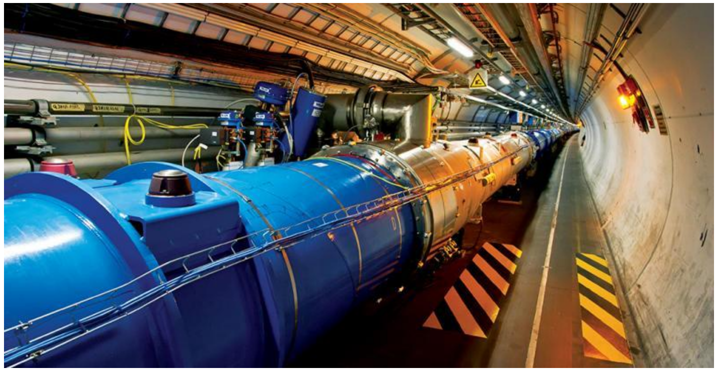




From Electrons Paired to Electrons Delivered

-Challenges Facing the Path Forward for High Temperature Superconductivity from Its Fundamental Understanding to Eventual Societal Deployment-

Paul Michael Grant

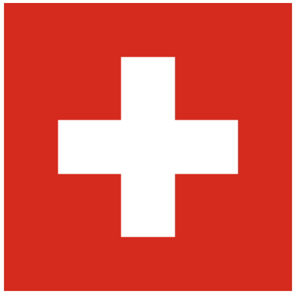
EPRI Science Fellow (Retired)

IBM Research Staff Member/Manager Emeritus

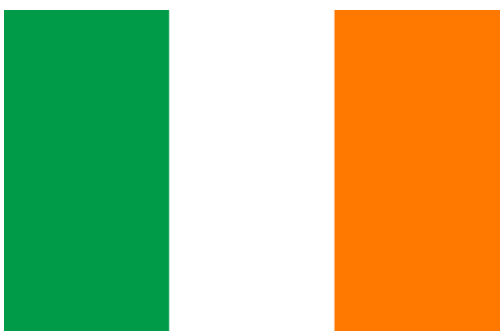
(etc, etc...& so forth and so on)

W2AGZ Technologies, USA (w2agz@w2agz.com)

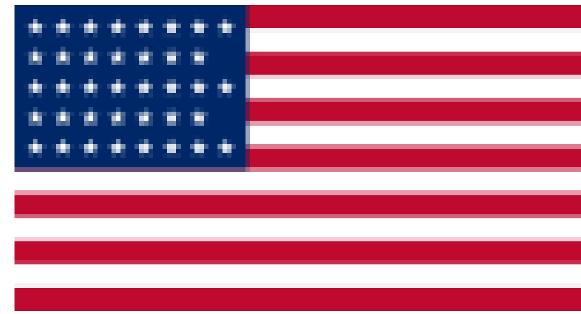
Aging IBM Pensioner



Grandson of Two Proud Lands

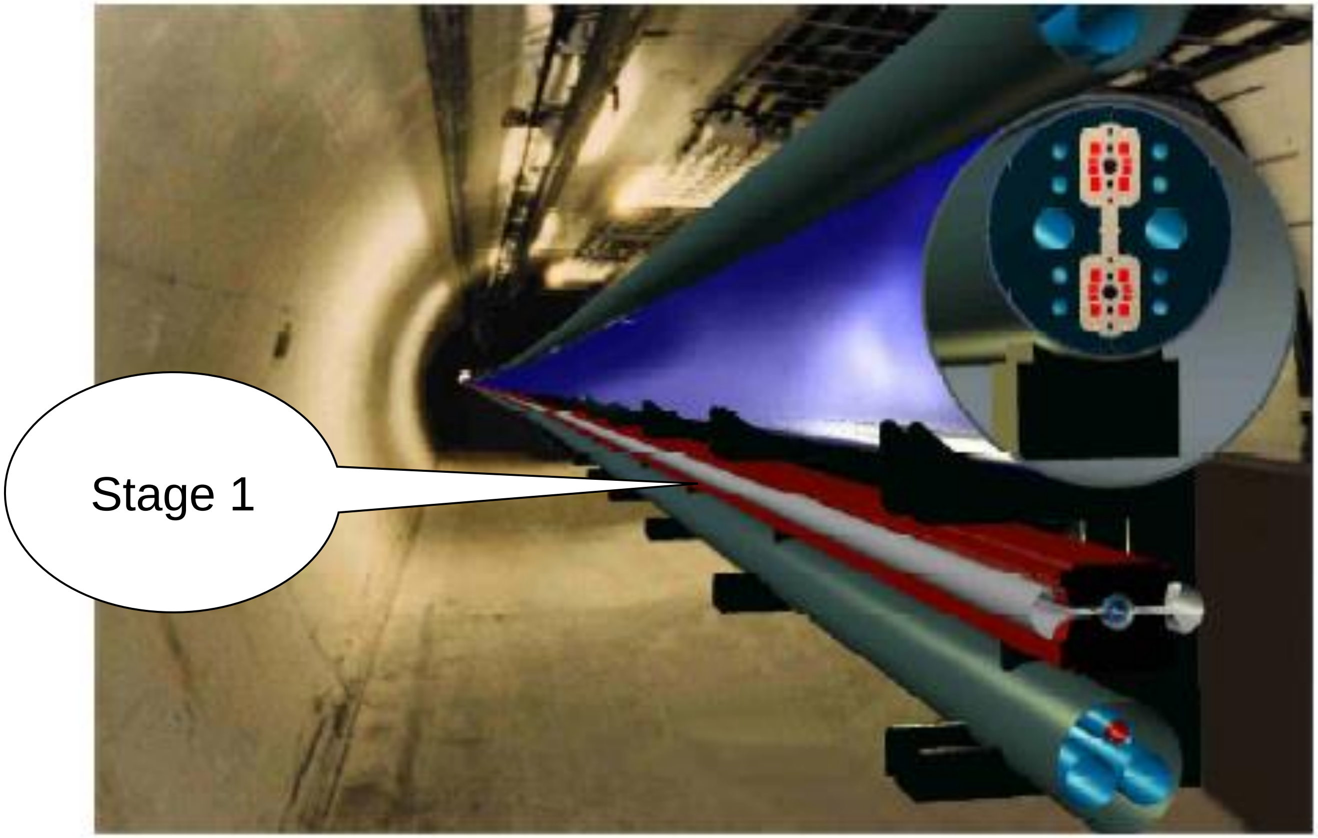


Bridget Ann Mullen-Whalen



"The Pipetron"

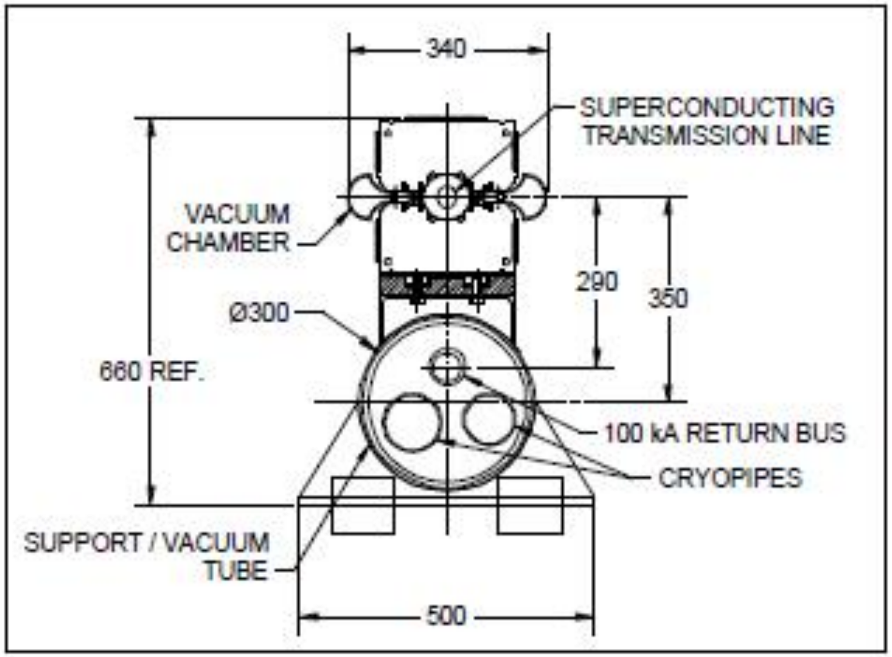
Design Study for a Staged Very Large Hadron Collider



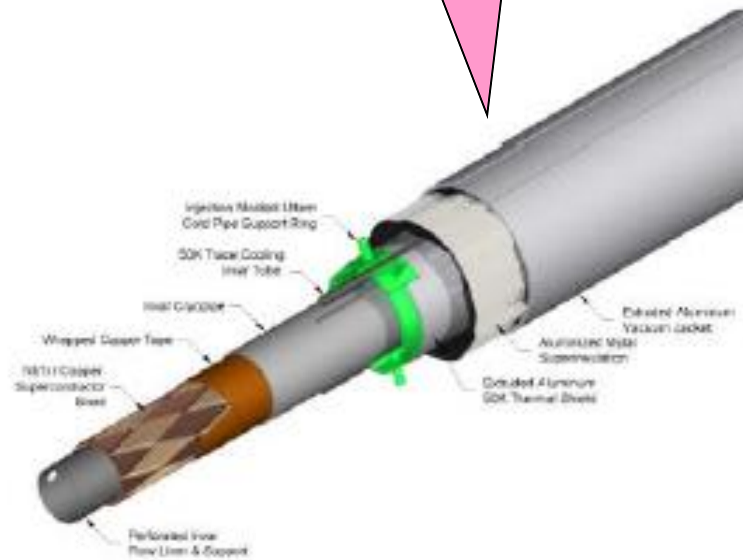
Peter Limon & Bill Foster (Fermilab VLHC Proposal, 2001)

Stage 1

Replace with HTSC?



Cross-section of Stage-1 superferric magnet



100 kA superconducting transmission line

40 Tev CoM, 233 km Circumference Ring

Interlaken 1988

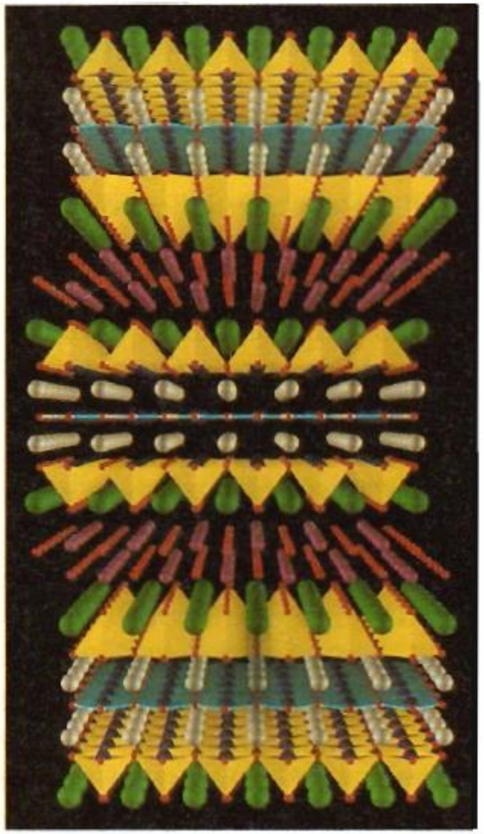


Fig. 6. $Tl_2Ba_2Ca_2Cu_3O_{10+y}$; same representation as $Tl_2Ba_2CaCu_2O_{8+y}$ (Fig. 5). For the remaining color coding see Figure 1.

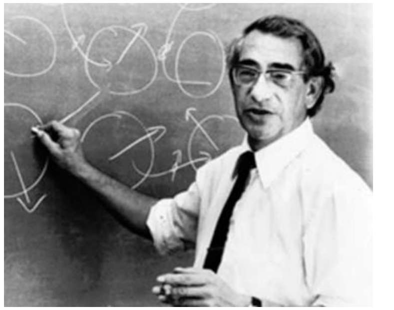
M2S Interlaken '88 – Tc 125 K Tl-2223

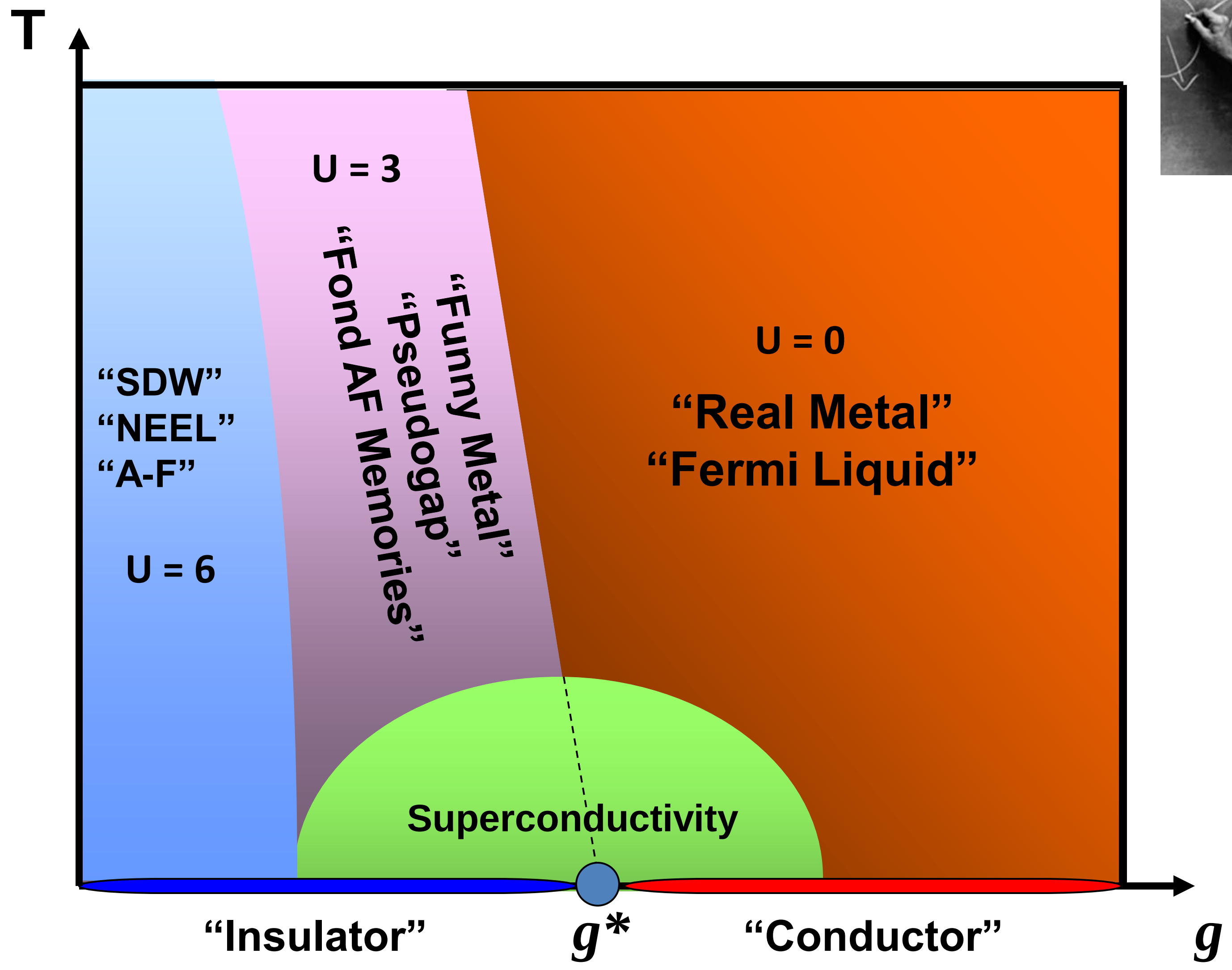
My Mexican Connection

Diego Patrick Lopez-Morales de Grant

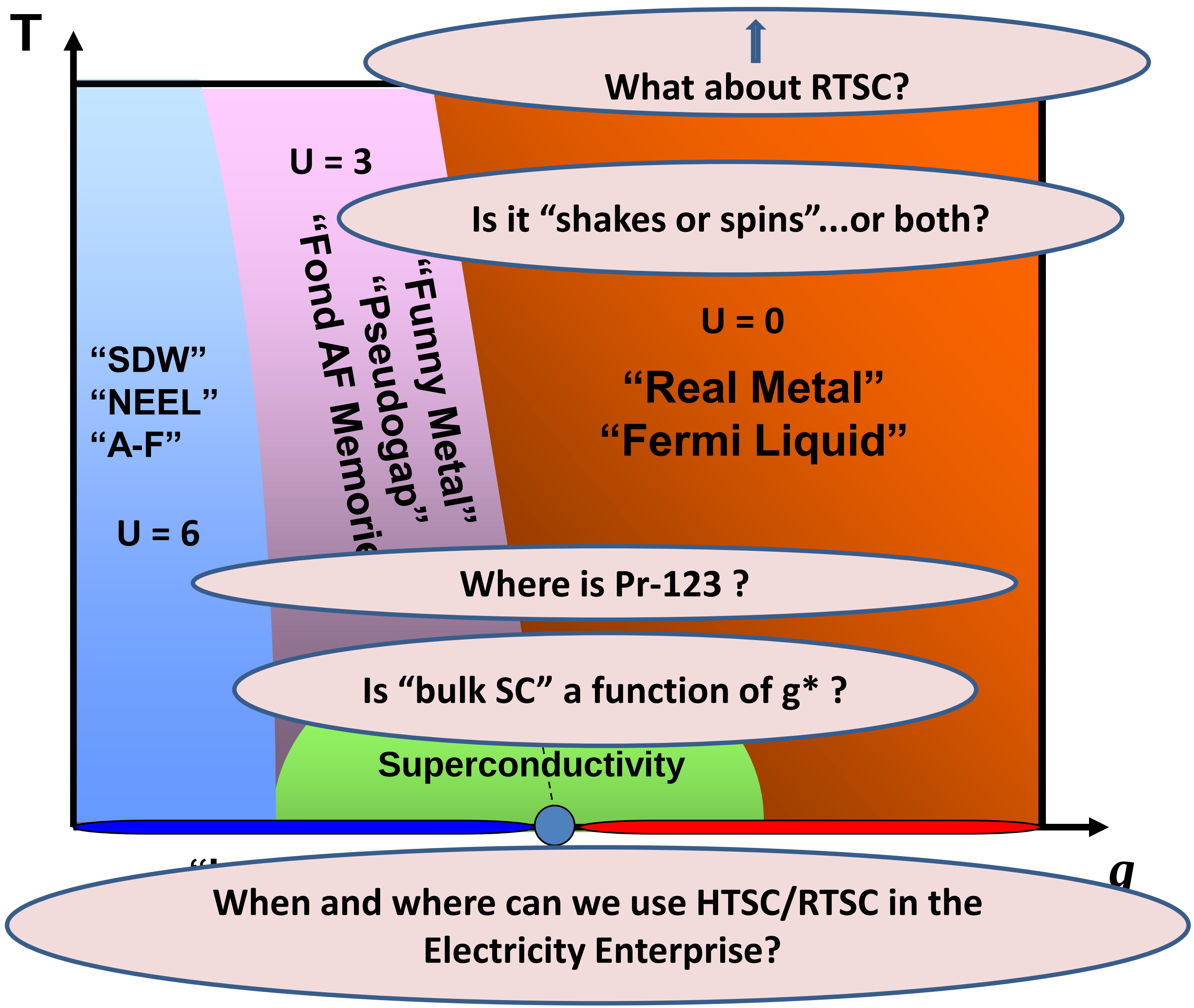
…hanging out with the Swiss!

The Colossal Quantum Conundrum (According to John Hubbard)

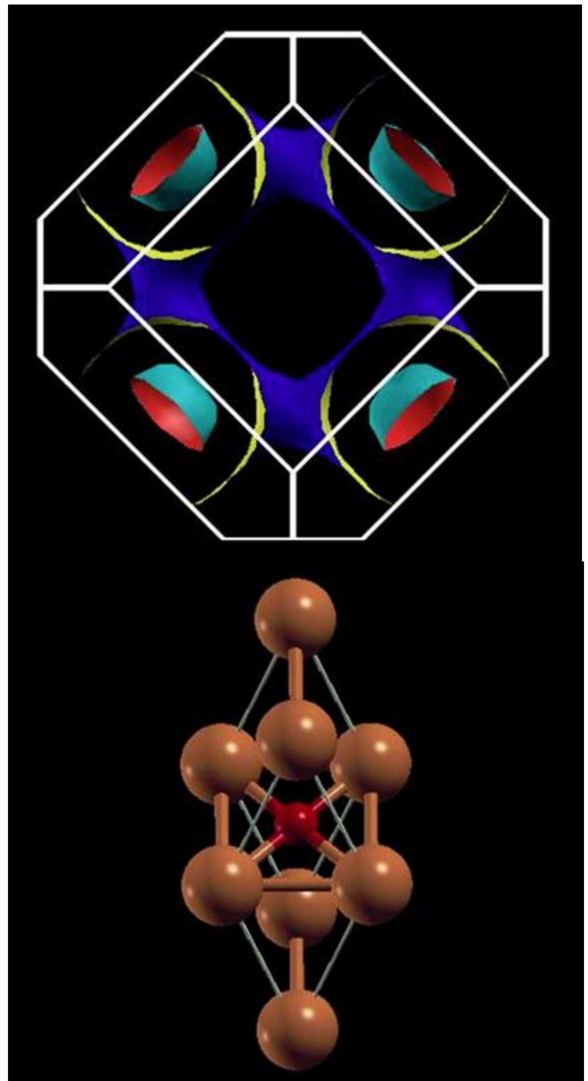




Five HTSC "In Your Face" Questions



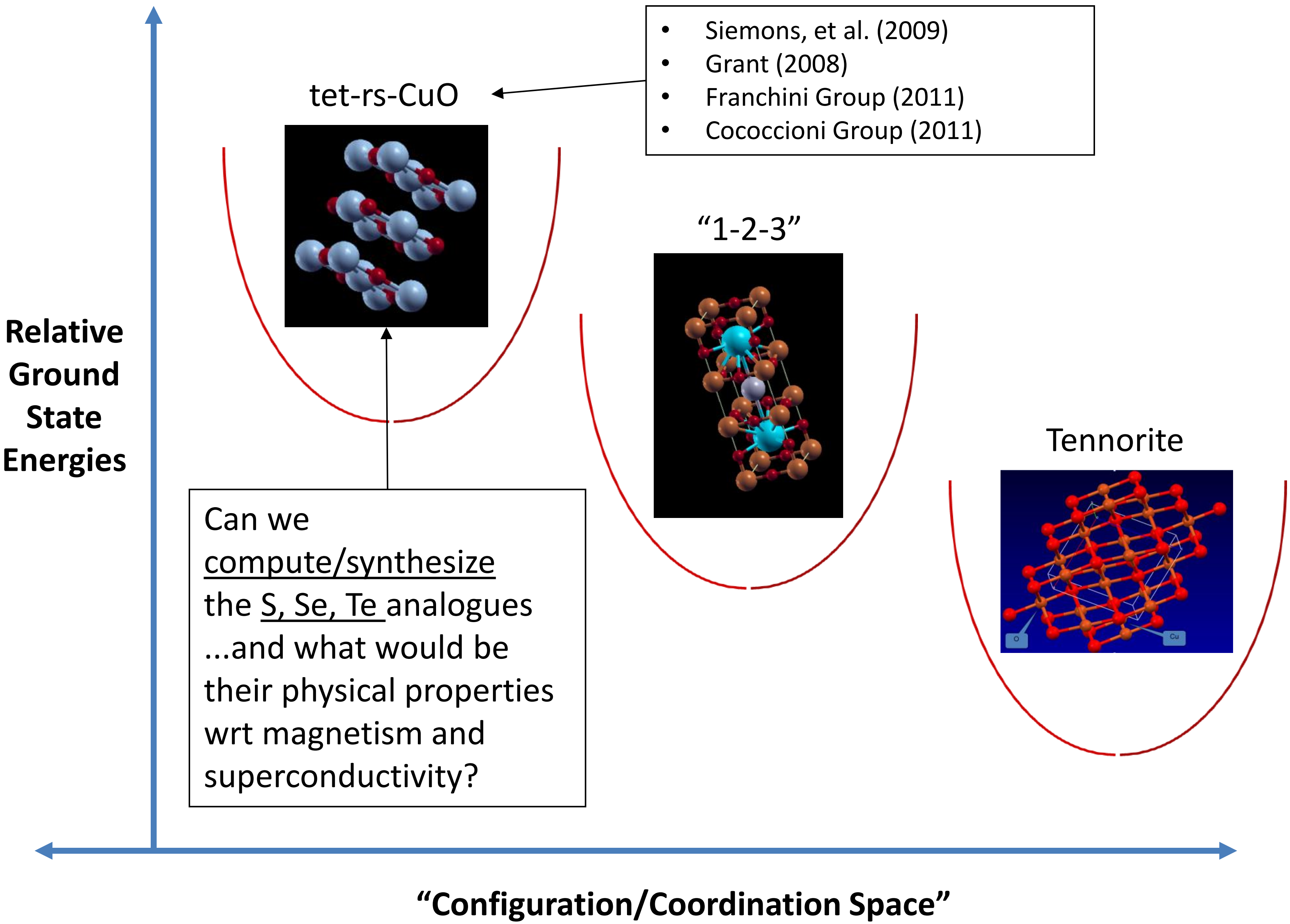
The Holy Grail of HTSC



Shakes and/or Spins?

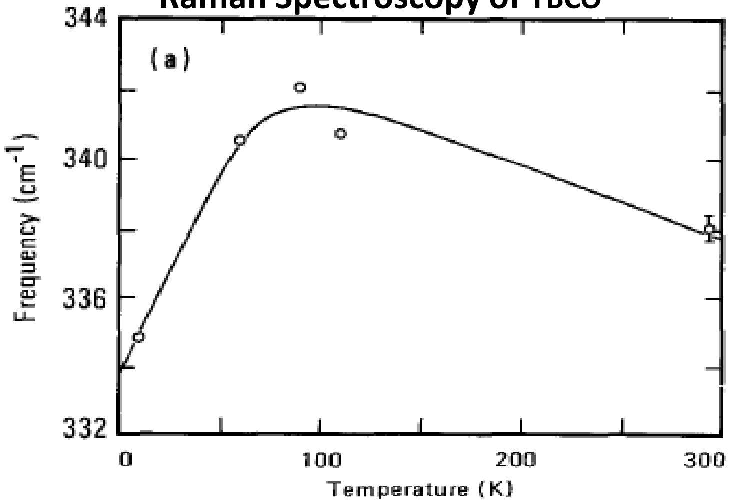
It takes two to Tango

The Various Flavors of Copper “Monoxide”

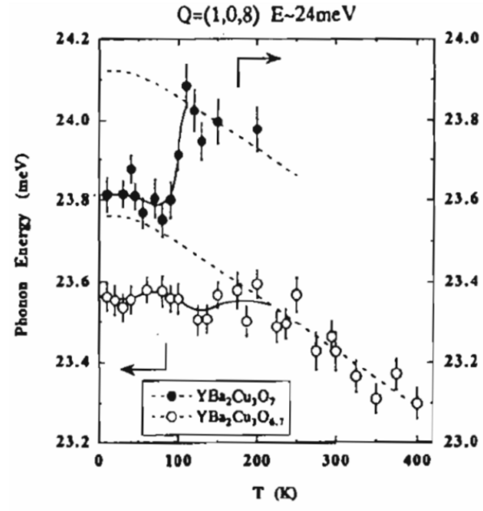


So What Else is New?

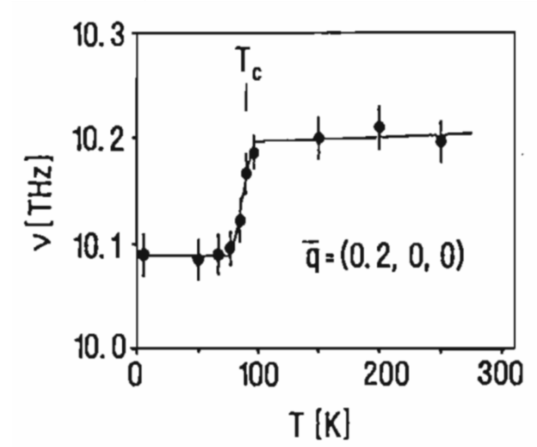
Macfarlane, Rosen, Seki, SSC 63, 831 (1987)
Raman Spectroscopy of YBCO



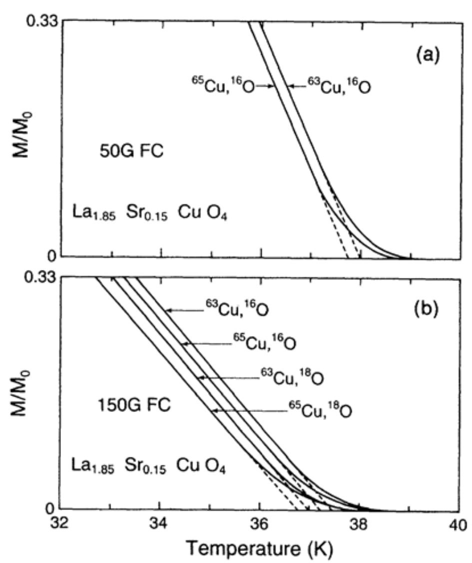
Harashima, et al., Physica C263, 257 (1996)



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

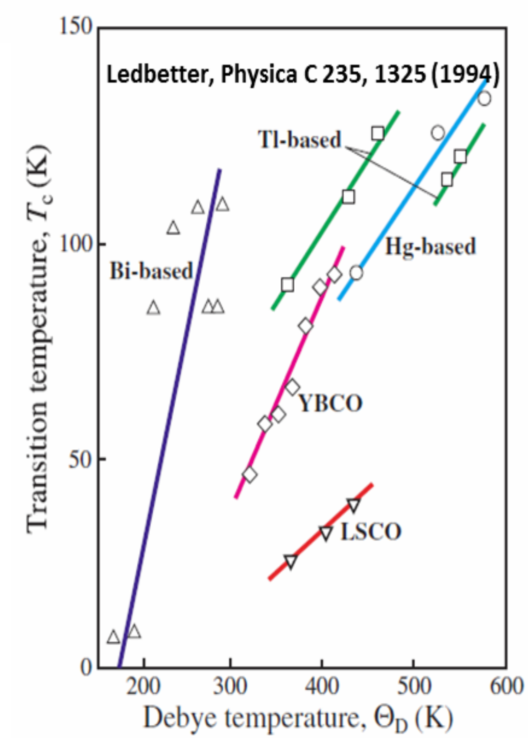


Franck, Harker, Brewer, PRL 71, (1993)
Cu and O Isotope Effects in $La_{2-x}Sr_xCuO_4$

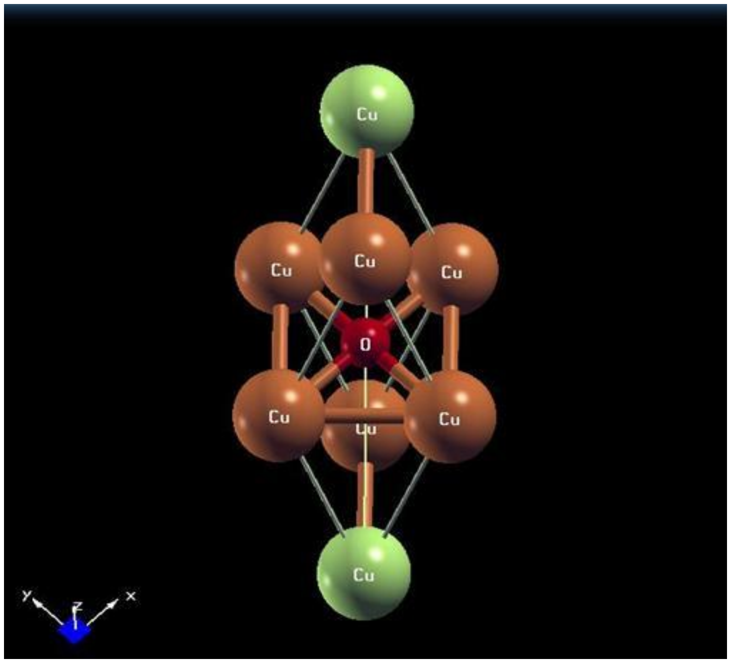


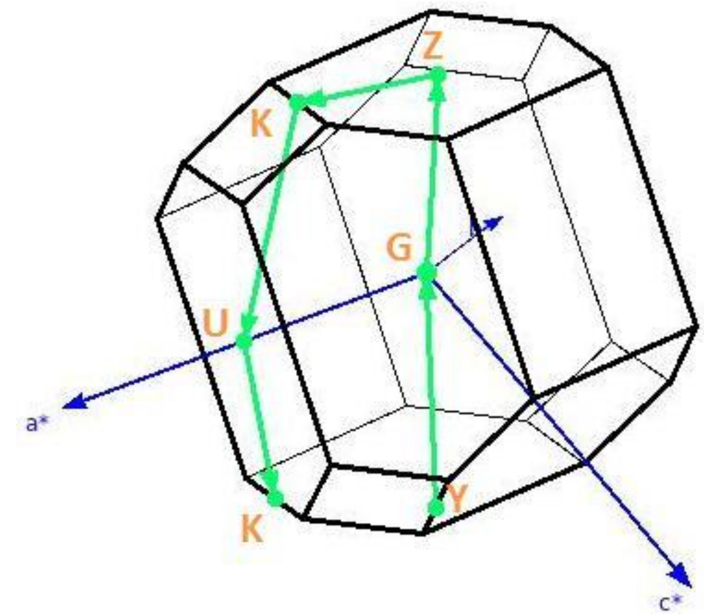
We can see Phonons have been there ever since the Creation!

Ledbetter, Physica C 235, 1325 (1994)



Well, how about the "U = 0, Fermi Liquid" limit for doped proxy tet-CuO?





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

The International Conference on Theoretical Physics 'Dubna-Nano2008'
IOP Journal of Physics: Conference Series 129 (2008) 012042
doi:10.1088/1742-6596/129/1/012042

Superconductivity and Phonons

BCS via Eliashberg-McMillan

$$H_{el-ph} = \sum_{\mathbf{k},\mathbf{q},\nu} g_{\mathbf{k+q},\mathbf{k}}^{\mathbf{q}_\nu,mn} c_{\mathbf{k+q}}^{\dagger m} c_{\mathbf{k}}^{n} (b_{-\mathbf{q},\nu}^{\dagger} + b_{\mathbf{q},\nu})$$

$$\lambda_{\mathbf{q},\nu} = \frac{2}{N(\varepsilon_F)\omega_{\mathbf{q},\nu}} \sum_{mn} \sum_{\mathbf{k}} \left| g_{\mathbf{k+q},\mathbf{k}}^{\mathbf{q}_\nu,mn} \right|^2 \delta(\varepsilon_{\mathbf{k+q},m} - \varepsilon_F)\delta(\varepsilon_{\mathbf{k},n} - \varepsilon_F)$$

$$\alpha^2 F(\omega) = \frac{1}{N(\varepsilon_F)} \sum_{mn} \sum_{\mathbf{q},\nu} \delta(\omega - \omega \quad \ldots \quad \varepsilon_F)$$

$$\lambda = 2\int_0^\infty \frac{\alpha^2 F}{\omega} \ldots$$

NB! The "double deltas" will be approximated by two Gaussians of width "sigma (σ)" whose numerical convergence is governed by imposed precision limits and basis set symmetry. Con Quidado!

To get λ, need to compute $g_{\mathbf{k+q},\mathbf{k}}$!

e-p Interaction in the DFT/LDA Formalism

$$g_{\mathbf{k}+\mathbf{q},\mathbf{k}}^{\mathbf{q}\nu,mn} = \sqrt{\hbar / 2\omega_{\mathbf{q},\nu}} \left\langle \psi_{\mathbf{k}+\mathbf{q},m} \left| \Delta V_{KS}^{\mathbf{q},\nu} \right| \psi_{\mathbf{k},n} \right\rangle$$

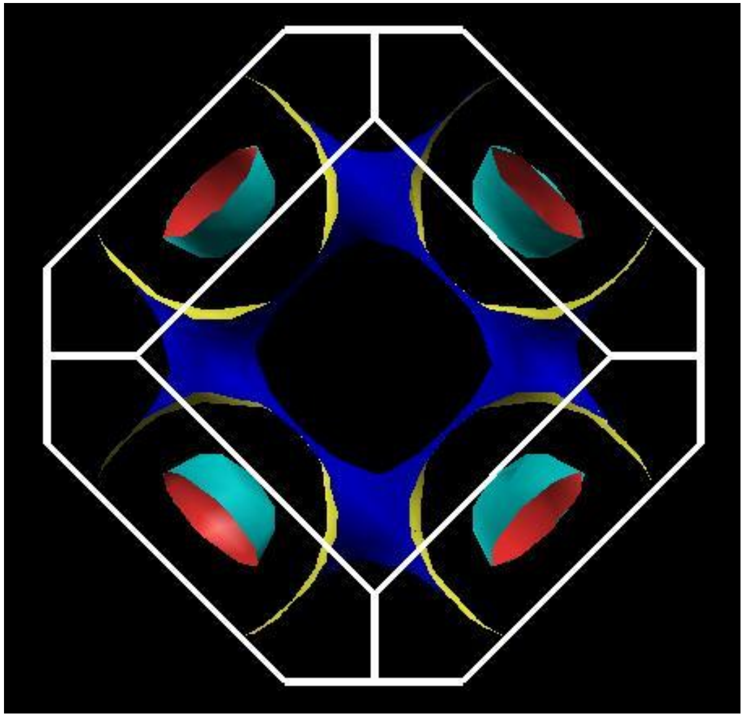
$$\Delta V_{KS}^{\mathbf{q},\nu} = \sum_{\mathbf{R}} \sum_{s} \frac{\partial V_{KS}}{\partial \vec{u}_{s,\mathbf{R}}} \cdot \vec{u}_s^{\mathbf{q},\nu} \frac{e^{i\mathbf{q}\cdot\mathbf{R}}}{\sqrt{N}}$$

$$T_C = \frac{\Theta_D}{1.45} \exp\left(-\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)} \right)$$

So let's do it and "compute*" what happens!

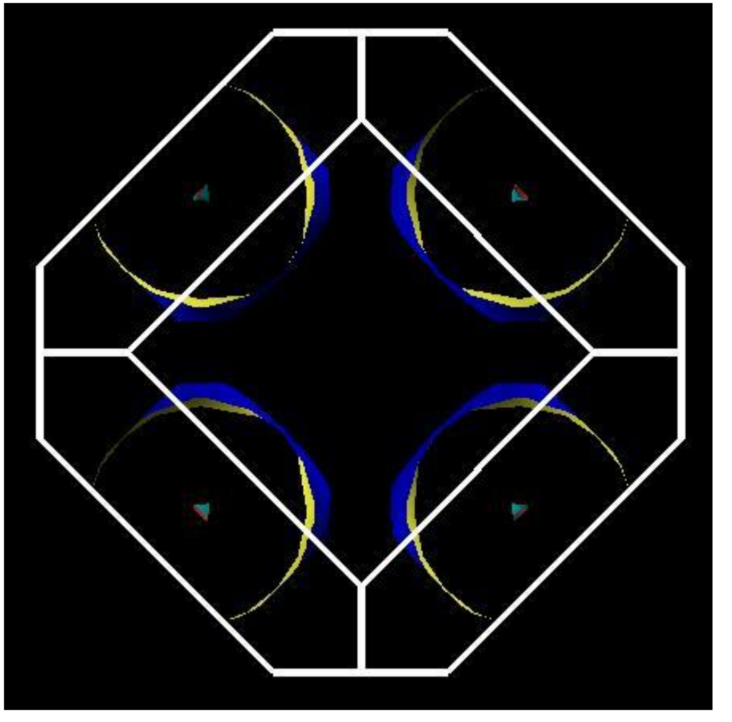
(*we use the Quantum-Espresso & Gibbs2 DFT packages)

q = 0.15 |e|/CuO (holes)



≈ 43 °K

q = -0.15 |e|/CuO (electrons)



≈ 25 °K

Apply DFT to obtain $g^{\mathbf{q}\nu,mn}_{\mathbf{k+q},\mathbf{k}}$ between electrons and phonons, followed by application of the Eliashberg-McMillan-Allen-Dynes formalism to find Tc:

Copper Monochalcogenides

Grant-Hammond, APS March 2015

- For X = S, Se and Te, neither a finite U or a “5% basal” tetragonal distortion has much effect on their respective CuX Fermiologies, and likely transport/magnetic properties dependent thereon.
- However, the respective Fermi surfaces ...may...may... contain nesting topologies promoting itinerant antiferromagnetism a la Cr, but, unlike Cr, here for X = S, Se, Te, the DOS at Ef is dominated by p-like chalcogenide overlap.
- Future homework for proxy structure modelling, suggested by preliminary results on “doped” tet-CuO: Let’s look for electron-phonon mediated superconductivity!
- But ...most importantly... experiment *always* rules. Our fundamental computational finding is that equilibrium rocksalt CuS, CuSe and CuTe structures can in principle exist ...so let’s try to make and dope them and henceforth measure their properties!

Finally, there <u>is</u> something quite special about the Cu-O bond in square-planar symmetry!

<u>...but we knew that already... in 1986 B & M told us so!</u>

Paramagnetic Dispersion Measurements at 77.3°K*

C. STARR
Massachusetts Institute of Technology, Cambridge, Massachusetts

(Received June 7, 1941)

The dispersion of the magnetic susceptibility of some paramagnetic compounds of Fe, Mn, and Cr, was studied at 77.3°K over a frequency range of 2 to 10 megacycles/sec. with magnetic fields up to 60,000 gauss. The results substantiate the theory of Casimir and du Pre, which is based upon the thermal coupling between the magnetic spin system and the lattice vibrations.

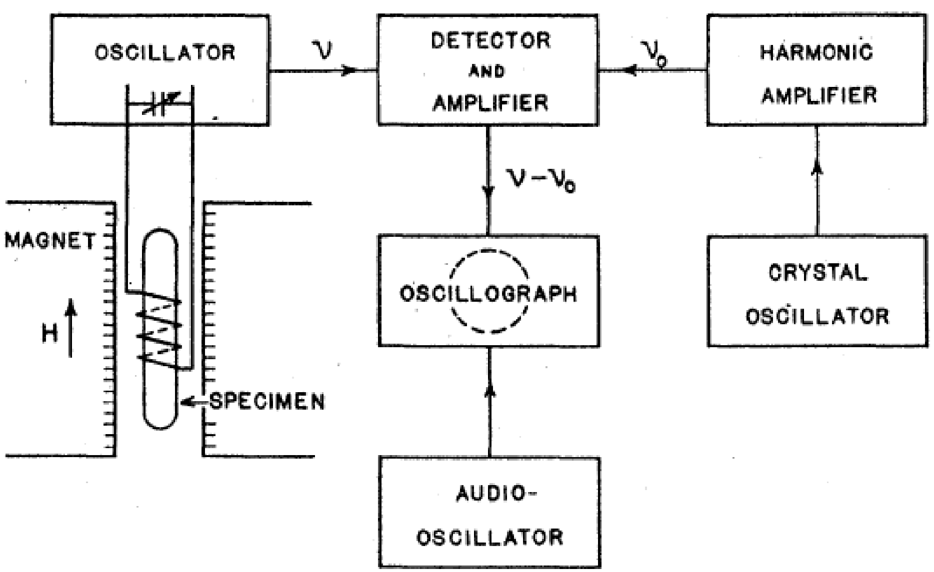


TABLE I. *Spin system data determined from dispersion measurements.*

	$10^{-6}a/c$ STARR 77°	TEUNISSEN AND GORTER 77°	DU PRE 1°–4°	$10^{-6}a$	η	δ
$FeNH_4(SO_4)_2\cdot12H_2O$	0.263	0.248	0.256	1.14	0.0472°	0.193°
$CrK(SO_4)_2\cdot12H_2O$	0.64	0.7	0.80	1.19	0.0204	0.231
$CrNH_4(SO_4)_2\cdot12H_2O$	2.68			4.99	0.0200	0.486
$MnSO_4\cdot4H_2O$	4.2	6.2		18.2	0.126	0.903
$MnCl_2\cdot4H_2O$	19.8	19.5		85.9	0.135	2.11

What's Needed

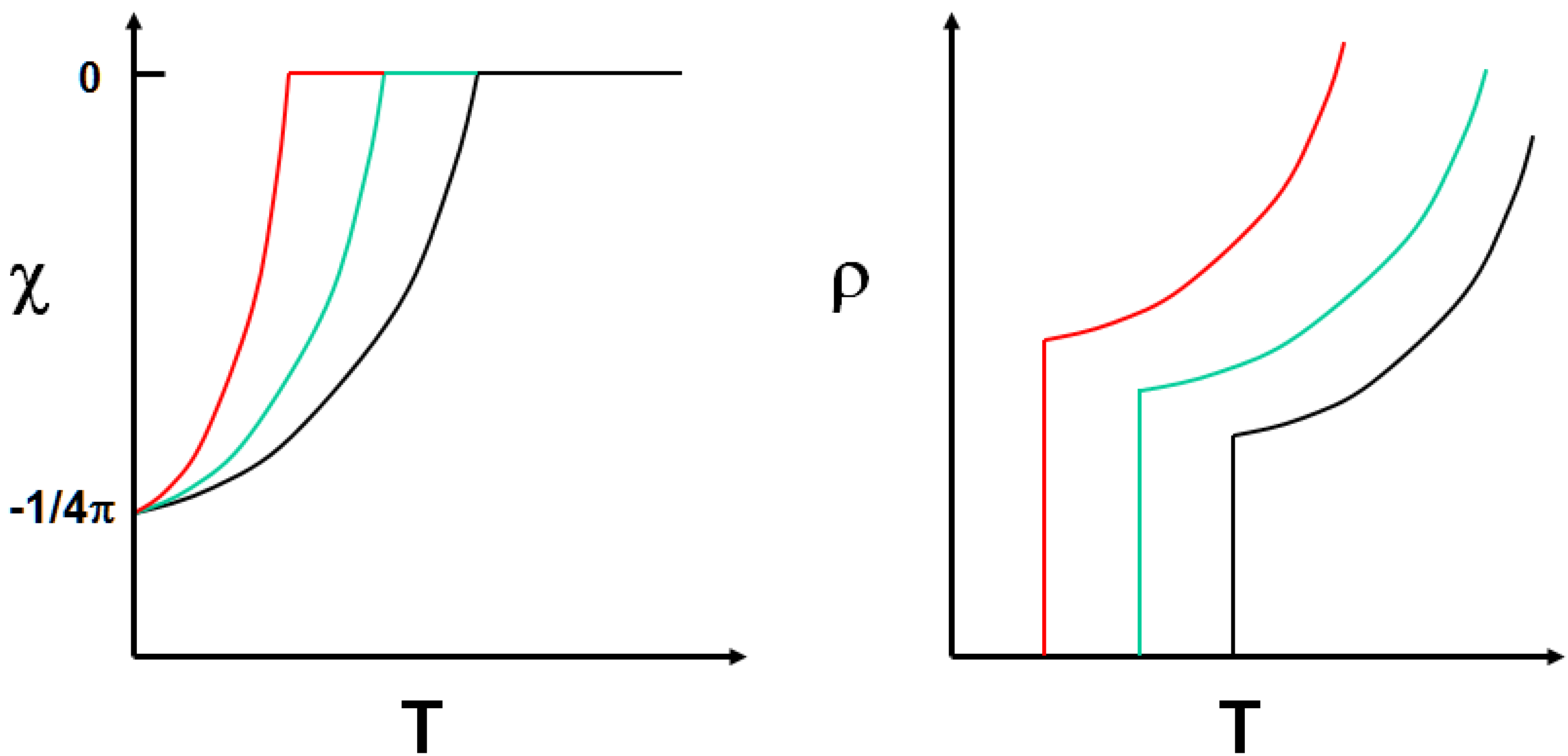
A DFT + U package (Elk?) that will allow the simultaneous calculation of electron-phonon interactions as well as spin-spin excitations, and thus enable an estimation of the Casimir/de Pre coupling…and maybe a combined phonon-spin pairing λ ?

Bulk or Not-Bulk?

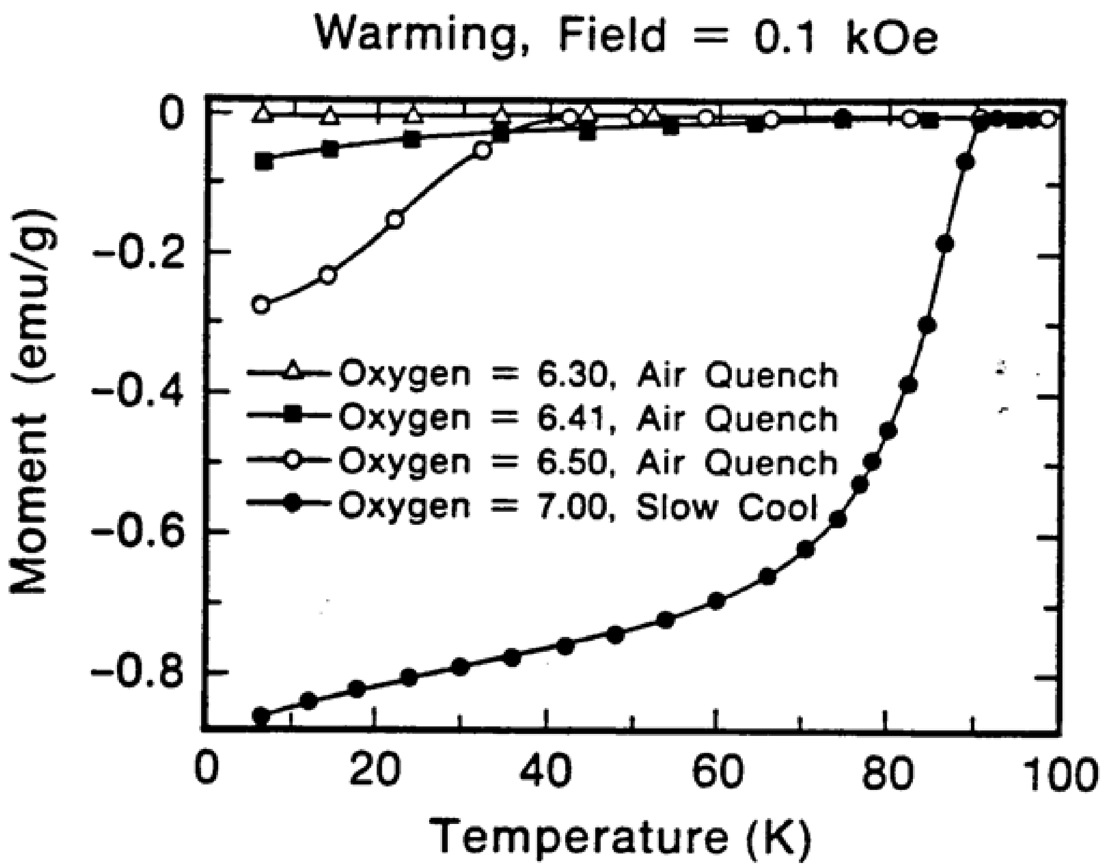
Field Dependence of Diamagnetic Shielding Fraction with Carrier Concentration in HTSCs

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

WC25.03: 14:24 24 March 1999



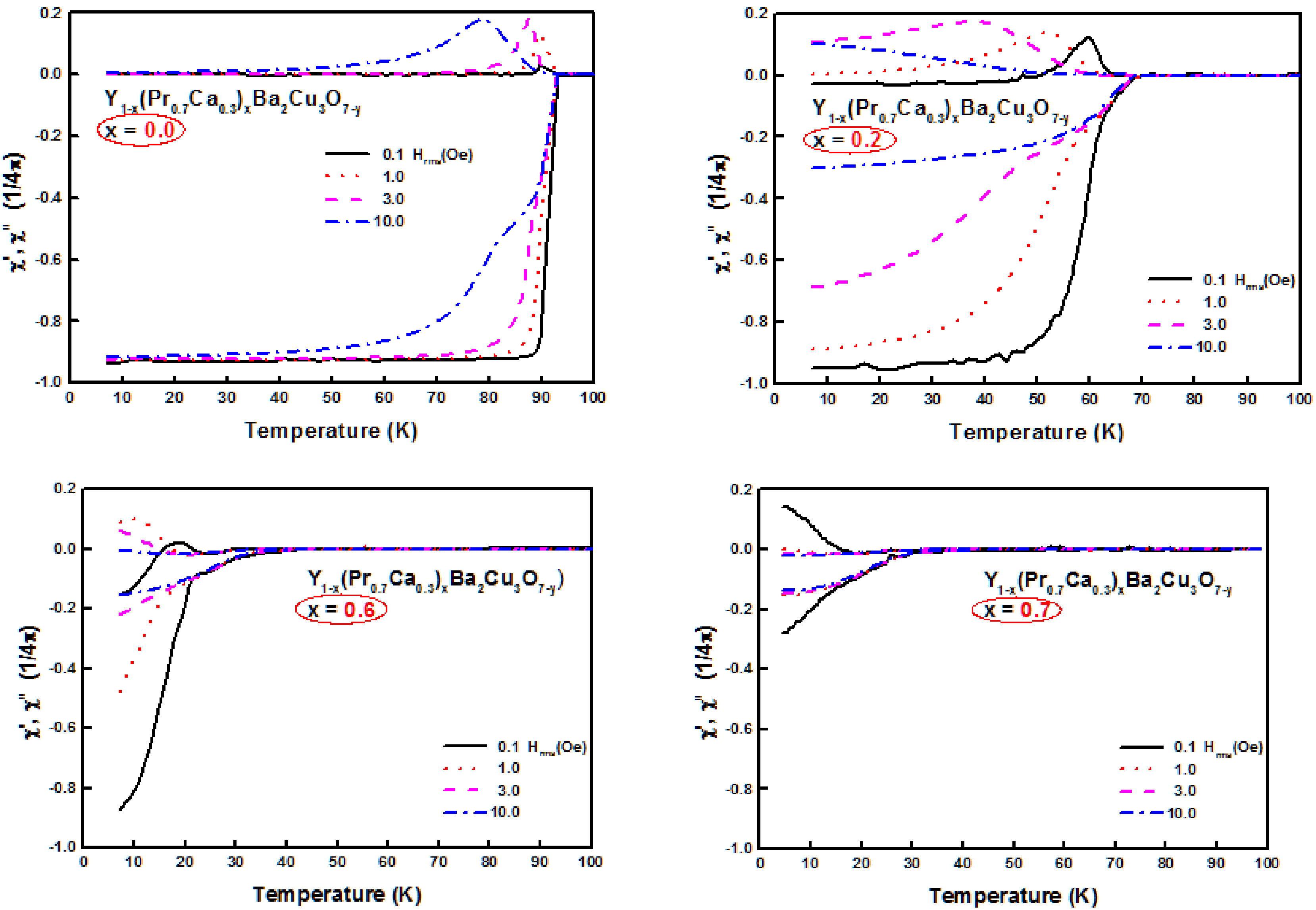
M vs. T,H
$YBa_2Cu_3O_{7-y}$



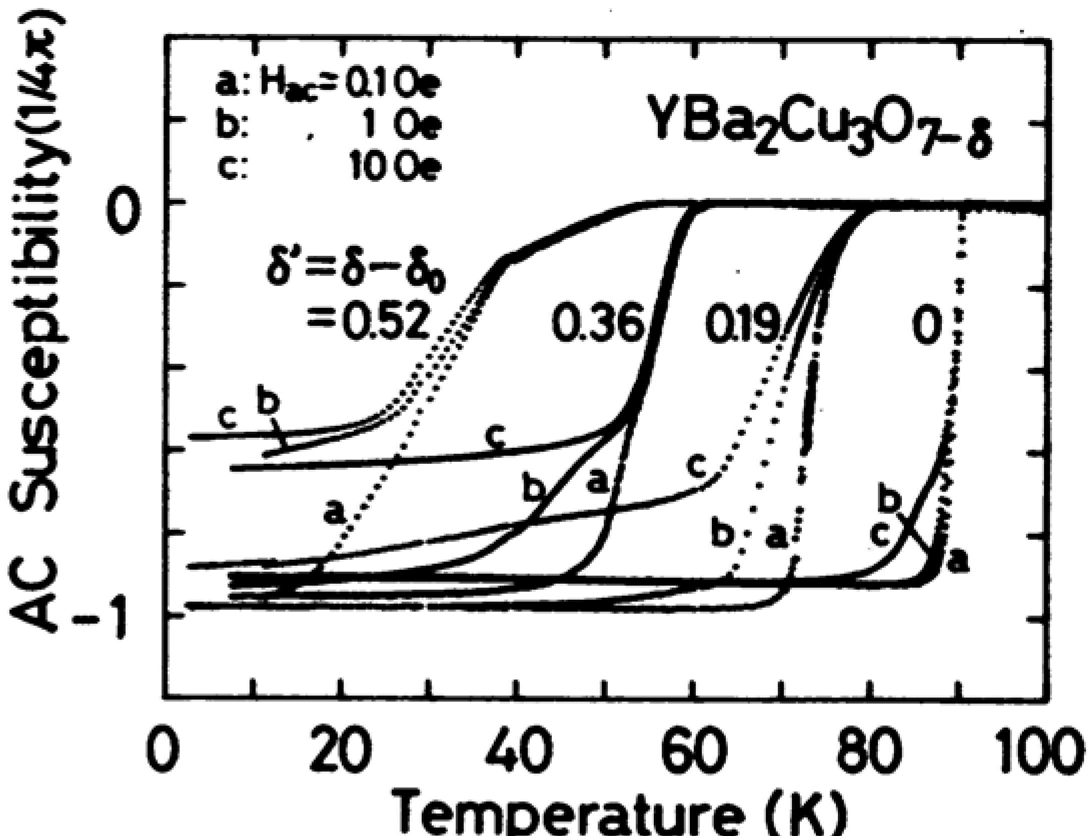
- IBM ARC Group Data <u>16 March, 1987</u>
- MRS Proc, April, 1987

$(\chi', \chi'')_{ac}$ vs. T,H,x

$Y_{1-x}(Pr_{0.7}Ca_{0.3})_xBa_2Cu_3O_{7-y}$



χ_{ac} vs. T,H,y
$YBa_2Cu_3O_{7-y}$



- Kubo, et al., PRB <u>37</u>, 7858 (1988){1987}.
- Early H-Field Dependence on "Carrier Concentration."

In moderate magnetic fields, low-T shielding limit complete only for highest T_C carrier concentrations (a universal HTSC constant?)

Strong evidence for granular behavior, due to either spacial *or electronic* inhomogeneities, at all carrier concentrations other than optimum.

What's Needed

ac Susceptibility measurements made over a broad range of doping and probe magnetic fields on single crystals of copper oxide and iron pnictide perovskites.

Pr-123

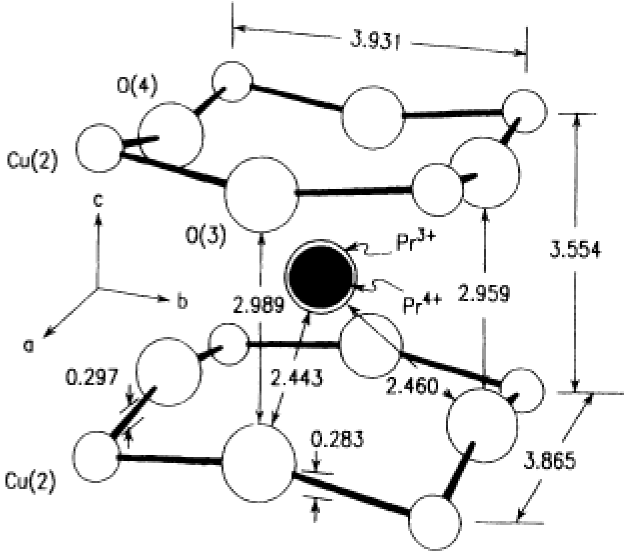
PHYSICAL REVIEW B VOLUME 41, NUMBER 10 1 APRIL 1990

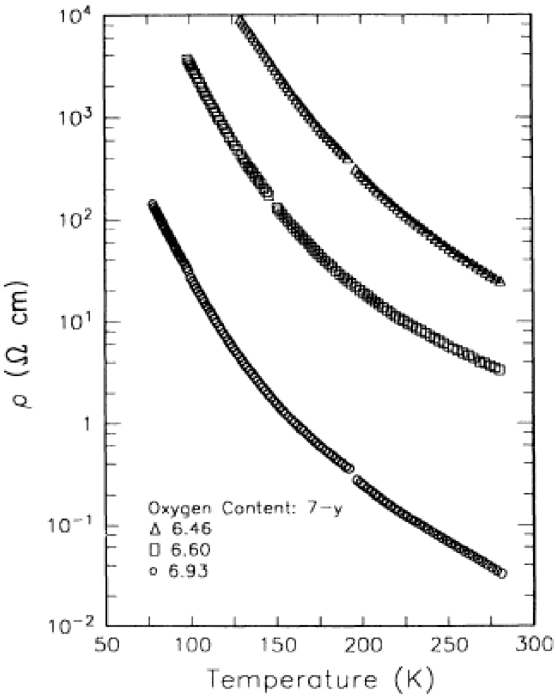
Role of oxygen in $PrBa_2Cu_3O_{7-y}$: Effect on structural and physical properties

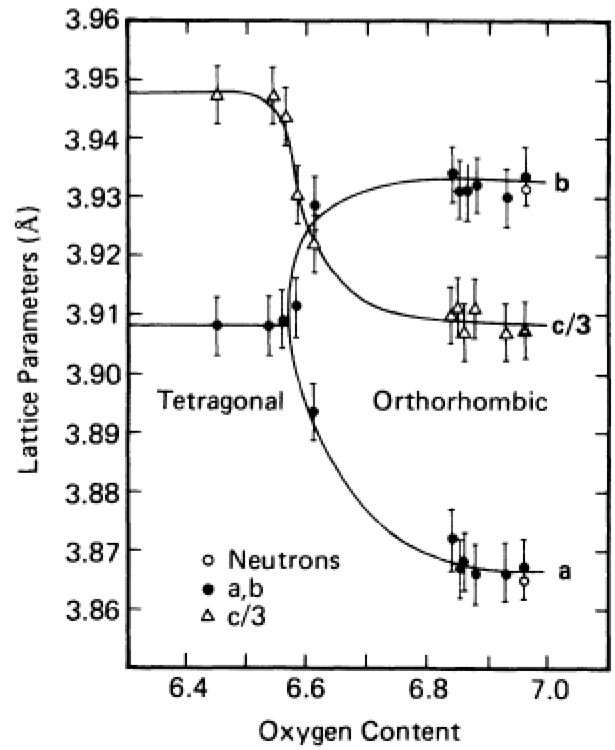
M. E. López-Morales,* D. Ríos-Jara, J. Tagüeña, and R. Escudero
Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, Apartado Postal 70-360, México, Distrito Federal, México

S. La Placa
Thomas J. Watson Research Center, Post Office Box 218, Yorktown Heights, New York 10598-0218

A. Bezinge,† V. Y. Lee, E. M. Engler, and P. M. Grant
IBM Research Division, Almaden Research Center, 650 Harry Road, San Jose, California 95120-6099





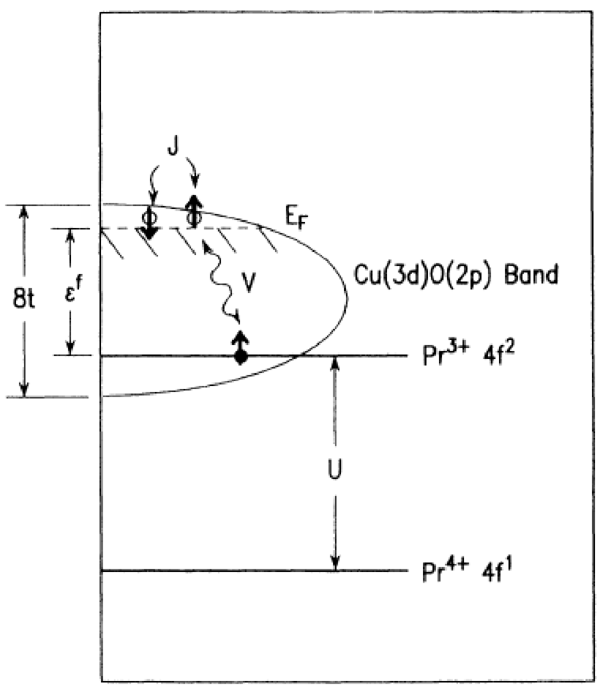


$$\mathcal{H} = \mathcal{H}_{\{R\}} + \mathcal{H}_{\{CuO_2\}} + \mathcal{H}_{\{R\},\{CuO_2\}}$$

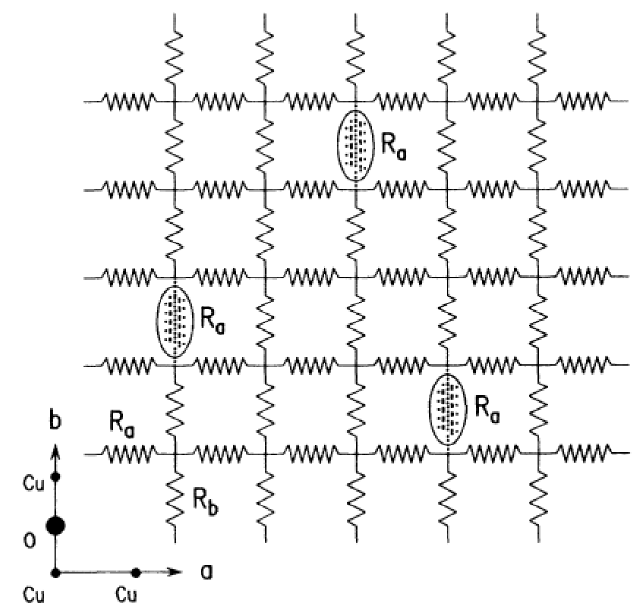
$$\mathcal{H}_{\{R\}} = \sum_{i\alpha} \varepsilon_\alpha^f f_{i\alpha}^\dagger f_{i\alpha} + \sum_{i\alpha\beta\gamma\delta} U_{\alpha\beta\gamma\delta} f_{i\alpha}^\dagger f_{i\beta}^\dagger f_{i\gamma} f_{i\delta}$$

$$\mathcal{H}_{\{CuO_2\}} = \sum_{j\neq j',\sigma} [t_{jj'}(1-n_{j,-\sigma}) d_{j\sigma}^\dagger d_{j'\sigma}(1-n_{J',-\sigma})] + J\sum_j \mathbf{S}_j \cdot \mathbf{S}_{j+1} ,$$

$$\mathcal{H}_{\{R\},\{CuO_2\}} = \sum_{ij\alpha(\sigma)} [V_{ij}^\alpha f_{i\alpha(\sigma)} d_{j\sigma} + \text{H.c.}]$$



Density of States



What's Needed

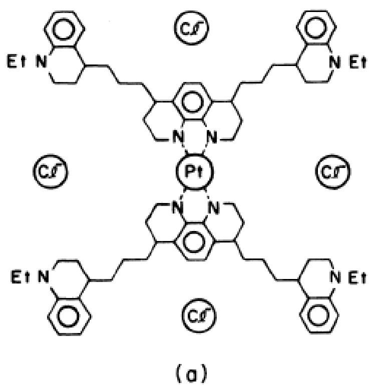
Quantum Monte Carlo calculations of the terms in the Hamiltonians defined in the previous slide, especially an estimation of the "trapping rate" resulting from interaction with the Pr 4f states.

Room Temperature Superconductivity?

PHYSICAL REVIEW B VOLUME 13, NUMBER 11 1 JUNE 1976

Proposed model of a high-temperature excitonic superconductor*

D. Davis,[†] H. Gutfreund,[‡] and W. A. Little
Physics Department, Stanford University, Stanford, California 94305
(Received 16 October 1975)

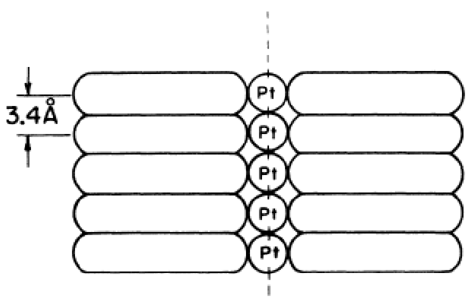


Kirzhnits, Maximov, Khomskii

$$F(\vec{p}, i\omega_n) = -G(\vec{p}, i\omega_n)G(-\vec{p}, -i\omega_n) \times \sum_m \int \frac{d^3k}{(2\pi)^3} V(\vec{p}-\vec{k}, i(\omega_n - \omega_m)) \times F(\vec{k}, i\omega_m),$$

$$\phi(p) = -\int_{-\pi/\alpha}^{\pi/\alpha} \frac{dk}{2\pi} \frac{U(p,k)\,\phi(k)}{[\xi^2(k)+\phi^2(k)]^{1/2}},$$

$$kT_c = 3.5\phi(k_F)_{T=0}$$



Interaction very dependent on the cutoff q of the electron-exciton coupling

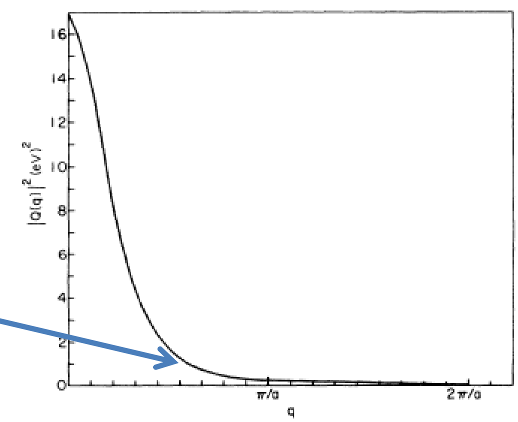


FIG. 4. Calculated electron-exciton interaction $|Q(q)|^2$ as a function of momentum transfer q.

PHYSICAL REVIEW B VOLUME 7, NUMBER 3 1 FEBRUARY 1973

Model for an Exciton Mechanism of Superconductivity*

David Allender,† James Bray, and John Bardeen
Department of Physics and Materials Research Laboratory, University of Illinois, Urbana, Illinois 61801
(Received 7 August 1972)

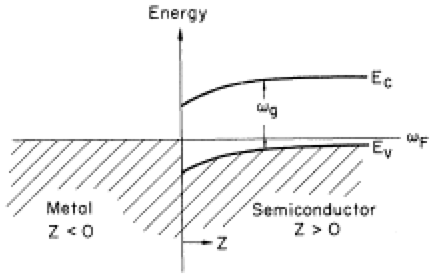
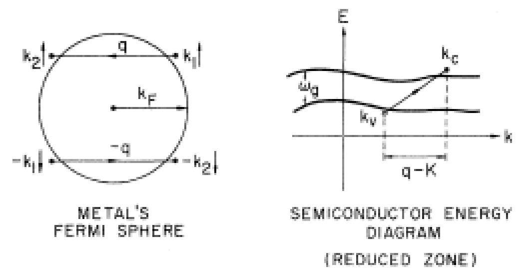
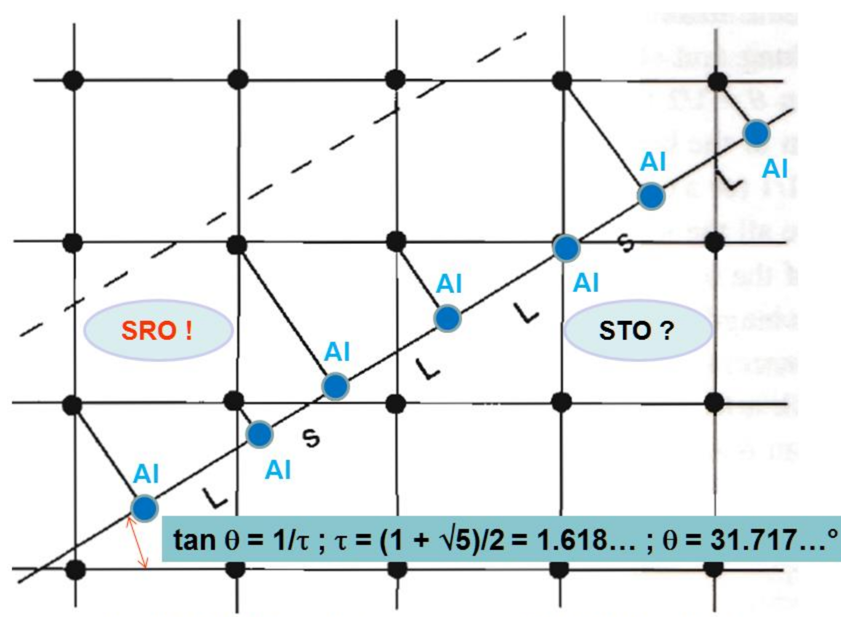


FIG. 1. Metal-semiconductor interface. E_c and E_v are the bottom of the conduction band and top of the valence band, respectively.



A Fibonacci "Dislocation Line"



Superconducting Fluctuations in One-Dimensional Quasi-periodic Metallic Chains

Does the
DAVINCI CODE
Hold the Key to Room Temperature Superconductivity?

Session T41: T41.00008, Room F152, Wednesday, 4:42 PM

Paul M. Grant

APS March Meeting 2010

What’s Needed

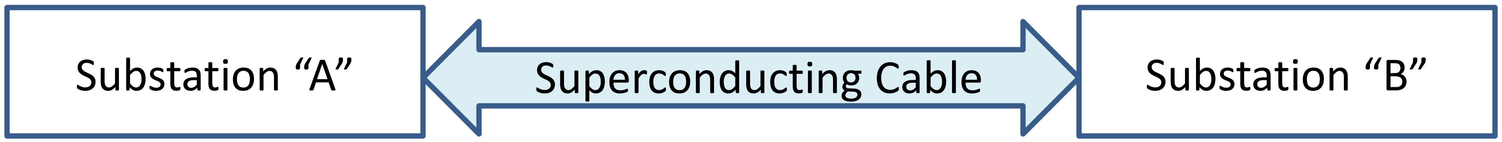
A DFT implementation of the KMK formalism (actually just coding the KMK formalism to analyze the eigenstates produced by a DFT calculation) applied to “proxy” structure models like ABB or the “DaVinci Code” chain proposed by Grant.

Power to the People

IFCL-HTS

"I" = "inherently"

What is it?



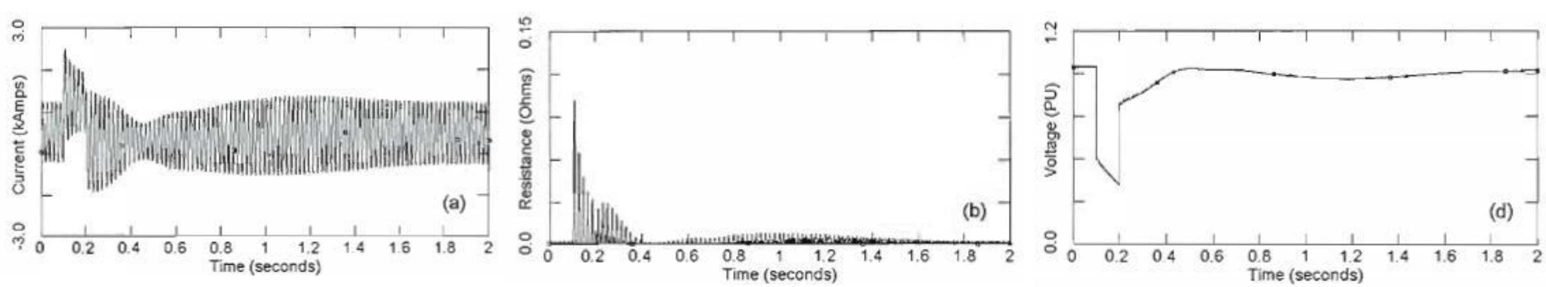
A Transient Model of High-Temperature Superconducting Cables in Electric Power Supply

Kim Hoj Jensen and Vladislav Akhmatov

(Tech. U. Denmark, 2005?)

$$\rho_{HTS} = \rho_C \left(\frac{I(t)}{I_C}\right)^{n-1}\left(\frac{T_C - T_0}{T_C - T(t)}\right)^n \qquad \rho_{HTS} = \alpha T(t) + \beta \qquad \rho_T = \left(\frac{1}{1+r}\rho_{HTS}^{-1} + \frac{r}{1+r}\rho_M^{-1}\right)^{-1} \qquad R(t) = \frac{l}{aN}\rho_T(t)$$

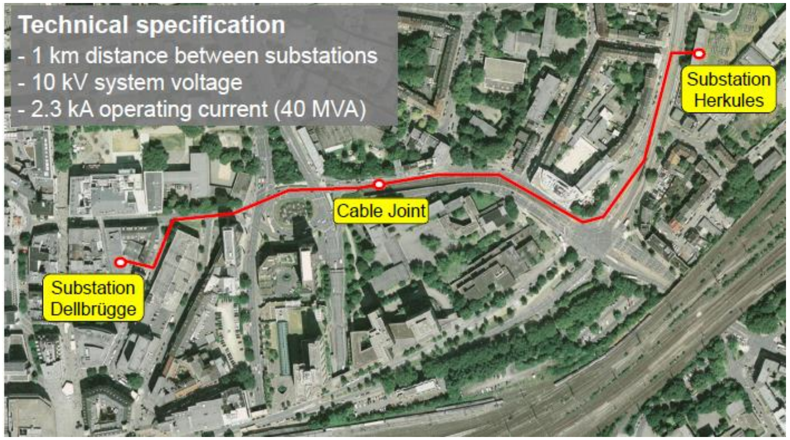
$$L\frac{dI(t)}{dt} = -R(t)I(t) - \Delta U(t) \qquad C_P\frac{dT(t)}{dt} = P(t) - h(\Delta T)A\Delta T(t)$$



AMSC US Patent 8,886,267,B2 Nov. 11, 2014

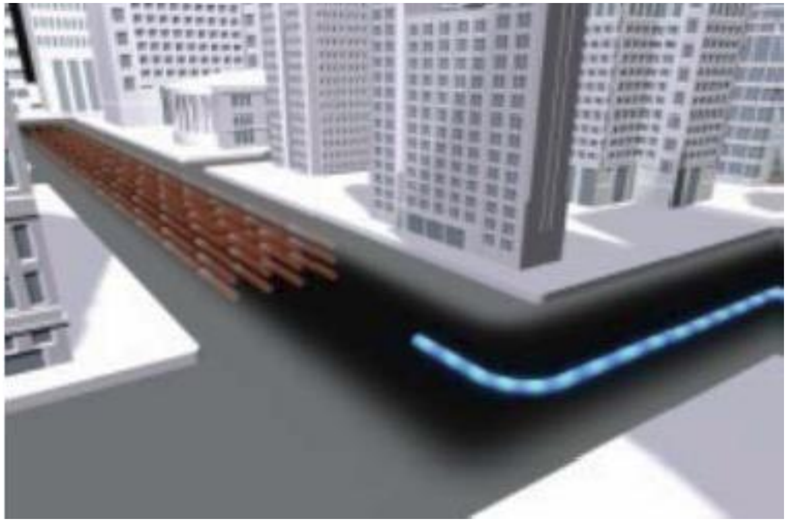
IFCL-HTS "Implementations"

AmpaCity – Essen (RWE, Nexans, KIT,...)



- Pilot operation in progress
- Funding: 13.5 M Euros
  - Nexans 36%
  - RWE 33%
  - BMWi 25%
  - KIT 6%
- Next...Muelheim (2020) ?

Project Hydra – (AMSC, ConEd, DHS,...)



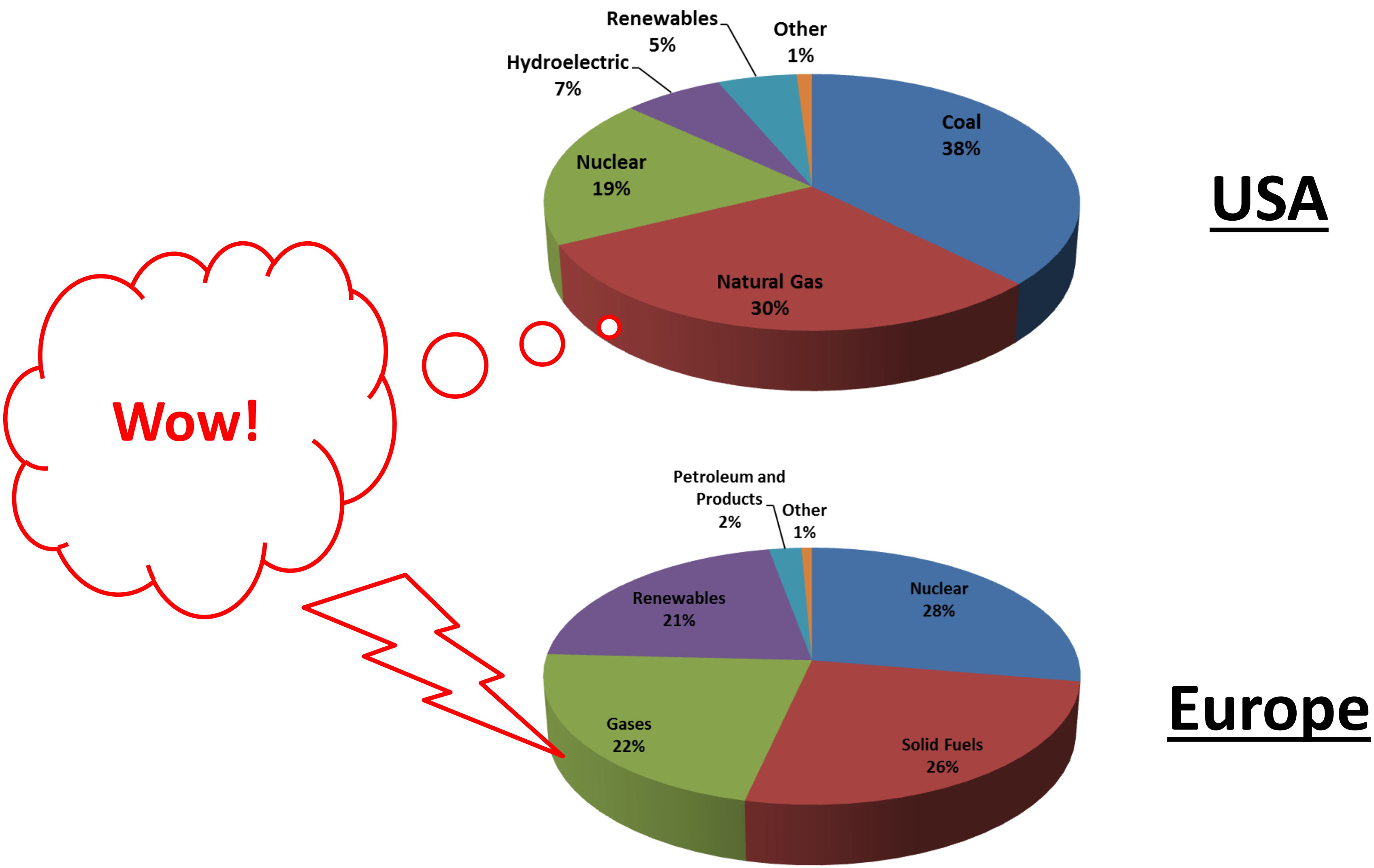
- First proposed in 2007 by DHS
- Funded by DHS at 30 M USD
- Contracted with AMSC & ConEd for installation in mid-Manhattan
- Put on hold in 2011
- Project moved to two adjacent substations in Yonkers
- Cable conductor now sits on site
- Future "uncertain"

DHS "Resilient Electric Grid" (2015)

- Objective: Protection of the US Grid against:
  - Natural Disasters
    - *e.g. "SuperStorm Sandy"*
  - "Unnatural" Disasters
    - *1960-70 attacks on California & Oregon substations by the SLA and environmental extremists*
    - *Most recent 2013 attack on PGE Metcalf transmission substation in San Jose*
- "Due Diligence" Study Underway
  - Objective: Assess the risk and readiness of the US (and some international) HTSC wire, cable, and cryogenic companies to undertake large scale production necessary to implement the REG
    - *e.g., would Gen I wire be sufficient, or is Gen II really needed, or both?*
  - DHS and EPRI have formed a 7 person team of "experts" to report their recommendations by 4Q15.
    - *Full Disclosure: I'm a member! Con Quidado!*

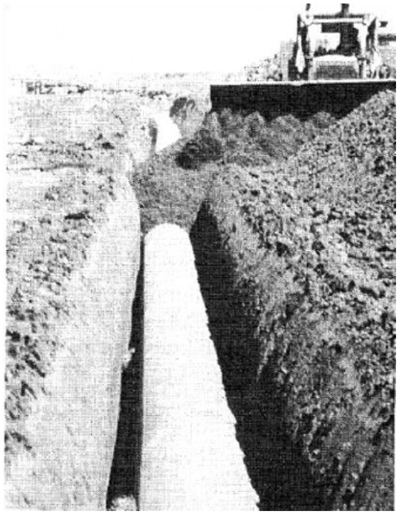
“Dual Use” of Energy Transport Corridors

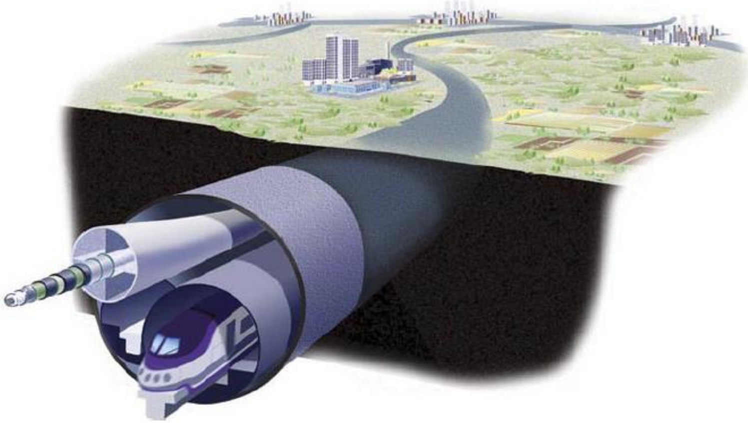
Electricity Generation by Primary Fuel Source (2011-12)



The “Dual Use” Concept Embodied

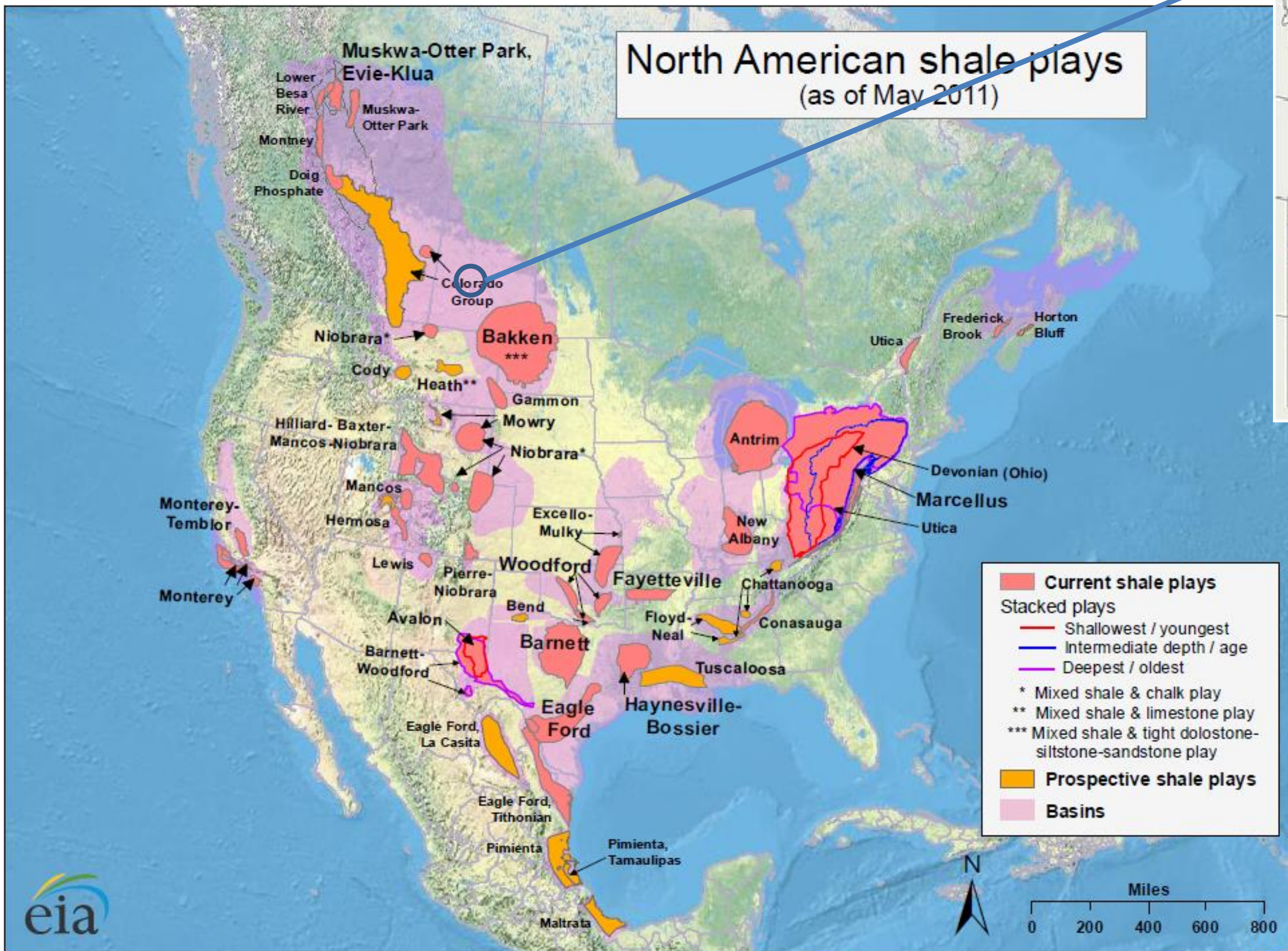
- Almost all NG used for electricity generation is “combusted” at a “local” delivery point using modern, efficient, combined cycle gas turbine (CCGT) technology.
- Why not “combust” that gas portion so-used at the “well-head” instead and deliver the “electrons” over a low-loss HTSC dc cable? As well as reducing volume...and...frictional loss due to NG transported by pipeline.
- ...and...consider “recycling” well-head generated CO_2 emissions into alcohols...and “pipe” those down the same ROW!





The ROW Dual Use concept has been documented in several peer reviewed journals as well as member magazines of the APS, IOP, IEEE, and Nature...contact the author/speaker for a linkable anthology.

Opportunities to Exploit the Keystone XL Pipeline ROW for the Dual Transport of Chemical and Electrical Energy



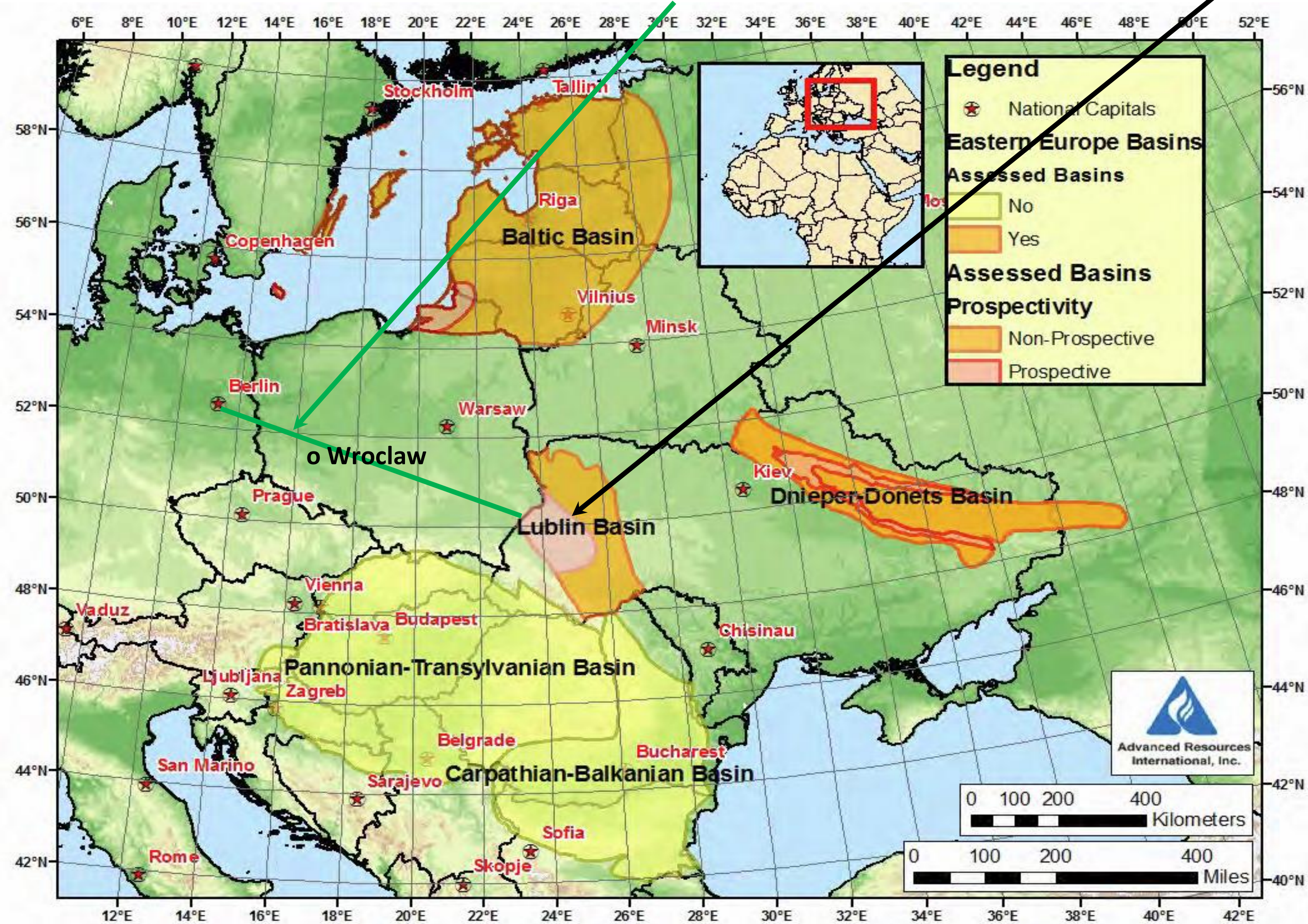
Smart Grid

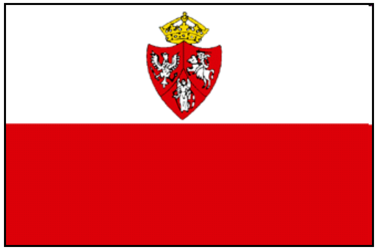
Fraternal Twins

2013 P. M. Grant's Editorial in Smart Grid News

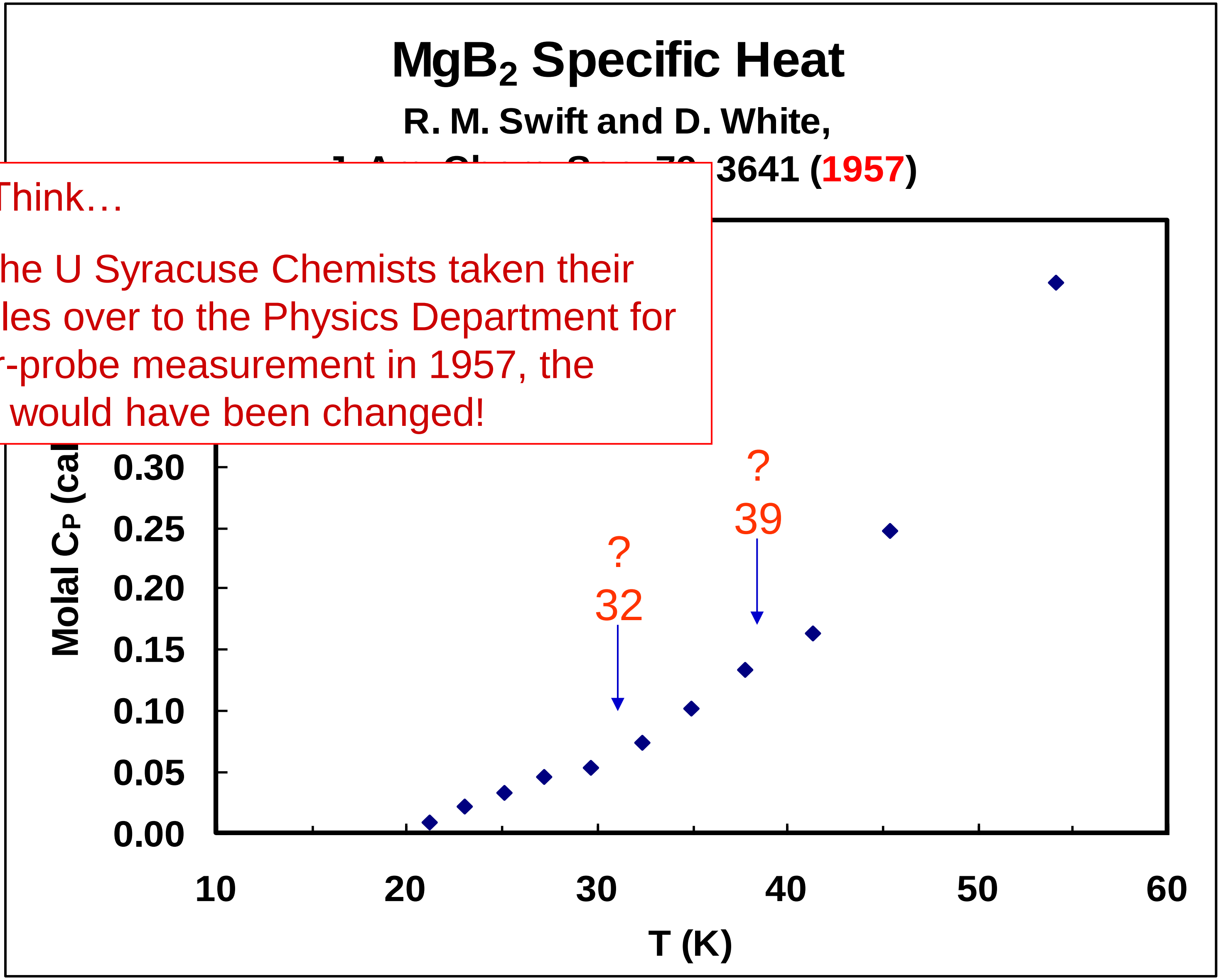
One European Scenario

The Wola Obszańska (Lublin) gas field in Poland/Ukraine was discovered in 1989. It began production in 1992 and produces natural gas. The total proven reserves of the Wola Obszańska gas field are around 37 billion cubic feet ($1×10^9 m^3$). "Dual-Pipe" to Berlin?





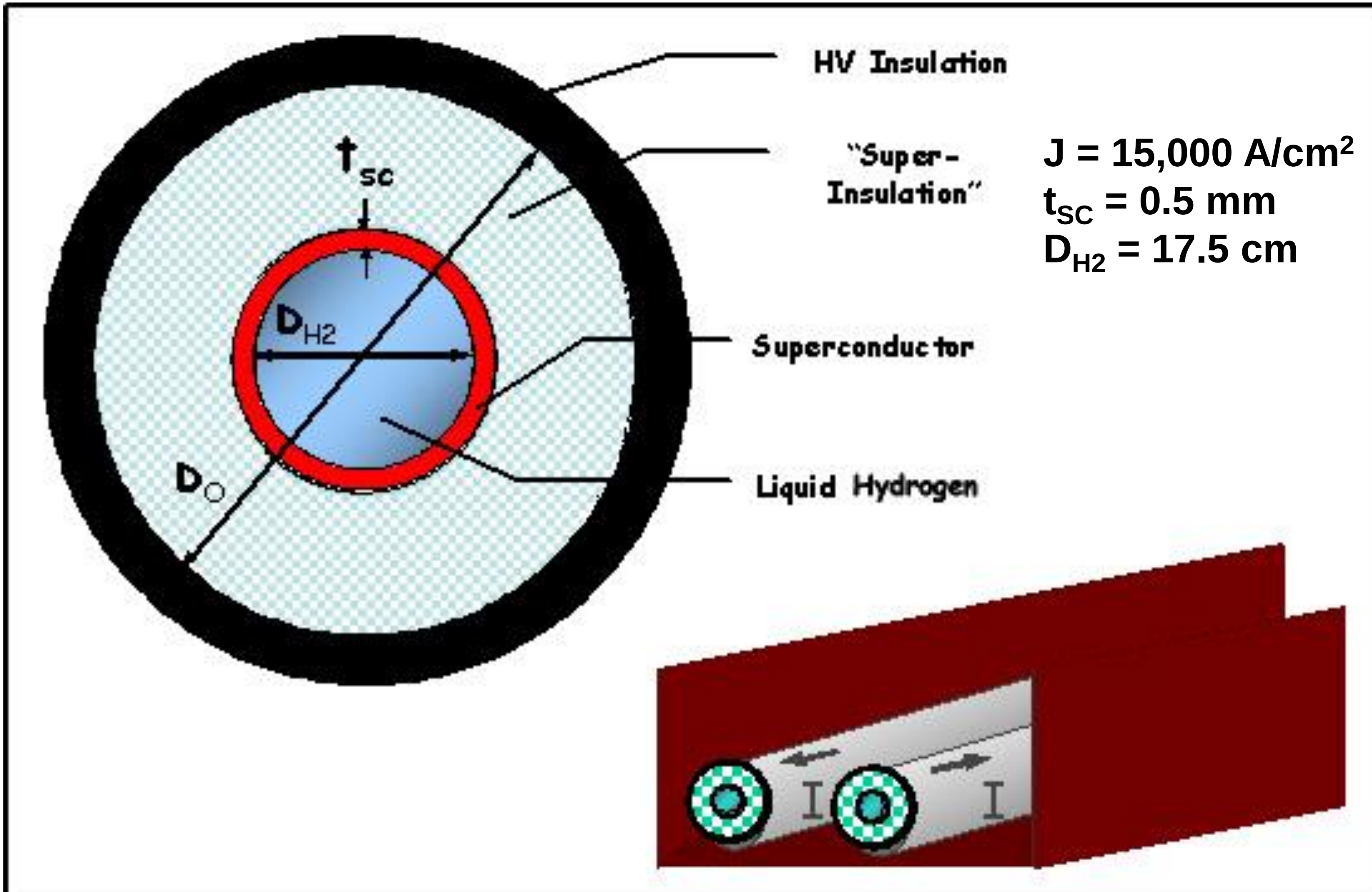
MgB_2 – How Was It Ever Missed?



Just Think…

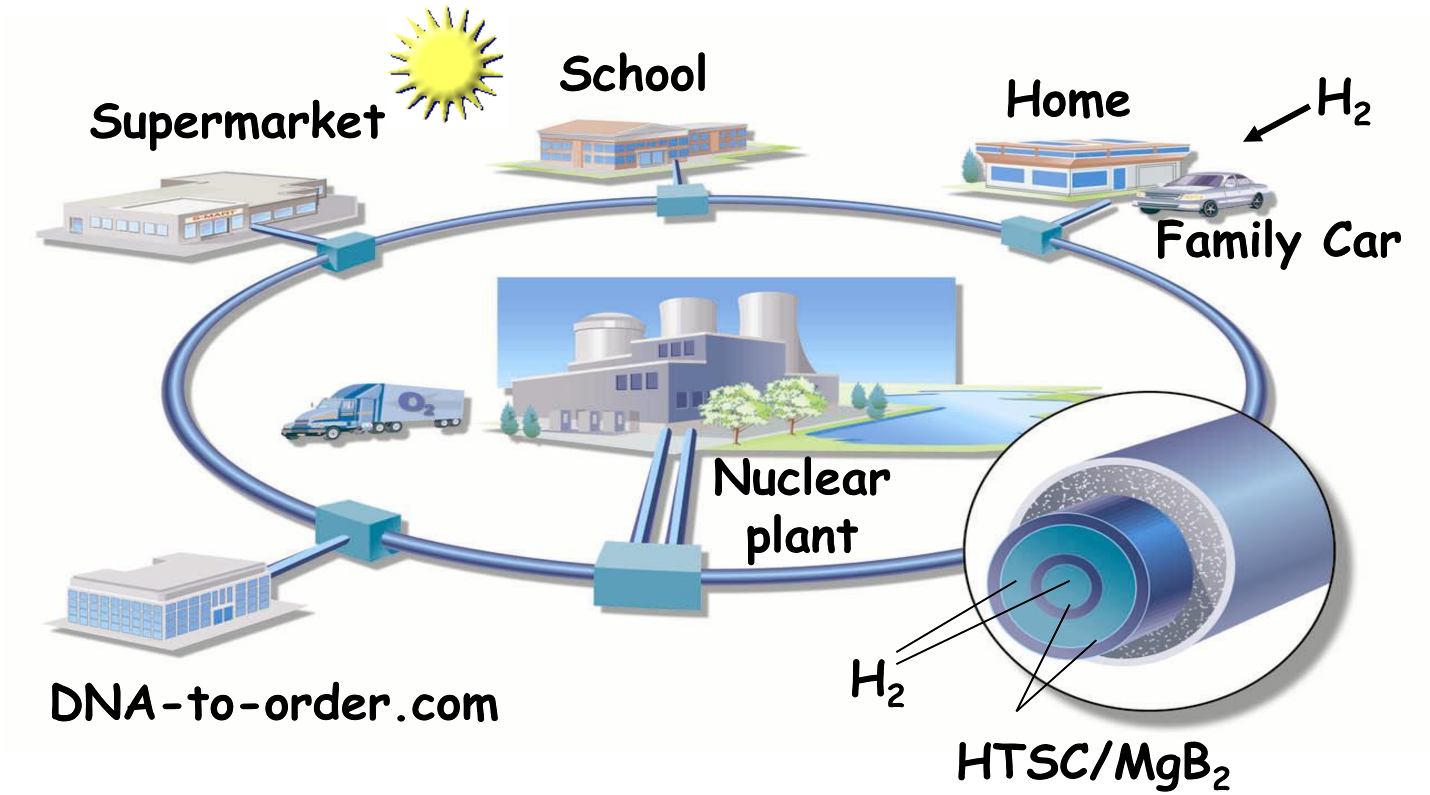
Had the U Syracuse Chemists taken their samples over to the Physics Department for a four-probe measurement in 1957, the world would have been changed!

The SuperCable



$J = 15{,}000\ A/cm^2$
$t_{SC} = 0.5$ mm
$D_{H2} = 17.5$ cm

SuperCity

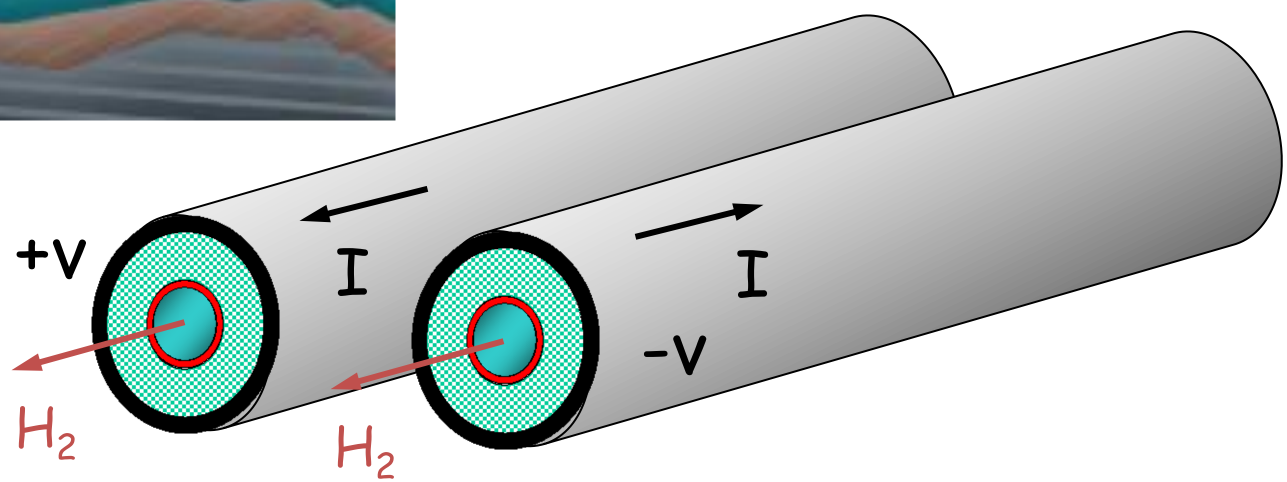


P. M. Grant, The Industrial Physicist, October/November 2001, p. 22
P. M. Grant, The Industrial Physicist, February/March 2002, p. 22

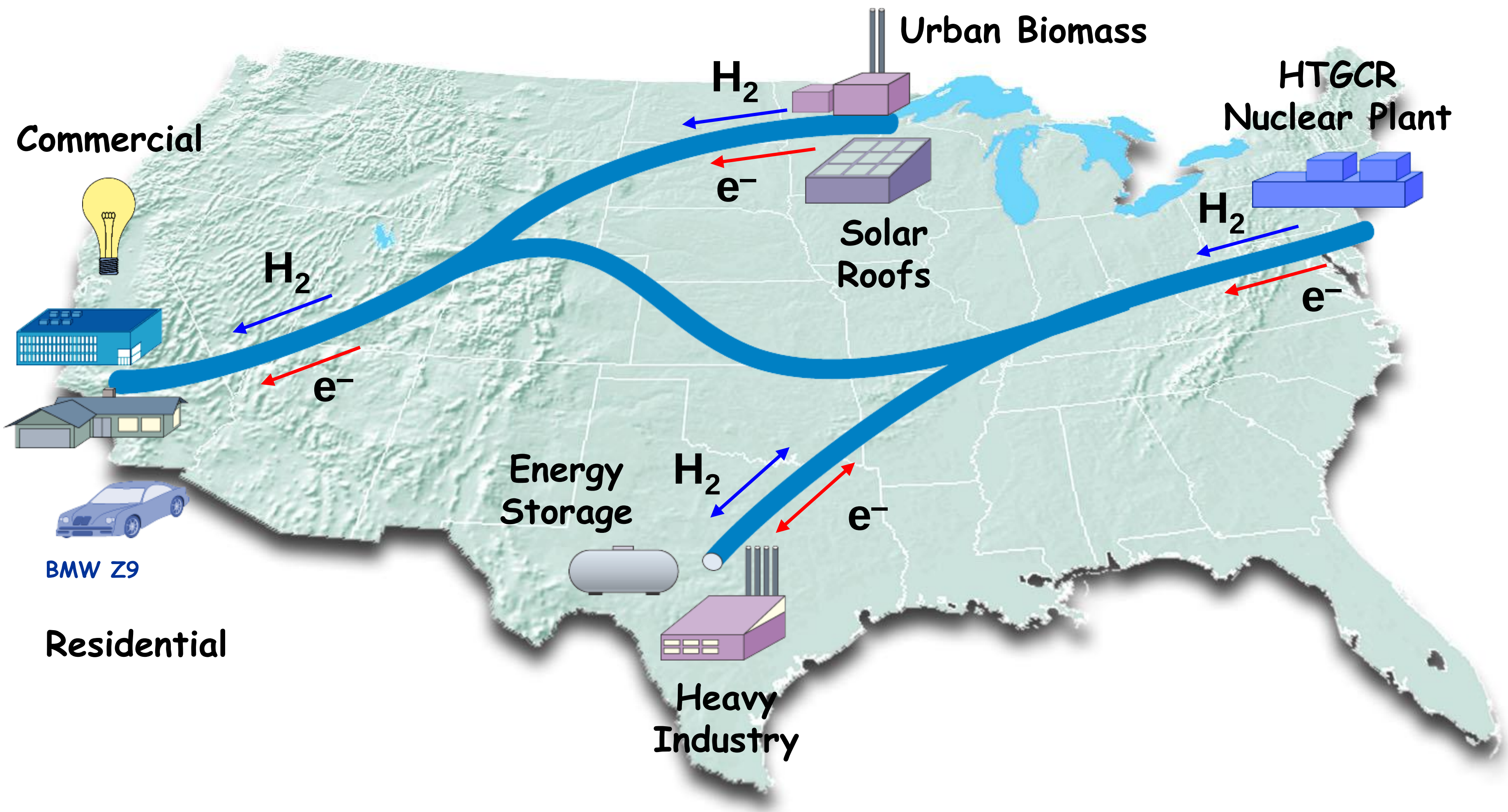
SuperGrid

Combining Superconducting Wires Cooled with Cryogenic Hydrogen
To Create a Dual-Energy Delivery Continental-Scale System

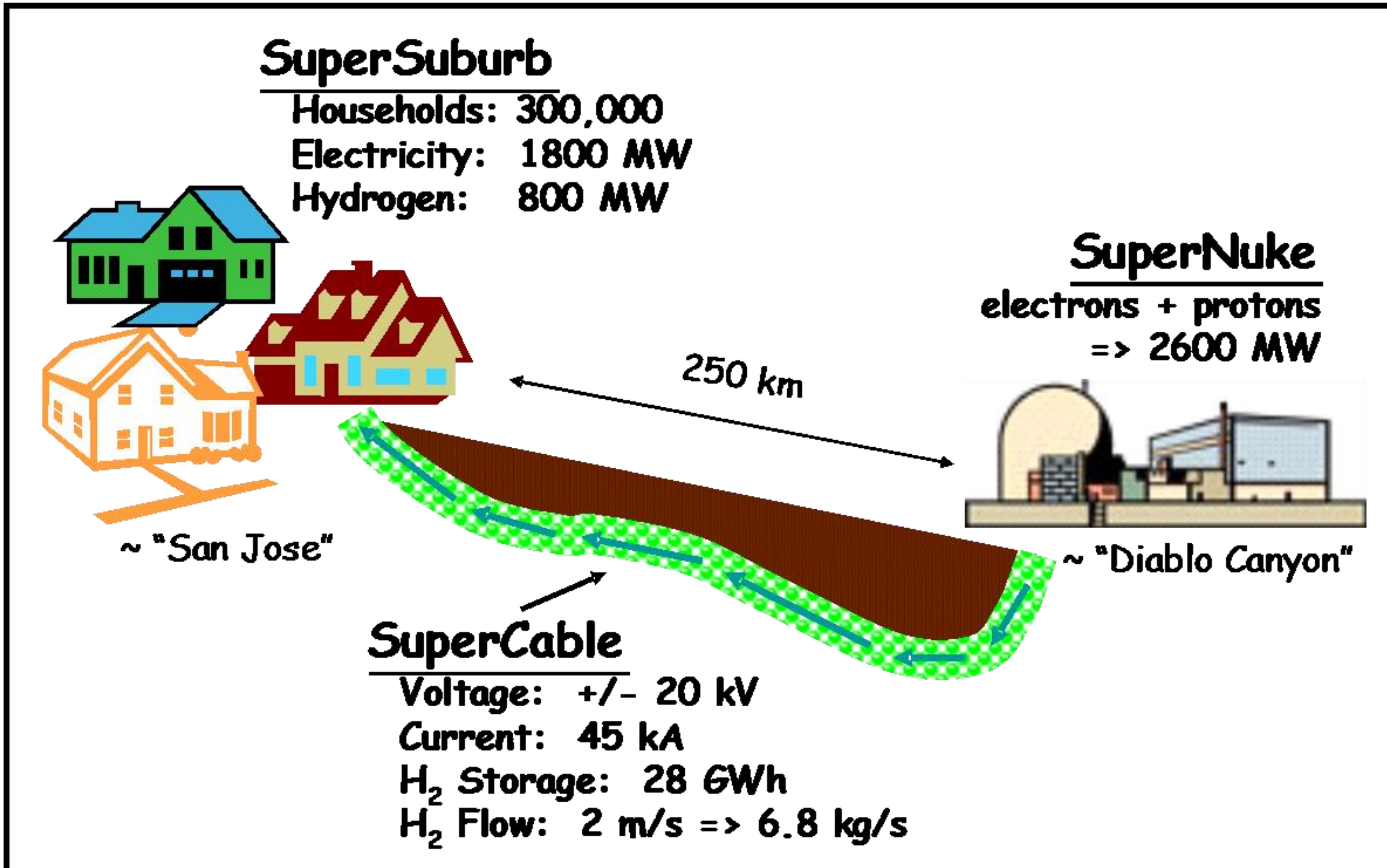
P. M. Grant, C. Starr, T. Overbye, "A Power Grid for the Hydrogen Economy," Scientific American, July 2003, p. 76.



North American 21st Century Energy SuperGrid



The Cryogenic Neighborhood



What's Needed

- Publicity!
  - Write your Congress-whatever
  - Contact your TV network (BBC, ZDF, PBS, FOX, CNN, CBS,...
  - Blurb Nature Physics, Physics World,...
- Funding!
  - Twitter your Parliament-whatever
  - Seriously... 500 K USD would more than support an in-depth "engineering economy" study of various scenarios worldwide to assess the "profitability" of the concept, both monetarily and socially.
- Follow-up:
  - Emphasize relationship to past, present and future high energy physics projects.
  - The current MgB_2 CERN "cable feeder" effort could indeed be the precursor to the worldwide SuperGrid of the future!

"You can't always get what you want…"

"…you get what you need!"