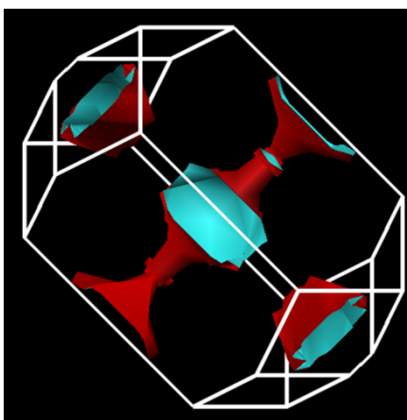
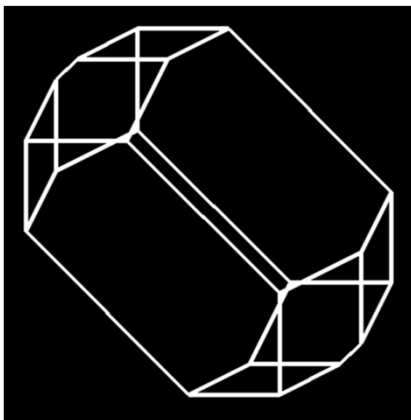
+0.15

-0.15

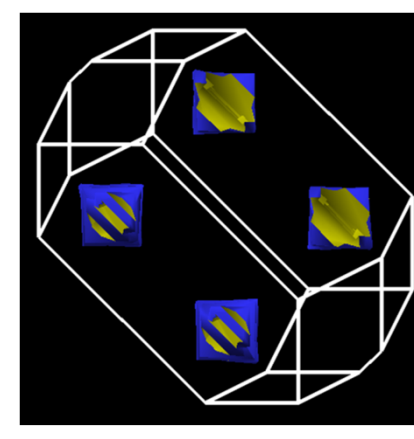
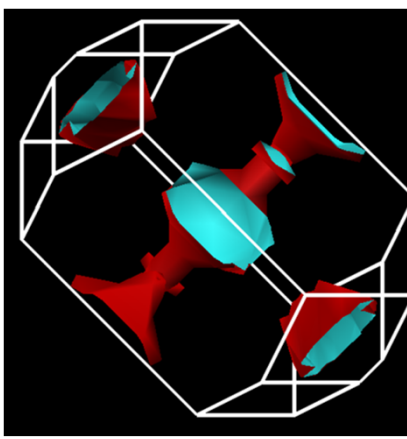
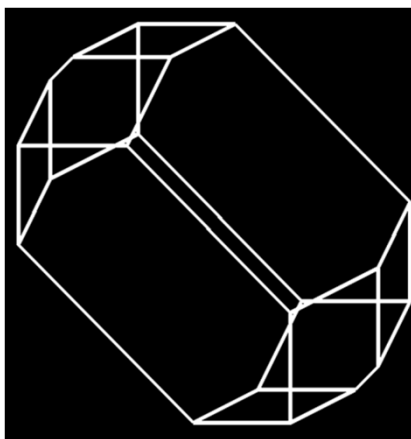
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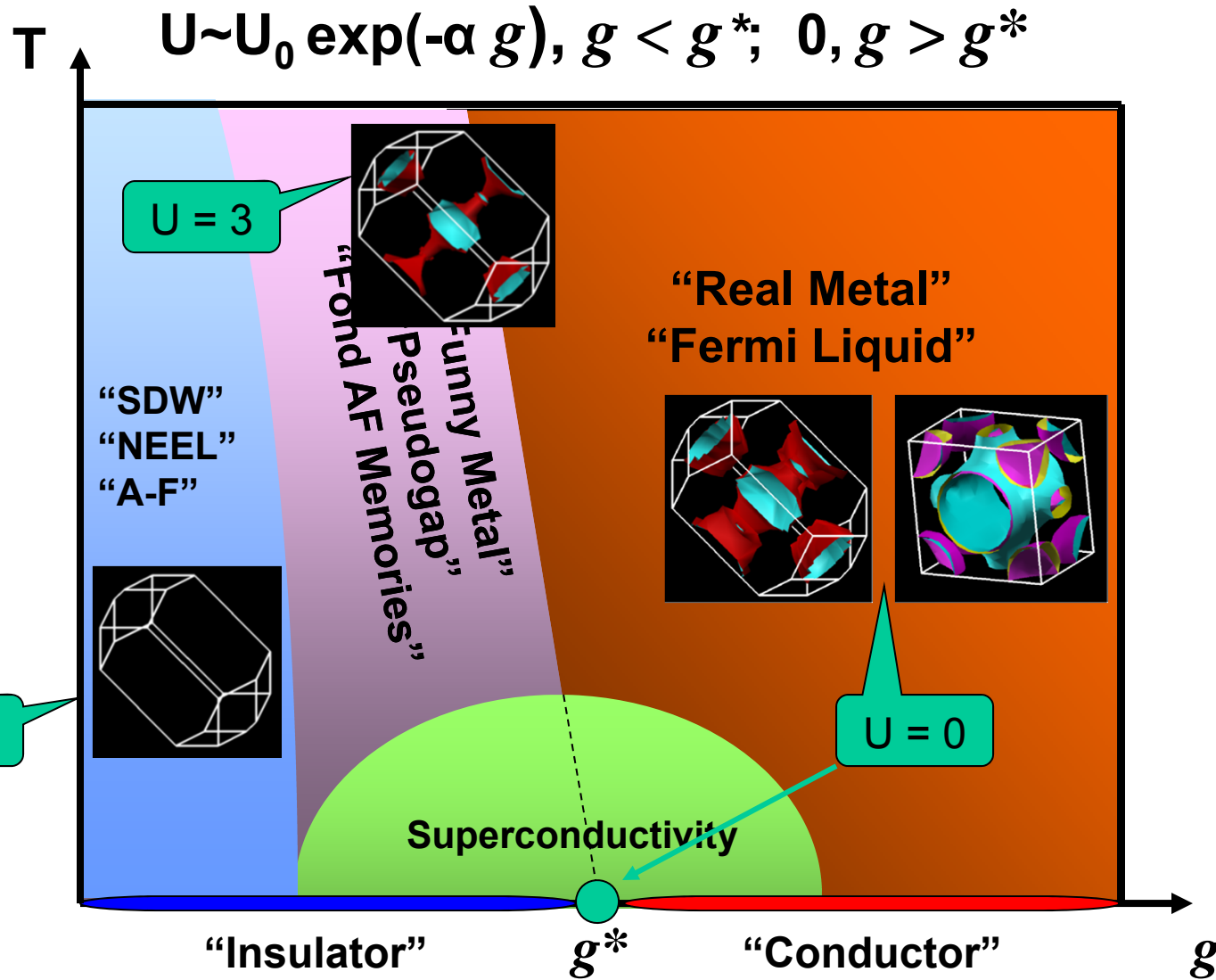
3



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)

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

What's the HTSC equivalent?

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

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

where the integral $\int d^2p$ is taken over the Fermi surface and the electron-phonon matrix elements are given by¹⁴

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

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

$$g_{\nu}(pp') = \int \psi_p^*(\mathbf{r}_{p-p'\nu}) \nabla \mathcal{U} \psi_{p'} d\mathbf{r}. \quad (21)$$

Generalized Linhard Function

$$\chi^0(\mathbf{q}, \omega) = \sum_{\mathbf{k}, \sigma} \frac{f(\mathbf{k}) - f(\mathbf{k} + \mathbf{q})}{\hbar\omega - (\varepsilon_{\mathbf{k} + \mathbf{q}} - \varepsilon_{\mathbf{k}}) + iDq^2}$$

$$D = \lim_{t \rightarrow \infty} \frac{1}{2t} \overline{\delta \mathbf{R}^2(t)}$$

$$V(\mathbf{q}) = 4\pi e^2 / q^2$$

$$\varepsilon(\mathbf{q}, \omega) = 1 - V(\mathbf{q})\chi^0(\mathbf{q}, \omega)$$

$$\varepsilon_1(x, y) = 1 + \frac{q_{\text{TF}}^2}{8k_F^2 x^2} \left\{ 1 + \frac{1}{8x} \left[(1 + b^2 x^2 - v_+^2) \ln \left[\frac{(1 + v_+)^2 + b^2 x^2}{(1 - v_+)^2 + b^2 x^2} \right] + (1 + b^2 x^2 - v_-^2) \ln \left[\frac{(1 + v_-)^2 + b^2 x^2}{(1 - v_-)^2 + b^2 x^2} \right] \right] \right. \\ \left. - \frac{b}{2} \left\{ v_+ \left[\arctan \left[\frac{1 - v_+}{bx} \right] + \arctan \left[\frac{1 + v_+}{bx} \right] \right] + v_- \left[\arctan \left[\frac{1 - v_-}{bx} \right] + \arctan \left[\frac{1 + v_-}{bx} \right] \right] \right\} \right\}$$

where

$$x = \frac{q}{2k_F}, \quad y = \frac{\hbar\omega}{4\varepsilon_F}, \quad q_{\text{TF}}^2 = \frac{4me^2 k_F}{\pi \hbar^2}, \quad b = \frac{2mD}{\hbar}, \quad v_{\pm} = x \pm y/x,$$

“Fluctuations?”
“Empirical?”

HO (1989)

Dielectric Response Function

$$G(\mathbf{k}, i\omega_n) = 1/(i\omega_n - \xi_{\mathbf{k}})$$

$$F(\mathbf{p}, i\omega_n) = -G(\mathbf{p}, i\omega_n)G(-\mathbf{p}, -i\omega_n)T_c \sum_{\mathbf{m}} \int [d^3k/(2\pi)^3] \\ \times V(\mathbf{p} - \mathbf{k}, i\omega_n - i\omega_{\mathbf{m}})F(\mathbf{k}, i\omega_{\mathbf{m}})$$

$$V(\mathbf{q}, i\omega_n) = \frac{4\pi e^2}{q^2} \left[1 - \int_0^\infty \frac{dE^2 \rho(\mathbf{q}, E)}{\omega_n^2 + E^2} \right]$$

In principle, KMK can calculate the BCS gap for general “bosonic” fields, be they phonons, magnons, spin-ons, excitons, plasmons...or morons!

Bottom Line

Can studying CuO proxies with DFT

+ LDA+U

+ phonons

+ spins

provide insight into the origins of High- T_C ?

I say “Yes,” but...

Size Matters...

...and I need a...

BIGGER COMPUTER!

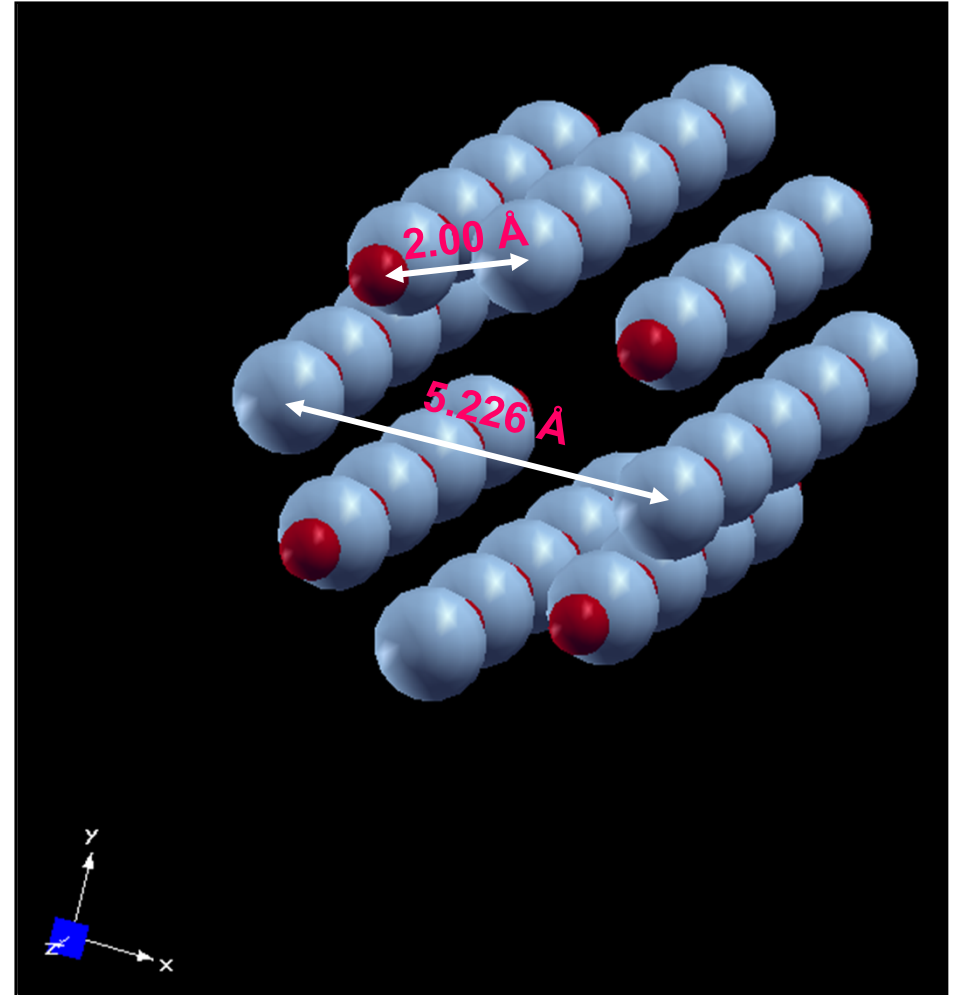
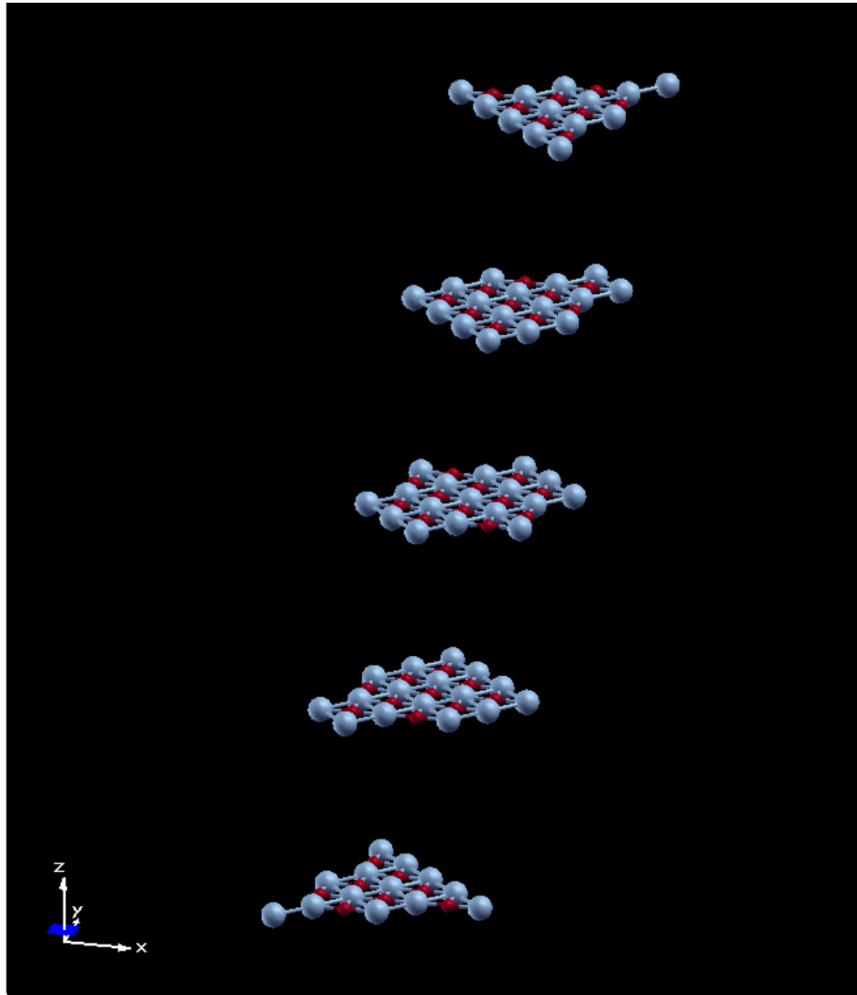
Other CuO Proxy Structures

- Studies in Progress -

Films

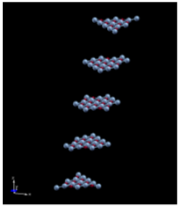
&

Tubes



$a = b = 3.905 \text{ \AA}$
 $c = 6 \times 3.905 = 23.43 \text{ \AA}$

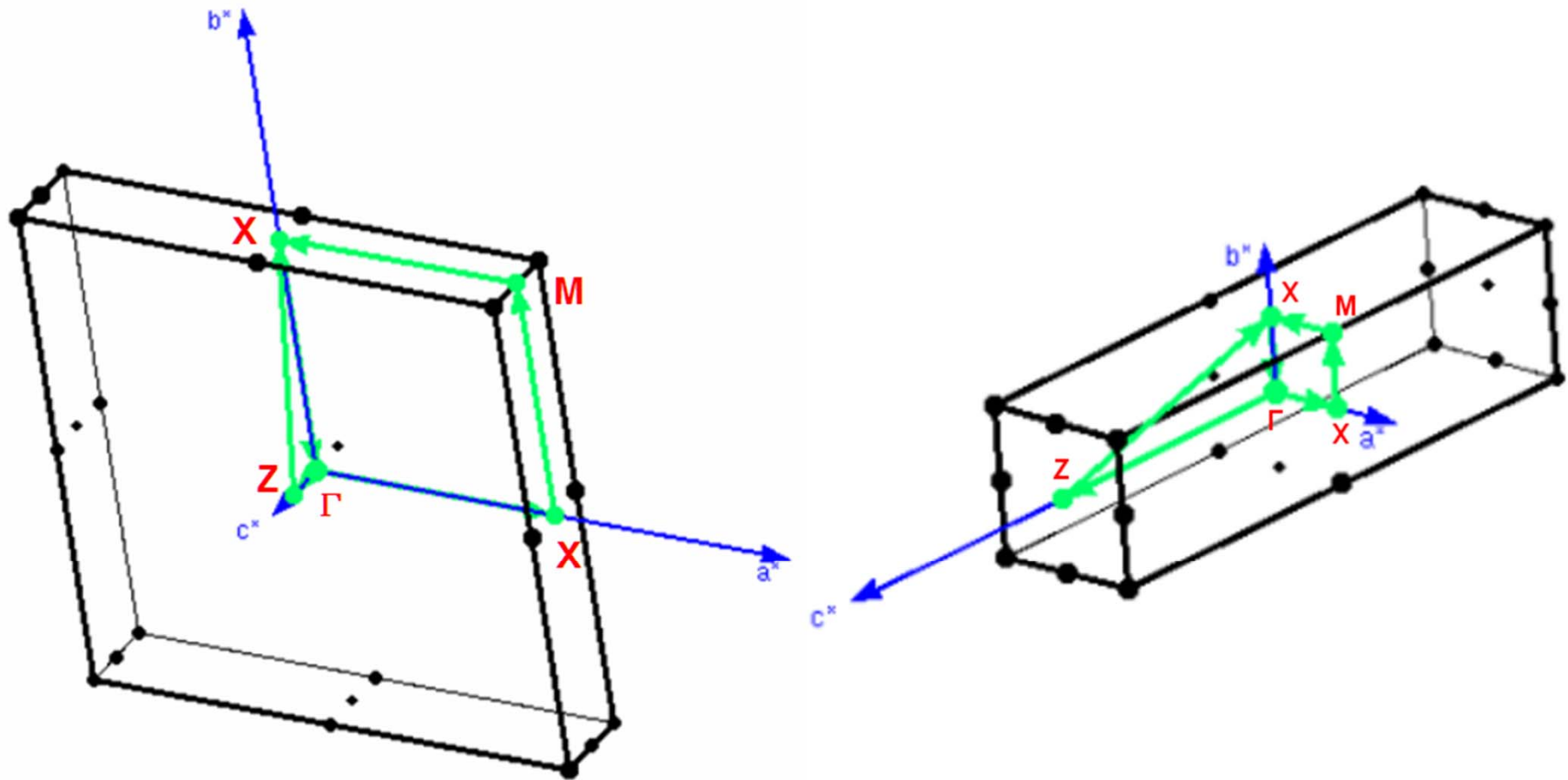
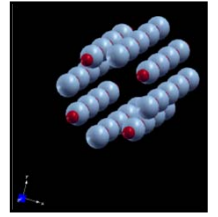
2 CuO segments per quadrant
16 \AA between tubes

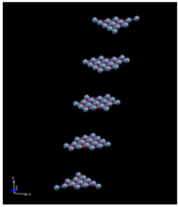


Films

&
Zones

Tubes

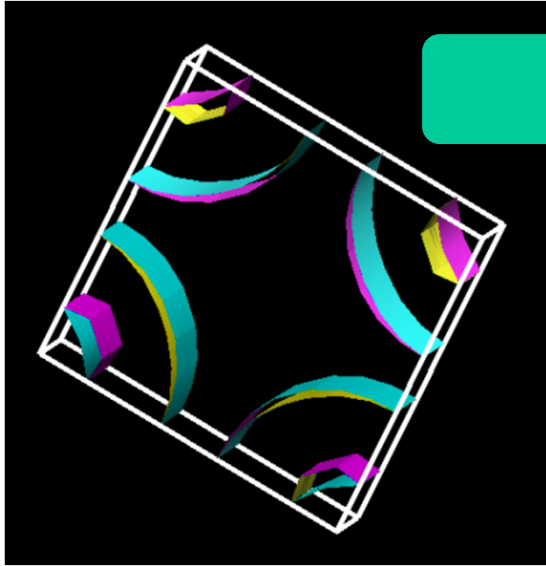
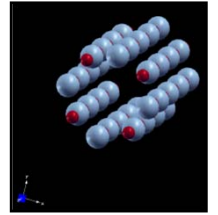




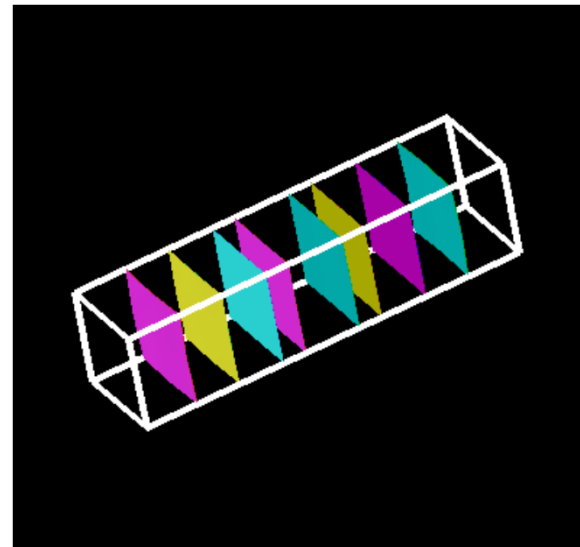
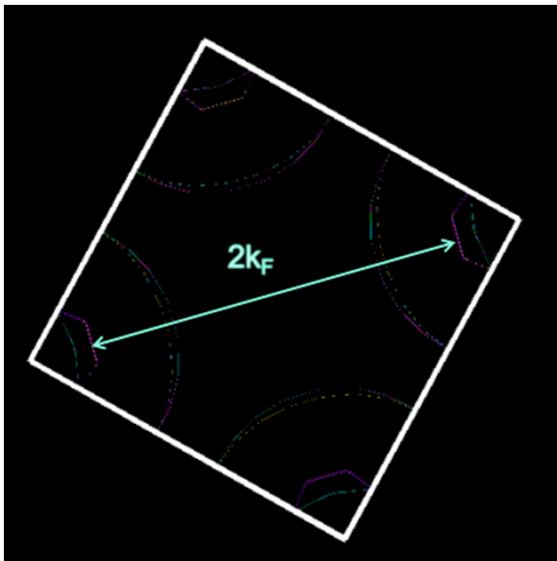
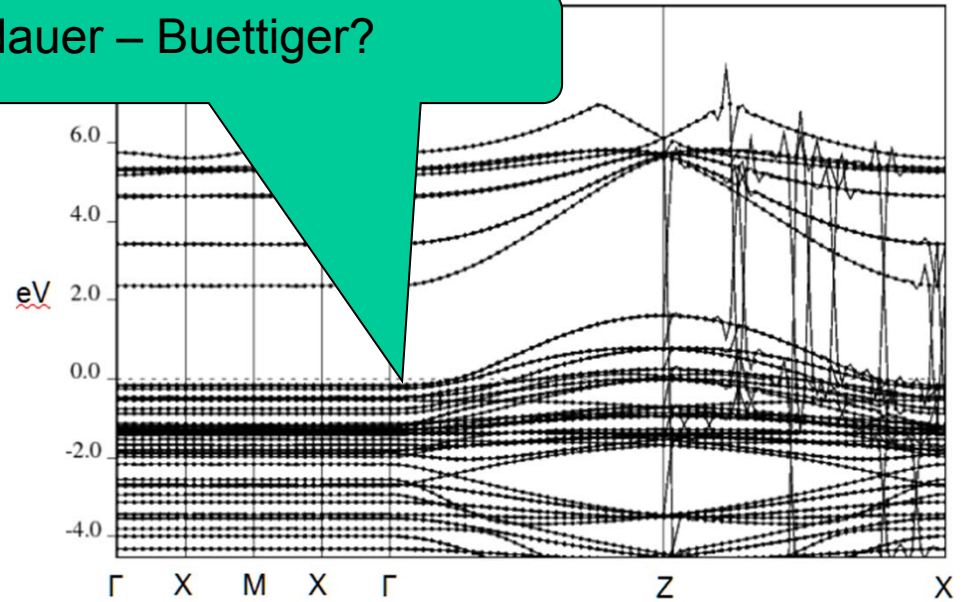
Films

&
States

Tubes



Landauer – Buettiger?



-- OK...Enough Already !

-- That's all for now !

-- But Stayed Tuned...