Setup

Physics Seminar…SJSU

Thursday, November 20, 2014
Science 242, 4:30 PM

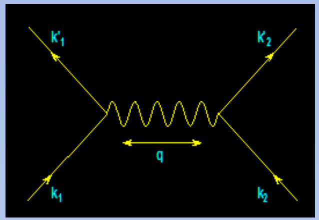
San Jose State, 1857 -> Today

"Challenges Confronting the Physics of Superconductivity in the 21st Century: From Nanoscale Theories to Exascale Energy Applications"

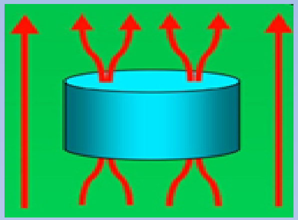
Paul Michael Grant
EPRI Science Fellow (Retired)
IBM Research Staff Member/Manager Emeritus
(etc, etc…& so forth and so on)
W2AGZ Technologies
San Jose, CA 95123, USA (w2agz@w2agz.com)

Aging IBM Pensioner

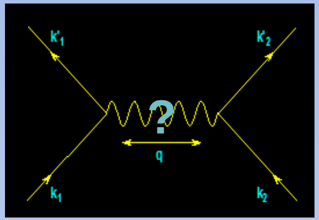
From
Electrons
Paired



To
Electric
Power Delivered



…And…
Back
Again



-- A Personal Journey in Applied Physics --
-- IBM, EPRI, and Beyond --

Paul M. Grant

IBM (1953-1993)

- Joined 1953 (age 17)
- SAGE/NORAD (MIT)
- Clarkson/Harvard
- Magneto-optics
- Displays/Printers
- Organic Conductors
- DFT
- Superconductivity
- High-Tc
- Sabbatical (UNAM)

EPRI (1993-2005)

- High-Tc Power Apps
- Wide Bandgap SCs
- Power Electronics
- “Hot” Fusion
- “Smart Grid”
- “SuperGrid”
- “Climate Change”
- Visionary Energy Societies

W2AGZ (2005-?)

- Due Diligence
- Tet-CuO (Stanford)
- “Proxy” DFT
- RTSC via DFT
- IASS Potsdam
- *Dual Use of NG Pipeline ROWs for Co-transport of Electricity via HTSC Cables (e.g., Keystone)*

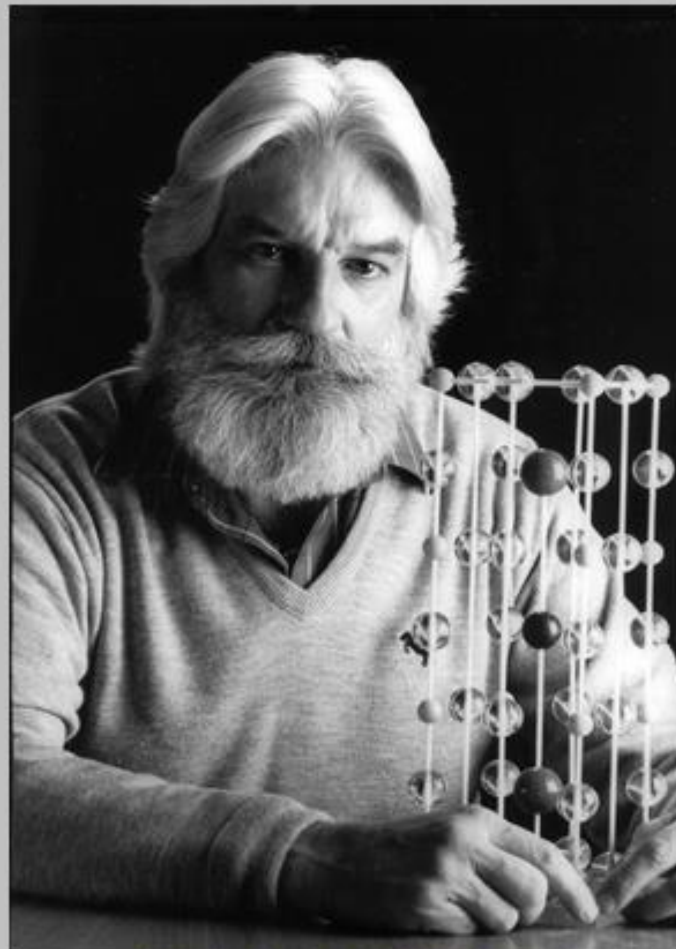
W2AGZ Technologies

Paul Michael Grant

Physicist and Science Writer

Principal, W2AGZ Technologies

Senior Life Fellow, American Physical Society

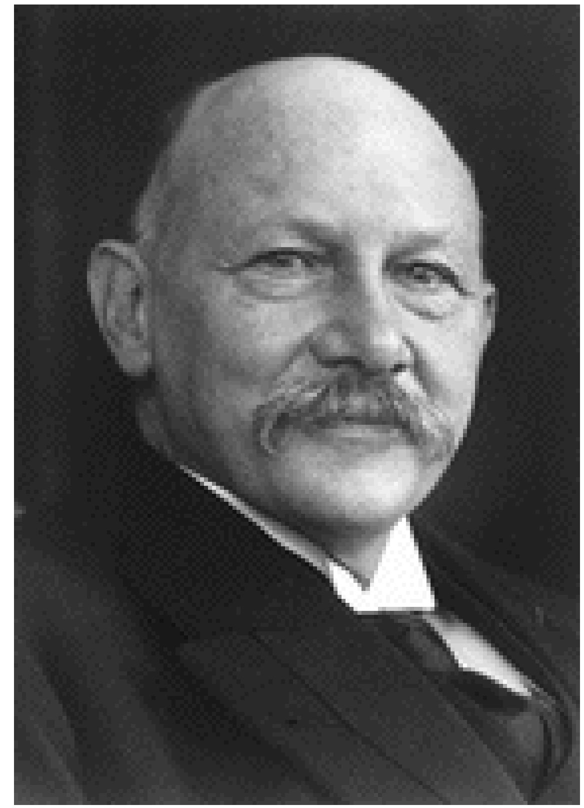


Read the Story Behind This Picture!

Fathers of Cryogenics

Dewar

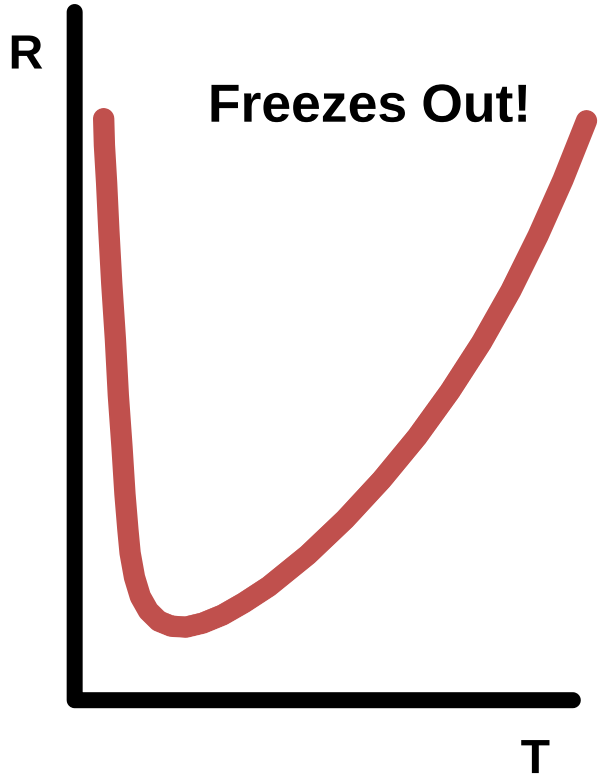
CH_4	112 K
O	90
N_2	77
Ne	27
H_2	20
He	4.2

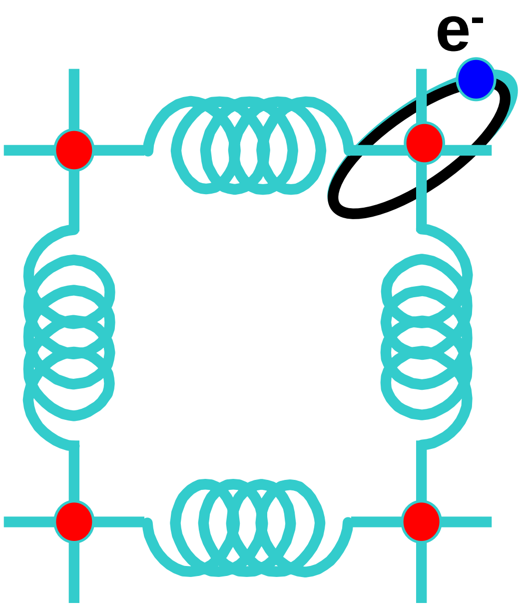


Kammerlingh-Onnes

Models of
Electrical Conductivity

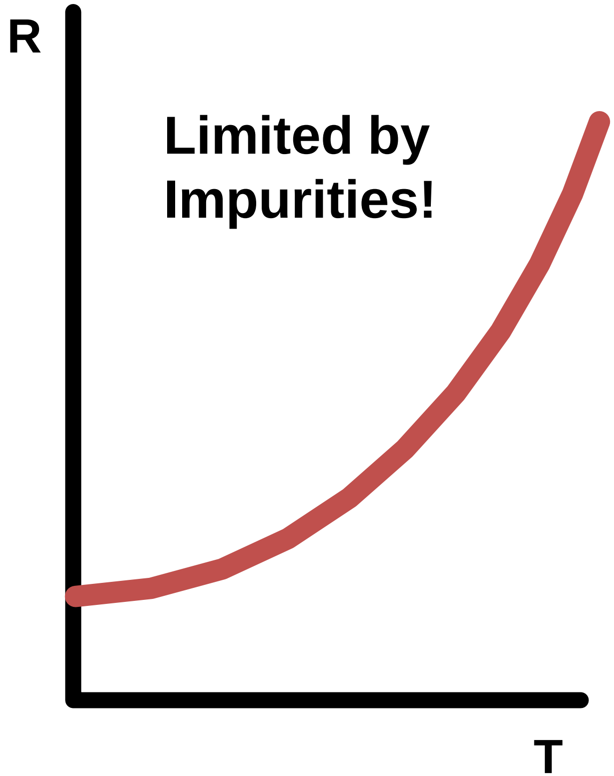
The Most Popular:

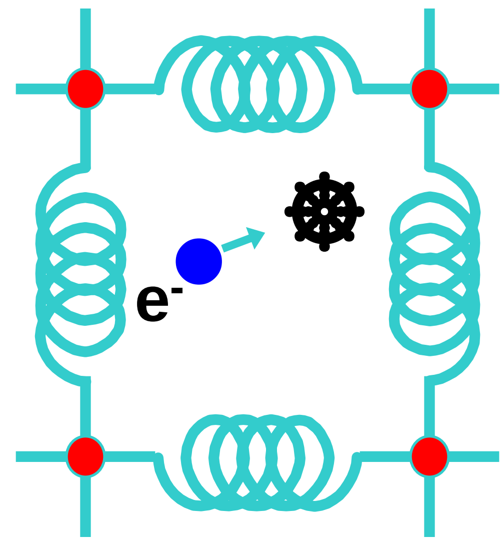




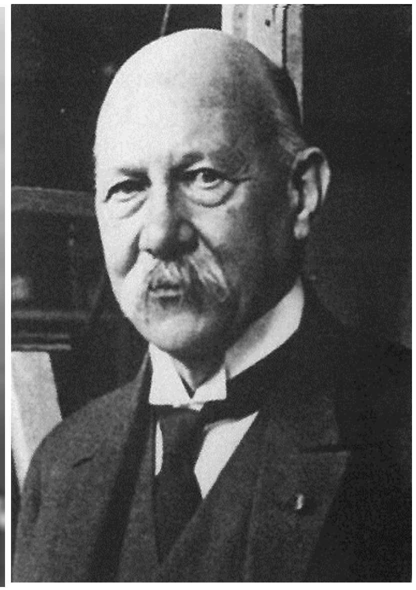
Models of Electrical Conductivity

Reality:



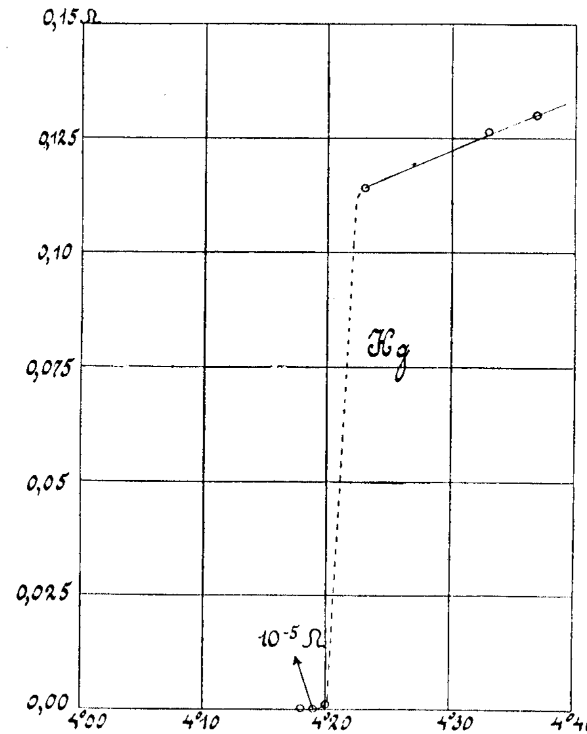


1911
A Big Surprise!

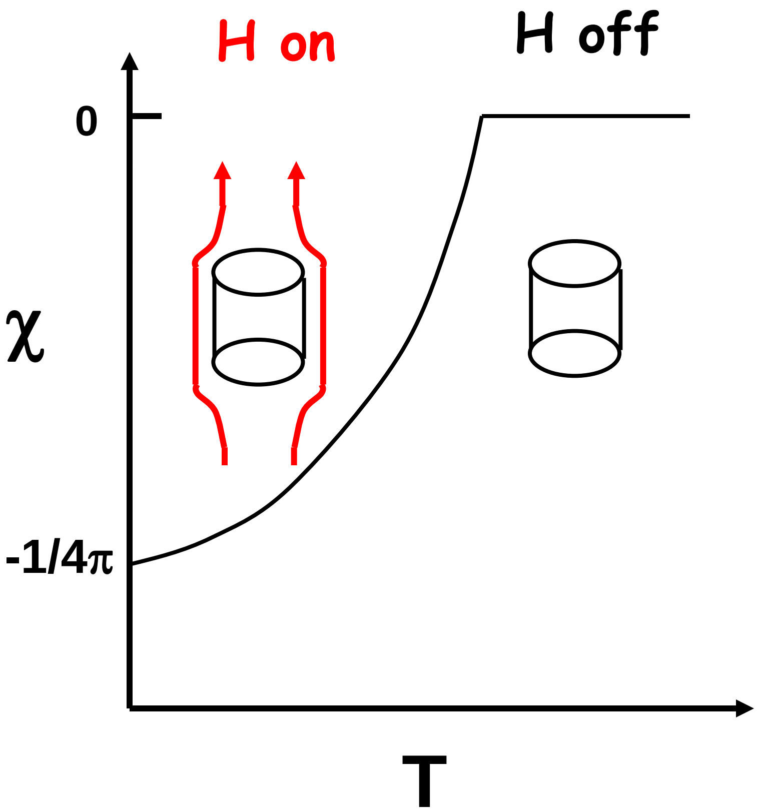


Thus the mercury at 4.2 K has entered a new state, which, owing to its particular electrical properties, can be called the state of *superconductivity*

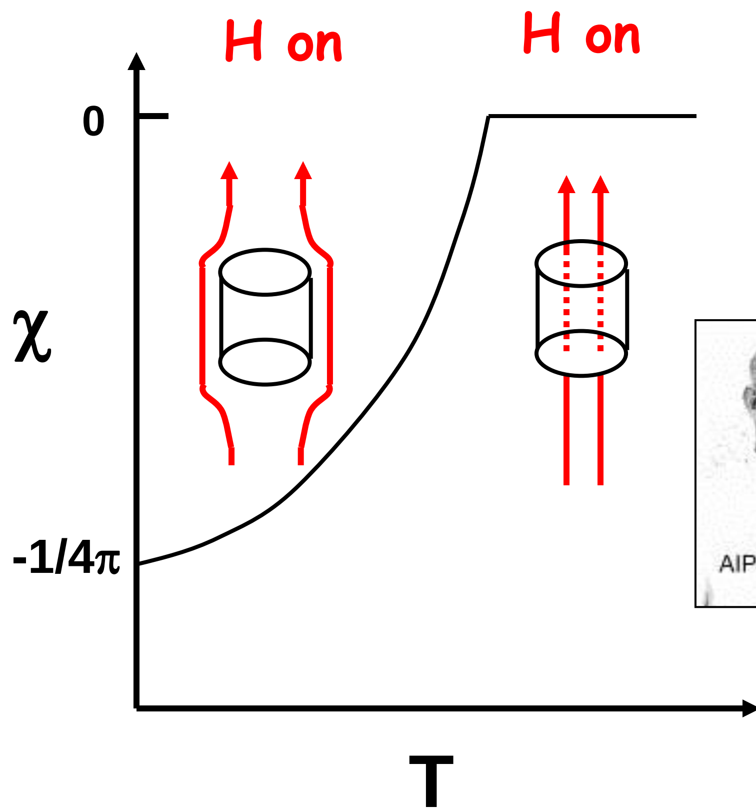
<u>Gilles Holst, H. Kamerlingh-Onnes (1911)</u>



Magnetic Properties

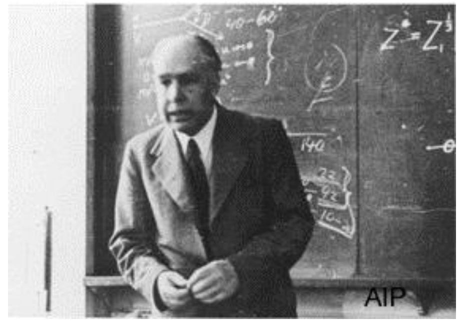


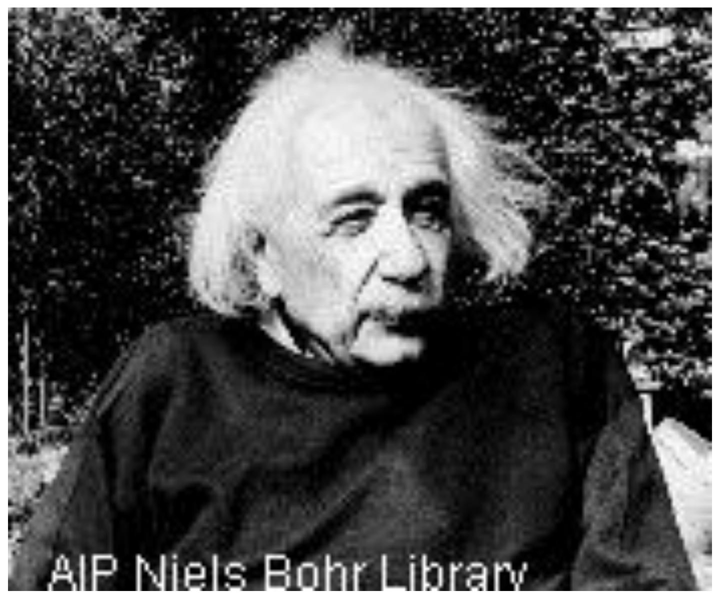
Expected (Lenz' Law)



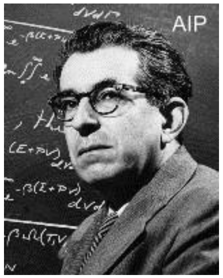
Weird ! (Meissner Effect)

They all tried…
and failed!





They came close...



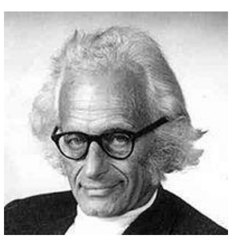
Fritz London

"The B-field does penetrate."

$$E \sim \lambda^2\, dJ/dt, \quad B \sim \lambda^2\, \nabla \times J$$

Lev Landau

"Since SC is a second-order phase transition, there must be an order parameter involved."



Herbert Froehlich

"T_C depends on the mass of the atoms (isotope effect), so the SC must be tied to lattice vibrations (phonons)."

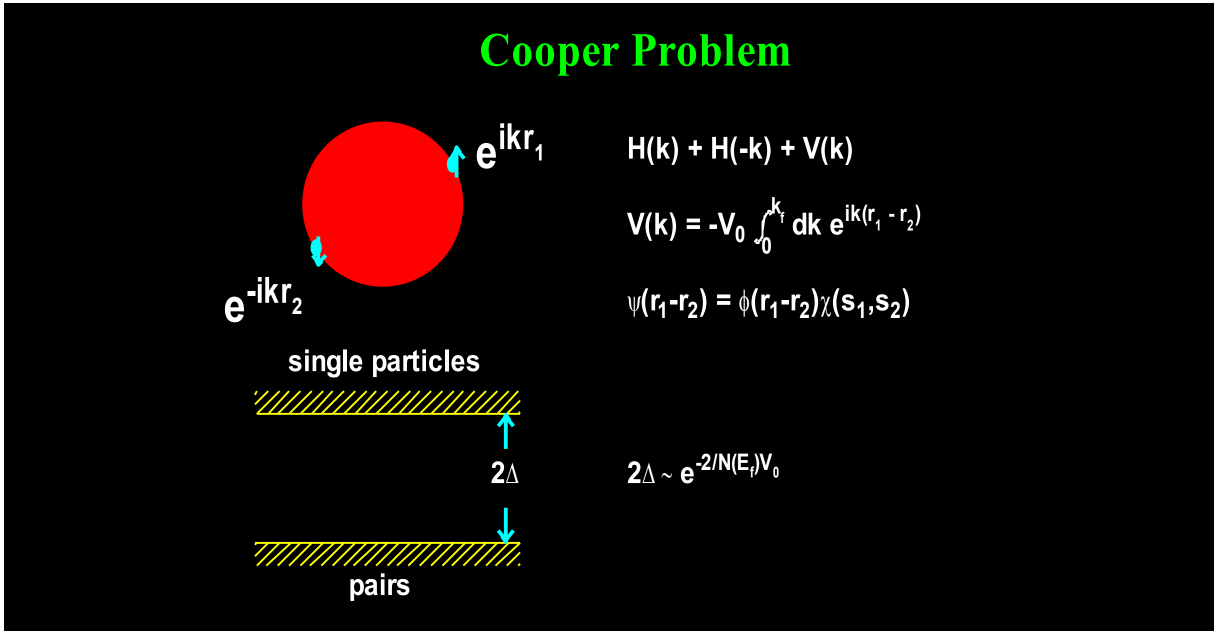
They Got It Right!

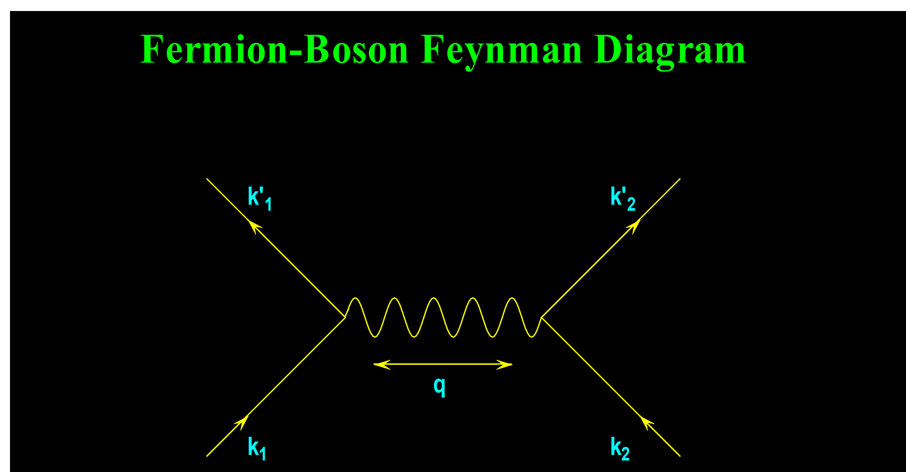
B ----- C ----- S

There has to be a regime where the lattice vibrations act to bind electrons together rather than scatter them with loss as given by Ohm's Law.

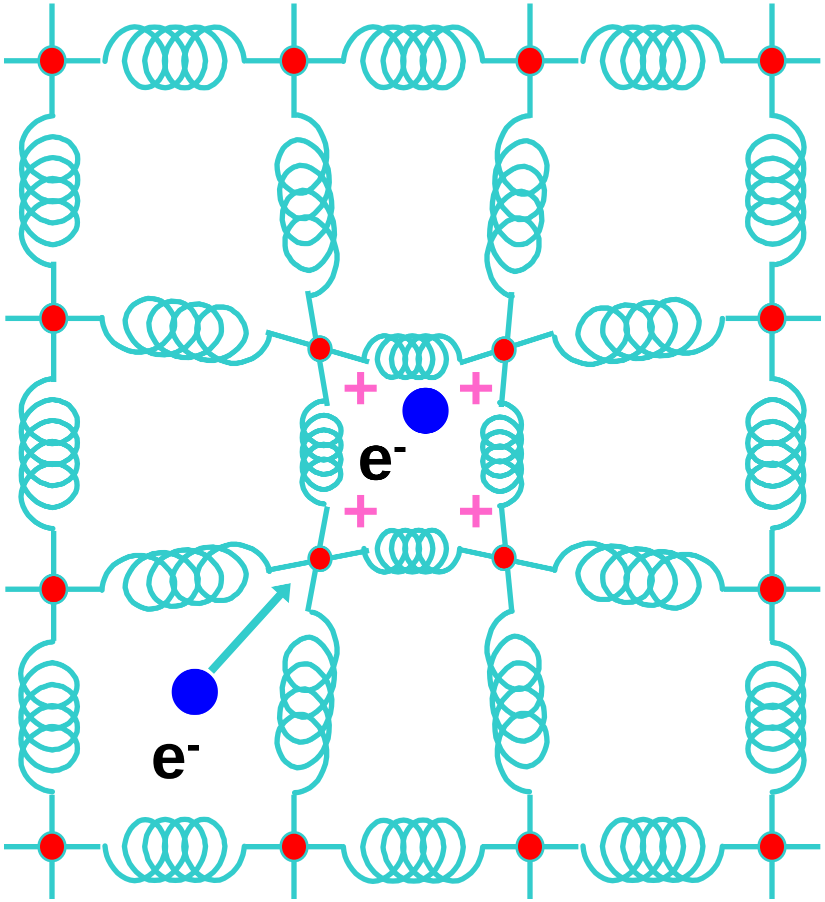
Bardeen: "It's a macroscopic quantum state"
Cooper: "It's got twice the charge you'd expect"
Schrieffer: "Ψ's a statistical wavefunction"

"Cooper's Problem"





Physics of Superconductivity



Electrons Pair Off!

BCS Equation

$$T_C = 1.14\,\theta_D \exp(-1/\lambda)$$

$$\theta_D = 275\,\mathrm{K},$$

$$\lambda = 0.28,$$

$$\therefore T_C = \underline{9.5\,\mathrm{K}} \quad \text{(Niobium)}$$

Electron-Phonon Coupling a la Migdal-Eliashberg-McMillan

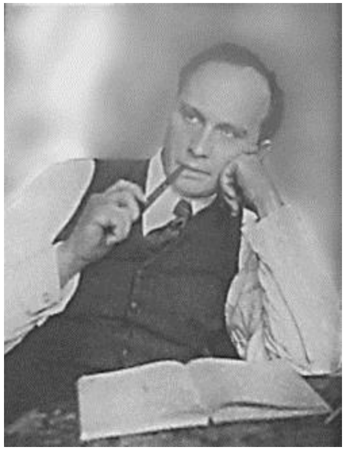
(plus Allen & Dynes)

$$H_{el-ph} = \sum_{\mathbf{k}\mathbf{q}\nu} g_{\mathbf{k}+\mathbf{q},\mathbf{k}}^{\mathbf{q}\nu,mn} \, c_{\mathbf{k}+\mathbf{q}}^{\dagger m} c_{\mathbf{k}}^{n} \, (b_{-\mathbf{q}\nu}^{\dagger} + b_{\mathbf{q}\nu}) \qquad (1)$$

$$\begin{aligned} \alpha^2 F(\omega) &= \frac{1}{N(\varepsilon_F)} \sum_{mn} \sum_{\mathbf{q}\nu} \delta(\omega - \omega_{\mathbf{q}\nu}) \sum_{\mathbf{k}} |g_{\mathbf{k}+\mathbf{q},\mathbf{k}}^{\mathbf{q}\nu,mn}|^2 \\ &\quad \times \delta(\varepsilon_{\mathbf{k}+\mathbf{q},m} - \varepsilon_F)\delta(\varepsilon_{\mathbf{k},n} - \varepsilon_F), \qquad (2) \\ \lambda &= 2 \int \frac{\alpha^2 F(\omega)}{\omega} d\omega = \sum_{\mathbf{q}\nu} \lambda_{\mathbf{q}\nu}, \qquad (3) \\ \lambda_{\mathbf{q}\nu} &= \frac{2}{N(\varepsilon_F)\omega_{\mathbf{q}\nu}} \sum_{mn} \sum_{\mathbf{k}} |g_{\mathbf{k}+\mathbf{q},\mathbf{k}}^{\mathbf{q}\nu,mn}|^2 \\ &\quad \times \delta(\varepsilon_{\mathbf{k}+\mathbf{q},m} - \varepsilon_F)\delta(\varepsilon_{\mathbf{k},n} - \varepsilon_F). \qquad (4) \end{aligned}$$

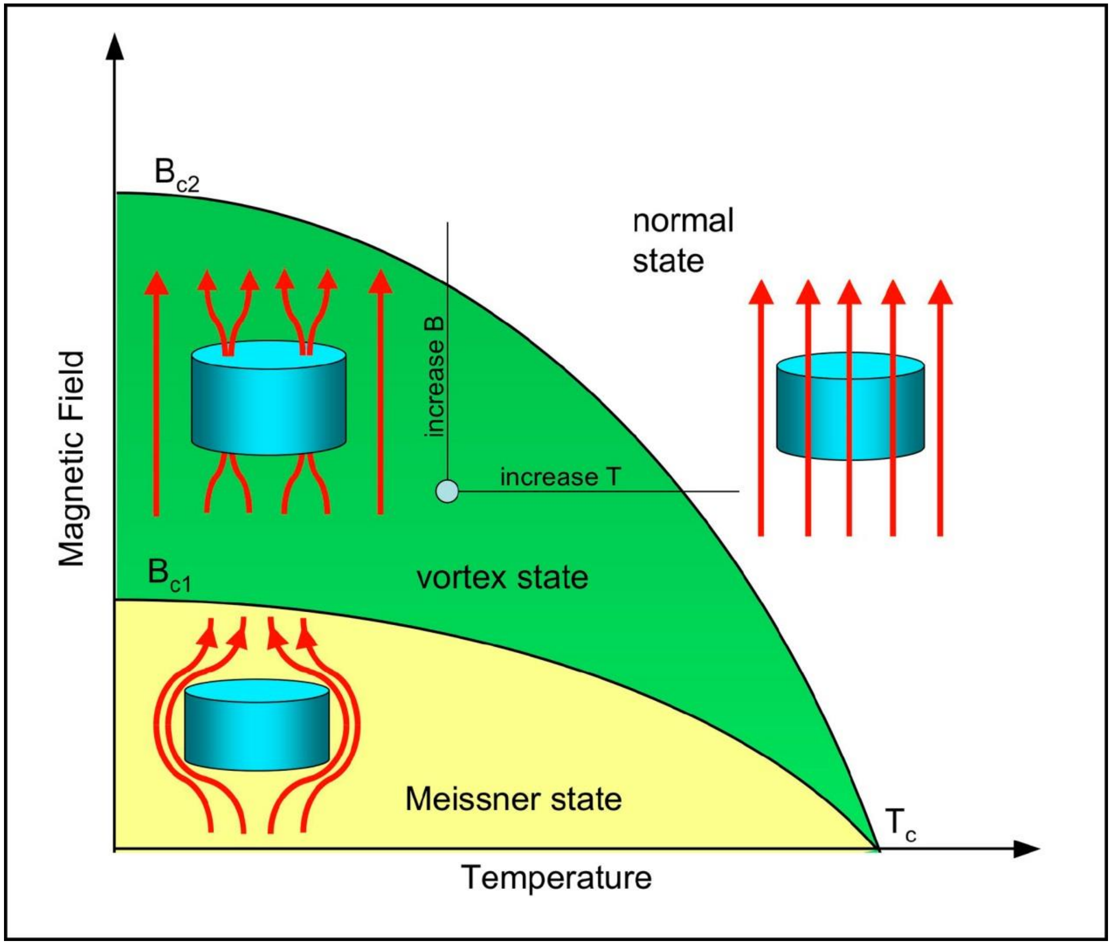
Wierzbowska, et al, arXiv:cond-mat/0504077 (2006) (Nb)

Type II (1930s +)



Lev Shubnikov

Lev Landau



"VL" Ginzburg

Aleksei Abrikosov

GLAG – "Engineering" Superconductors

$$G[\phi] \approx \int d^3r[\frac{1}{2m^*}(-i\hbar\nabla + e^*A)\phi^*(i\hbar\nabla + e^*A)\phi + a\phi\phi^* + \tfrac{1}{2}b\phi\phi^*\phi\phi^*]$$

$$-(i\partial\nabla - \mathcal{A})^2 f + f(1 - f^2) = 0$$

$$\kappa^2\nabla\times(\nabla\times\mathcal{A}) + \tfrac{1}{2}i(f^*\nabla f - f\nabla f^*) + \mathcal{A}f^2 = 0$$

$$\phi = (|a|/b)^{1/2} f$$

$$A = (\Phi_0 / 2\pi\xi)\mathcal{A}$$

$$\kappa = \lambda_L / \xi$$

$$\kappa < 1/\sqrt{2} \qquad \text{I}$$

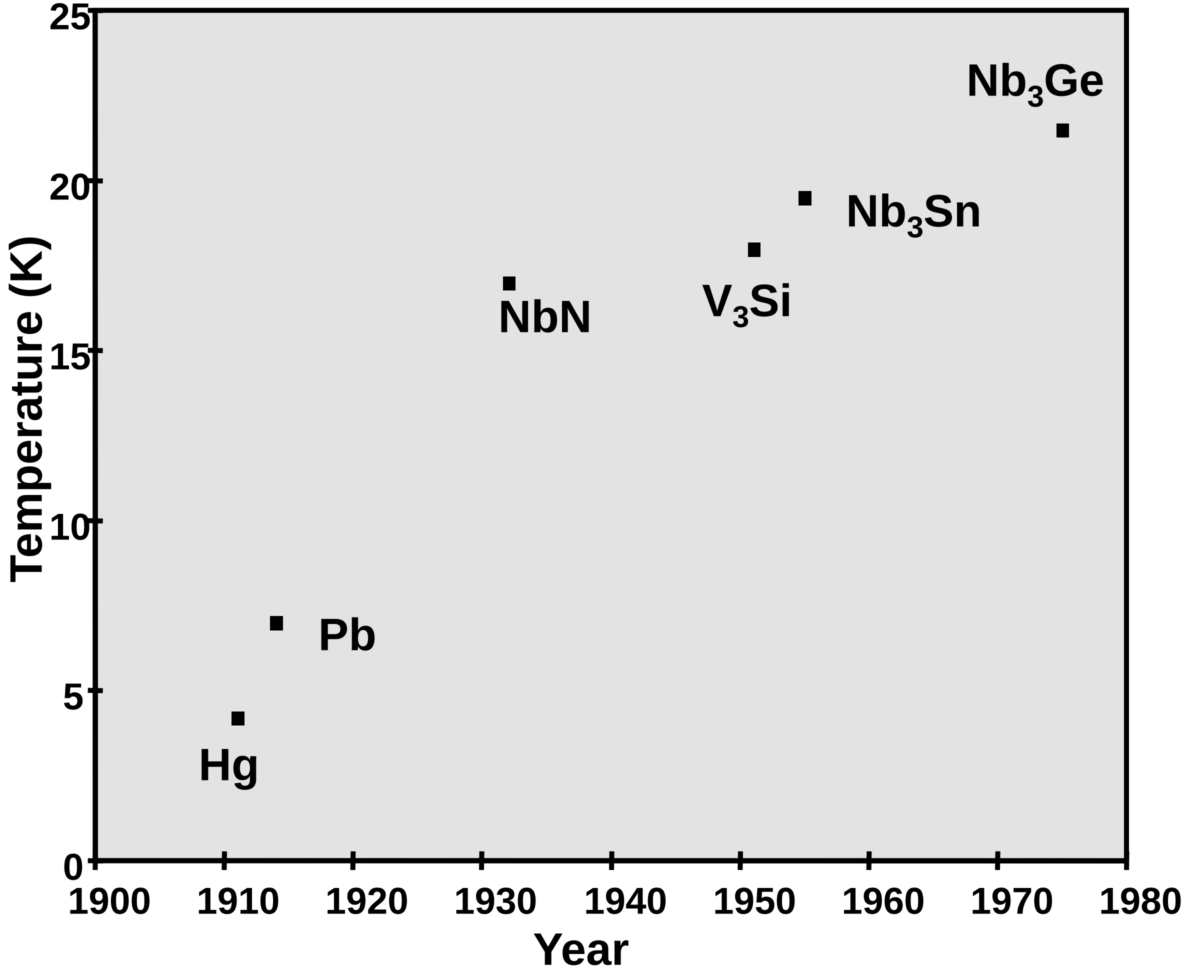
$$\kappa > 1/\sqrt{2} \qquad \text{II}$$

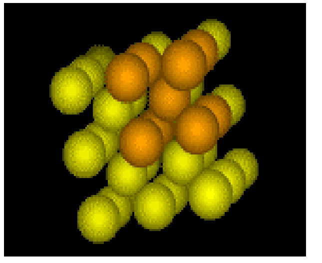
Important Numbers in Superconductivity

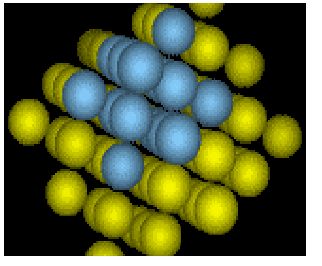
Transition Temperature, T_c	Way below 300 K
Critical Current Density, J_c	10^{-2} - 10^{6} A/cm^2
Critical Magnetic Field, H_c	10^{-4} - 10 T
London Penetration Depth, λ	10 - >1000 Å
Pippard Coherence Length, ξ	10 - >1000 Å
G-L Parameter, $\kappa = \lambda/\xi$	0.01 - 100

NB! All these numbers depend on each other. E.g., $H_c \sim \lambda\ \xi$

T_C vs. Year: 1911 - 1980

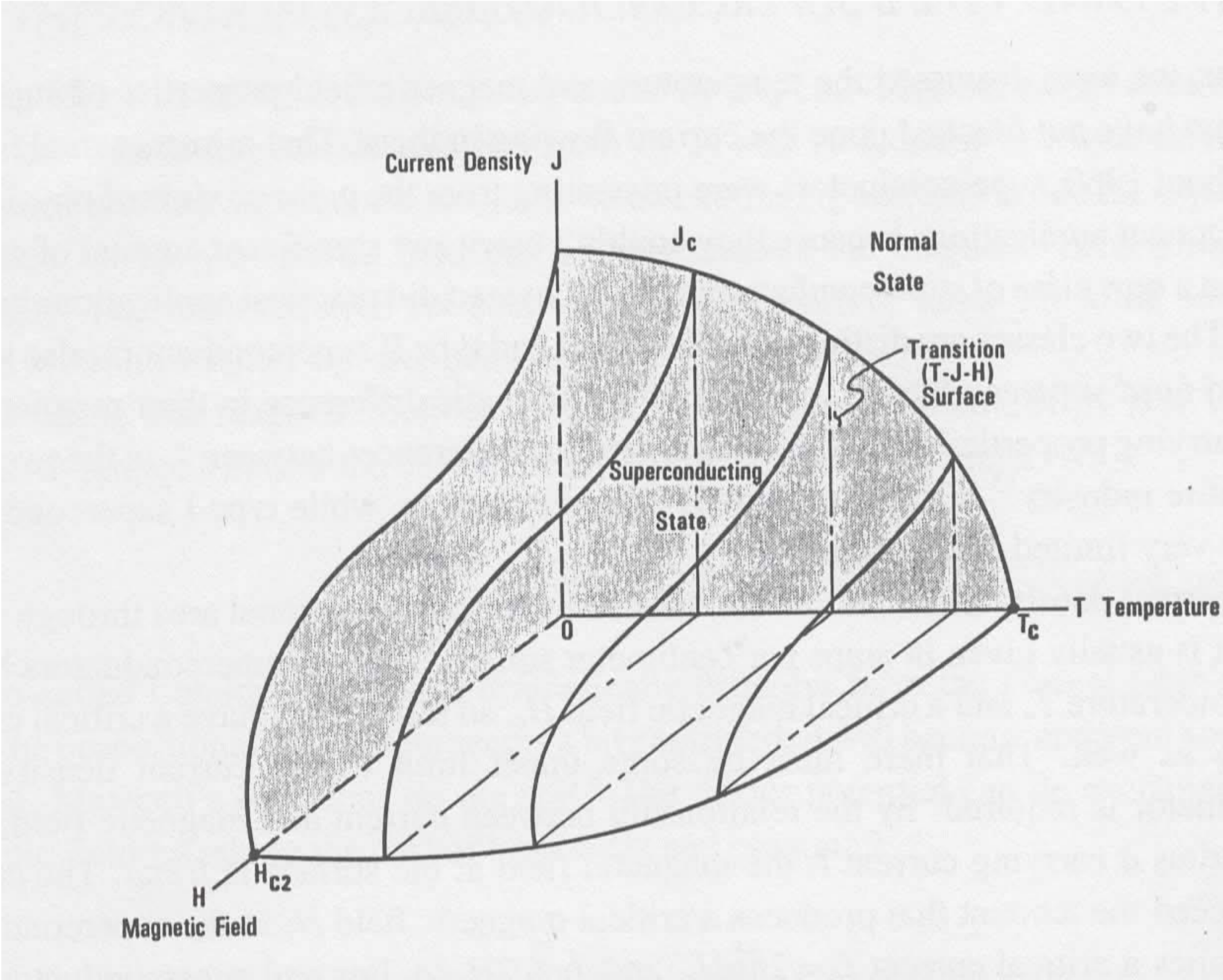






Cubic Metals

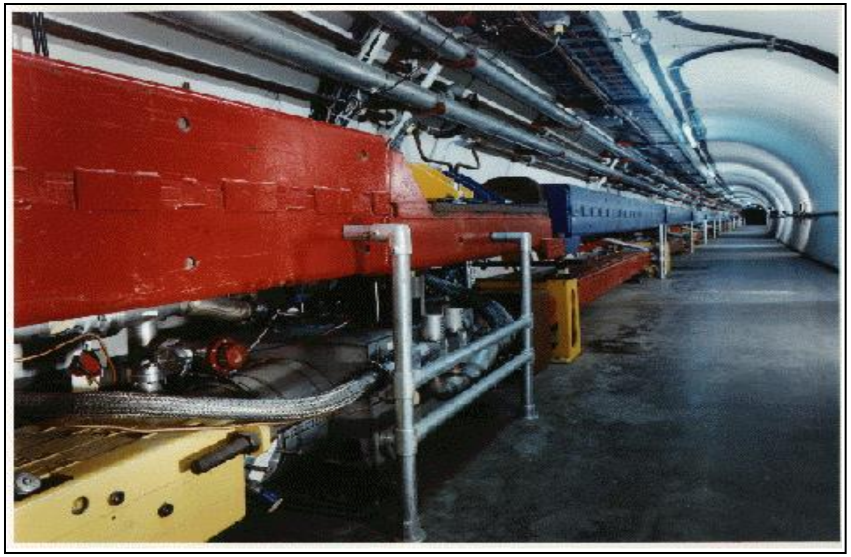
Properties



Current Density J
J_c
Normal
State
Transition
(T-J-H)
Surface
Superconducting
State
0
T Temperature
T_c
H_{c2}
H
Magnetic Field

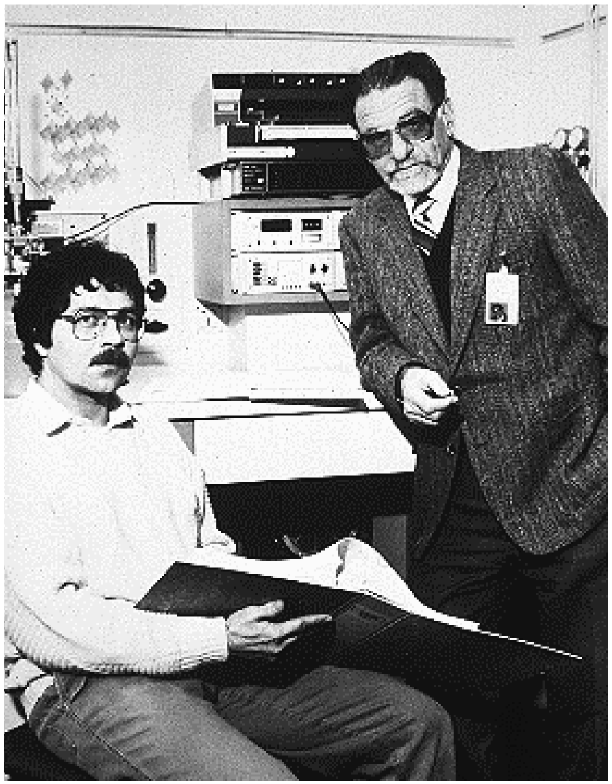
MRI & "Big Physics"

<u>Magnetic Resonance Imaging</u>
Philips

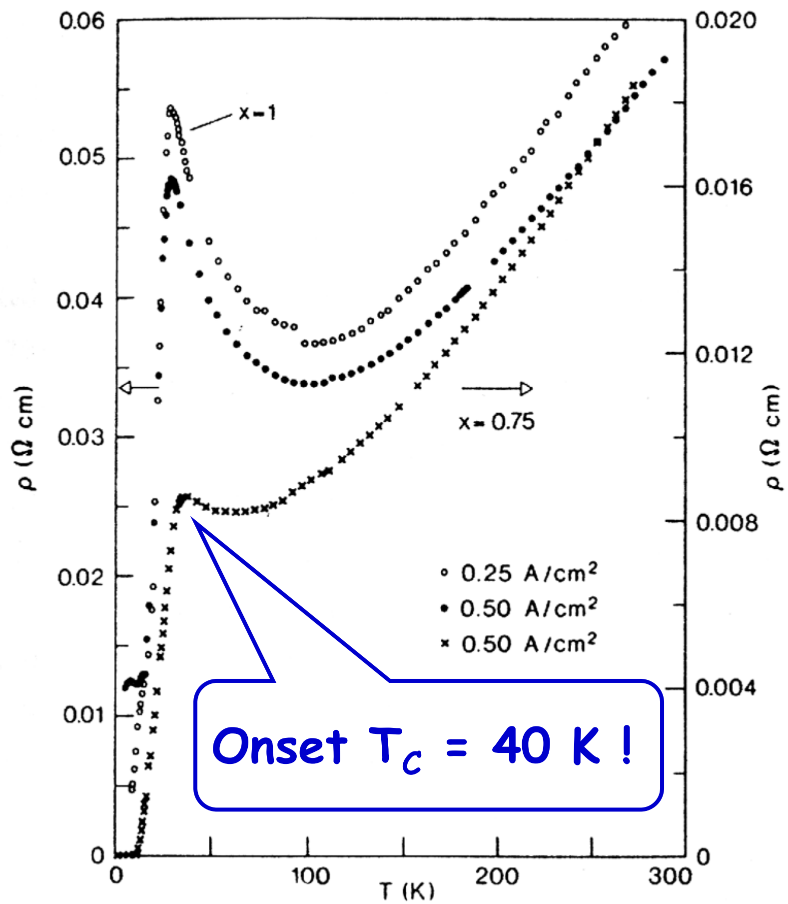


<u>Tevatron</u>
Fermi National Laboratory

1986
Another Big Surprise!



<u>Bednorz and Mueller</u>
<u>IBM Zuerich, 1986</u>



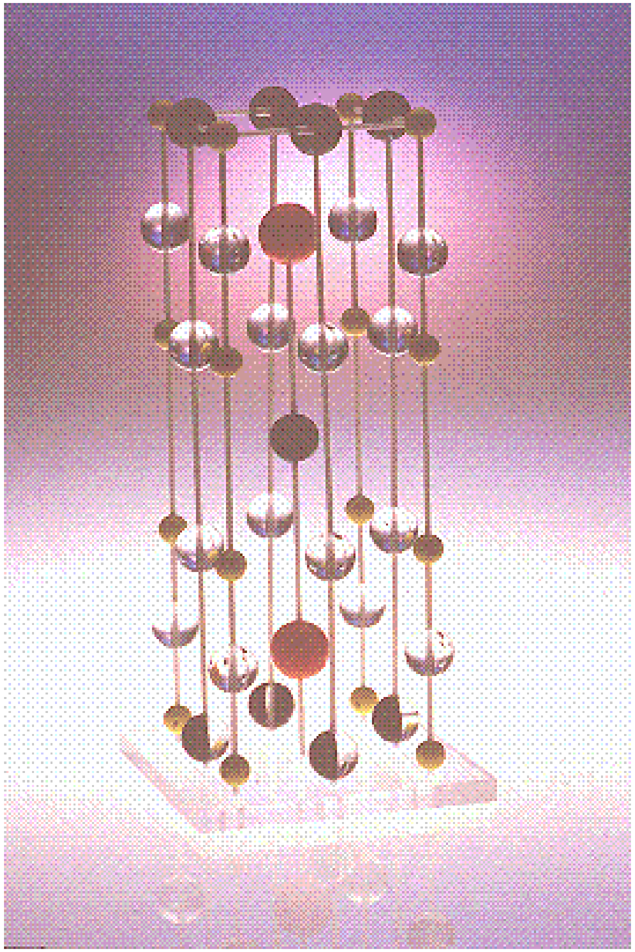
1987
"The Prize!"

Associated Press

J. Georg Bednorz, left, and K. Alex Müller after learning they had won the Nobel Prize in physics.

2 Get Nobel for Unlocking Superconductor Secret

March 3, 1987
“123” Discovered



Woodstock of Physics
NYC, 1987

Physicists' Night Out!

commentary

Woodstock of physics revisited

Ten years have passed since the now famous American Physical Society meeting that heard the first breathless accounts of high-temperature superconductivity. Now, in calmer times, practical applications are emerging.

Paul M. Grant

Snap quiz: who can tell me the winner of the 1987 Super Bowl? Not most physicists, I suspect, for whom it was certainly eclipsed by two events of far greater consequence that shared the early months of that year. One, the discovery of Supernova 1987A, perhaps portended the other: the announcement of superconductivity above liquid-nitrogen temperature on planet Earth — a dream fulfilled for many condensed-matter physicists like myself, whose careers had orbited around this elusive star.

The successful sighting[1] fell to W. K. Wu and C. W. (Paul) Chu and their teams of students and postdocs at the Universities of Alabama and Houston, following only five months after the publication in autumn 1986 by Georg Bednorz and Alex Müller[2] at IBM Zürich of their discovery of superconductivity in a previously unexplored class of compounds, the layered copper-oxide perovskites.

Rising stars: Müller and Chu with Shoji Tanaka (right), whose Tokyo laboratory provided one of the first confirmations of Bednorz and Müller's discovery.

The 'inside' story of the hectic interval between the first week in January 1987 — when an announcement of the confirmation of Bednorz and Müller's discovery first brought 'high-temperature superconductivity' to wide public attention — and the week of the American Physical Society's March meeting, remains to be told. Suffice it to say that this period, and the last three months of 1986, were replete with incredulity, credulity, excitement, secrecy and a sense of immediacy in competition with one's peers, all of which resulted in, frankly, a substantial amount of intrigue and suspicion. All who participated surely came to understand, if they had not done so before, that physics is not only a science but, perhaps more significantly, an intensely human pursuit — something they do not teach you in graduate school.

The programme of the March meeting, held each year in a different US city, is 'cast in concrete' early the preceding December; thereafter, an absolute policy of no alterations prevails. By the deadline of 5 December 1986, for the 1987 meeting at the Hilton hotel in New York City, only one abstract had been accepted on the new materials: "Specific heat of Ba–La–Cu–O superconductors" by Rick Greene and his collaborators at IBM Yorktown. But the explosion of results that appeared in the new year prompted the meeting's organizers to take an unprecedented step. Brian Maple of the University of California, San Diego, was asked to put together a special post-deadline evening session devoted entirely to the discovery.

All those wishing to report results would be granted five minutes each, in order of the arrival of their request to take part — and did the requests rain in, reaching a downpour in the two weeks before the meeting, as confirmations of the Wu–Chu measurements were made. All in all, 51 presentations were to be given throughout the evening and early morning of Wednesday and Thursday, 18 and 19 March. That memorable and riotous session was to become our "Woodstock of physics", so named in honour of the village only 50 miles north where, in an obscure farmer's muddy field in 1969, the rock concert occurred that defined a generation of youth the world over.

Fever pitch: the room filled to overflowing with physicists eager for news of superconductivity.

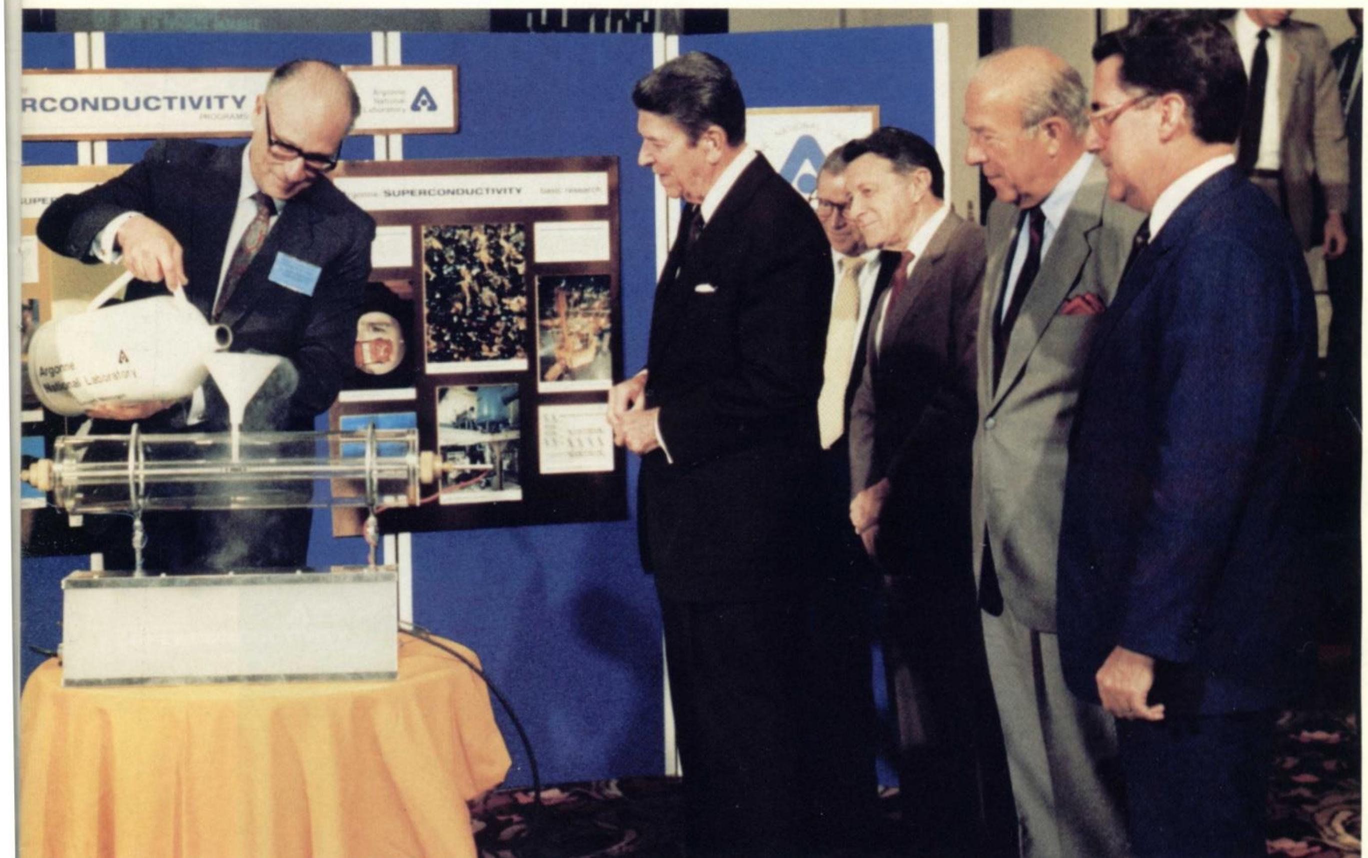
Opening act

A few personal observations and anecdotes may help to convey the colour of that week in midtown Manhattan. Excitement was running high even before Wednesday night. On Monday, the opening day, the press were already beginning to catch some of us to be interviewed. That noon my colleague Ed Engler and I went to lunch at a nearby Brew 'n' Burger and found Alex Müller sitting by himself in a corner booth, attempting to escape the turmoil at the Hilton. At the time he was not yet widely recognizable to those attending the meeting or to the press — a situation that would soon change.

HTSC Symposium, MRS Spring Meeting, Anaheim, 23–24 April 1987

"The Altamont of Materials"

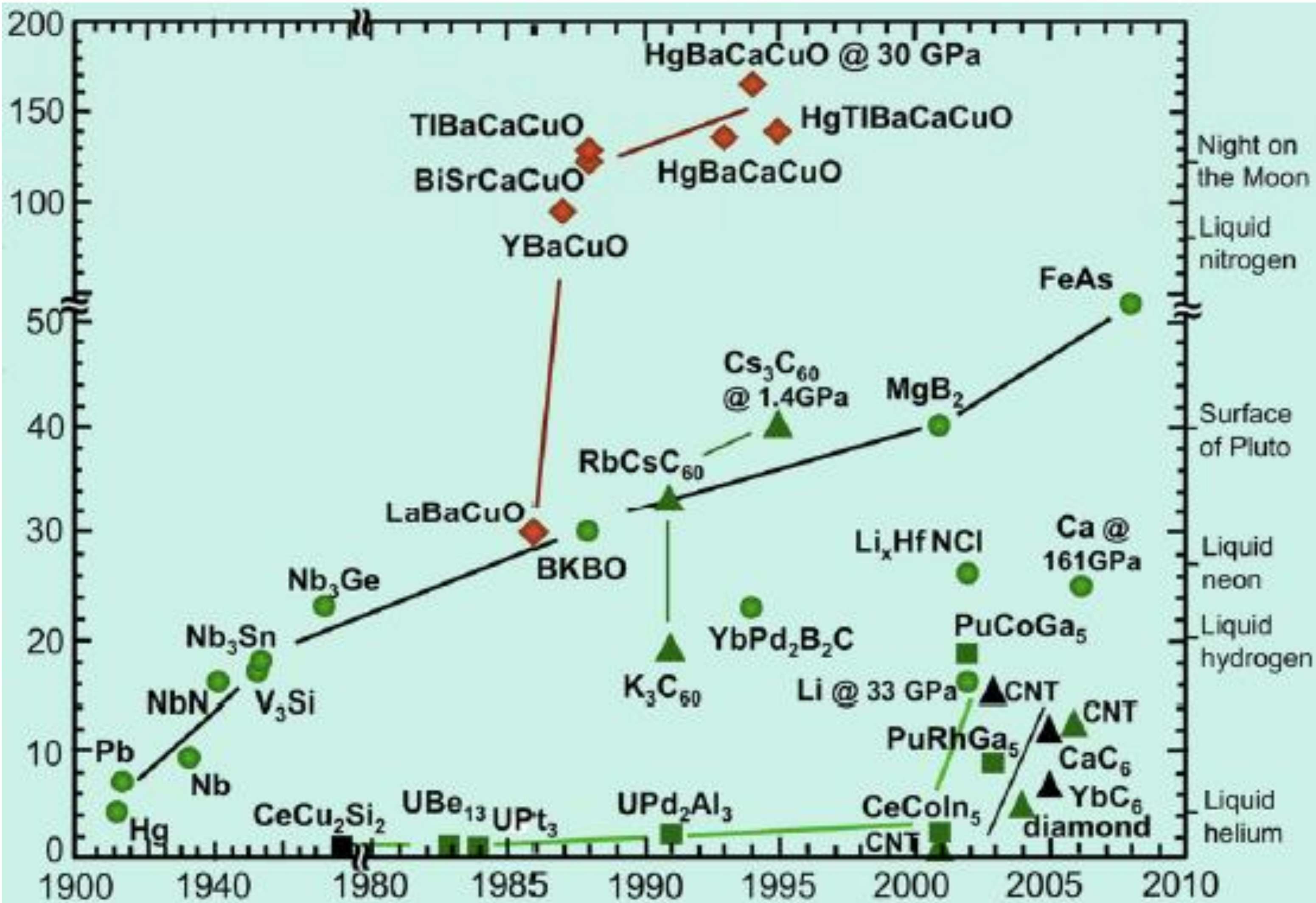
“The Great Communicator”



Alan Schriesheim, Director of Argonne National Laboratory, demonstrates superconductivity to the President, Chief of Staff Howard Baker, Secretary of Defense Caspar Weinberger, Secretary of State George Shultz and Secretary Herrington.

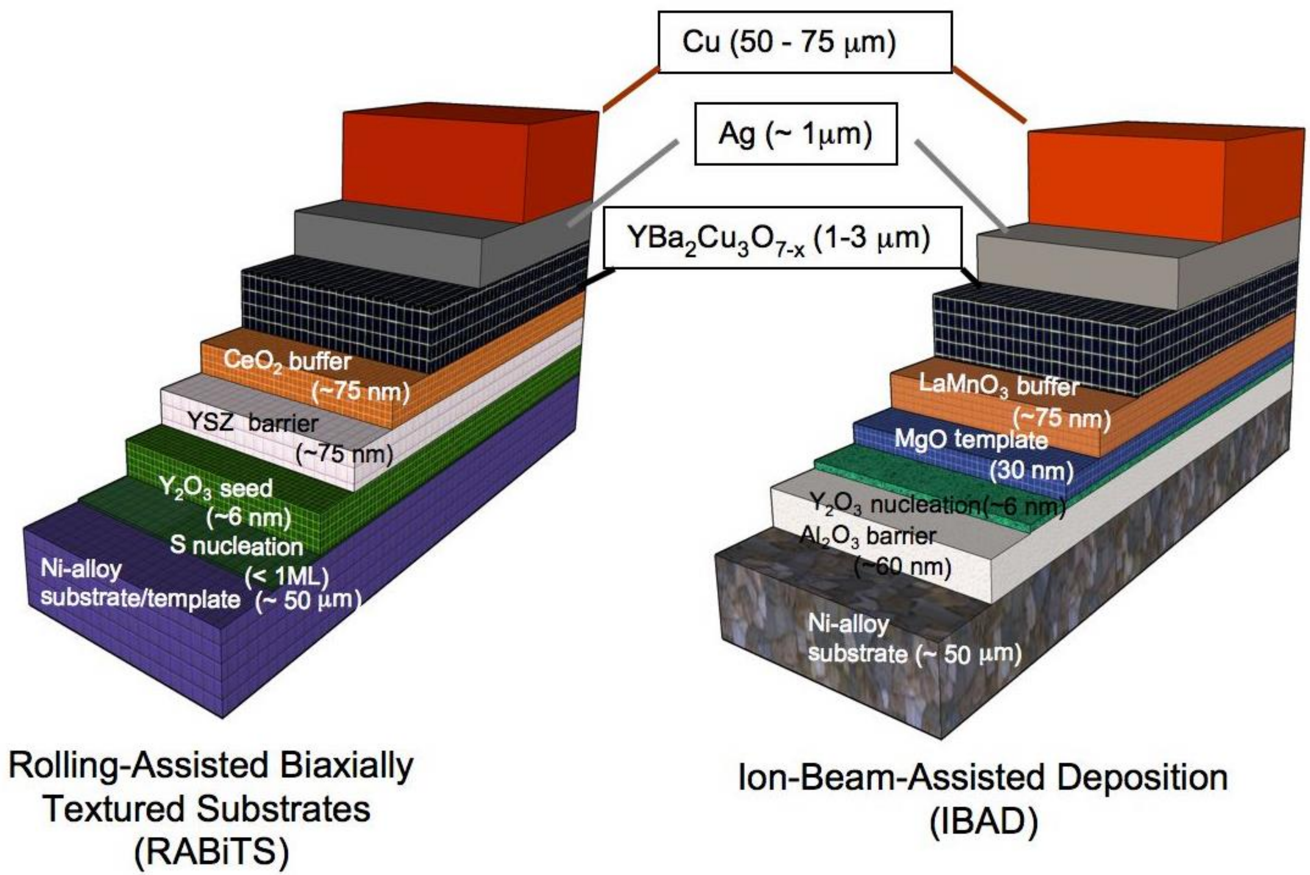
Today

Tc (K)



Year

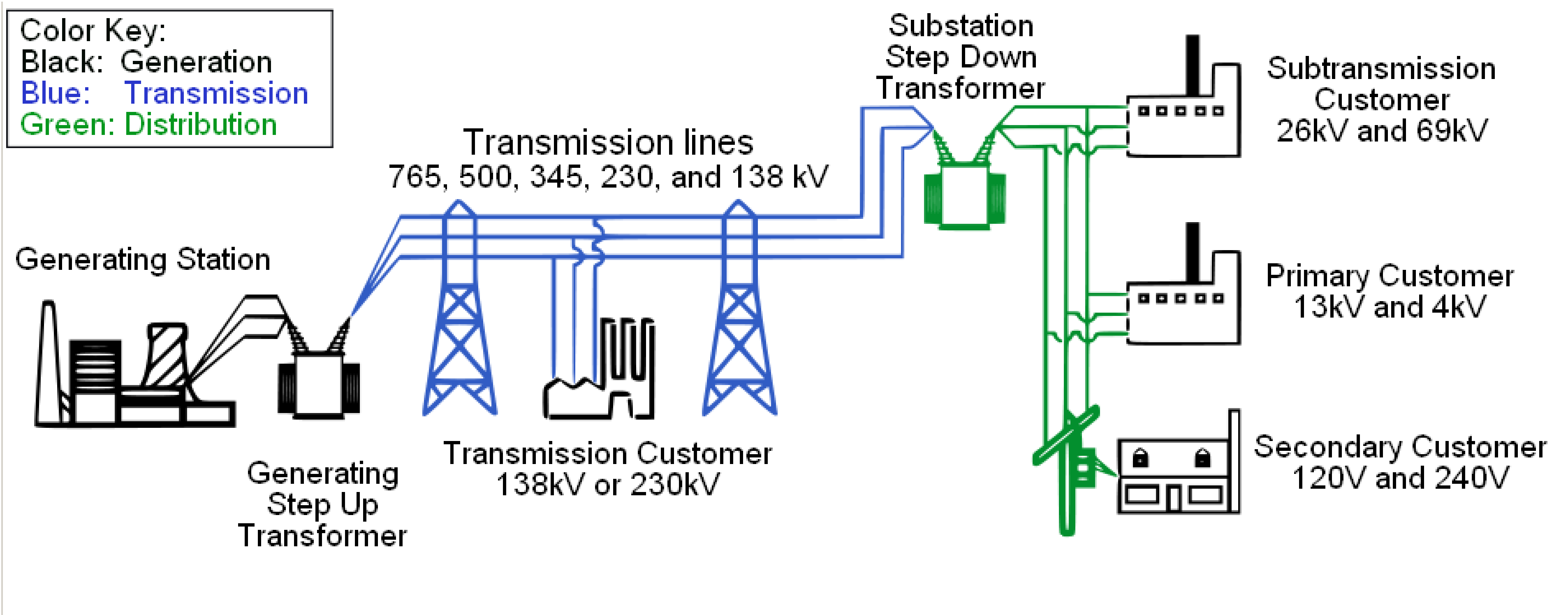
Gen II Coated Conductor



American Superconductor

SuperPower

Where Can We Apply Superconductivity to Electric Power?



Potentially Everywhere

It is now 27 years after "Woodstock and Altamont," yet two major issues remain unresolved:

"The Nanoscale:"

How does HTSC even occur? We know it's BCS, but what's the **"pairing glue?"**

"The Exascale:"

Despite more than 20 years of very successful HTSC wire development possessing outstanding critical state properties, and its use in equally outstanding and successful power application demonstrations in the US, Japan, China, Korea, Germany, Russia…, there remains no significant deployment of such technology by either government agencies or investor-owned utilities.

How come?

Hubbard Theory

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

One-electron "band" term

On-site "Hubbard" double occupation coulomb repulsion

Off-site repulsion

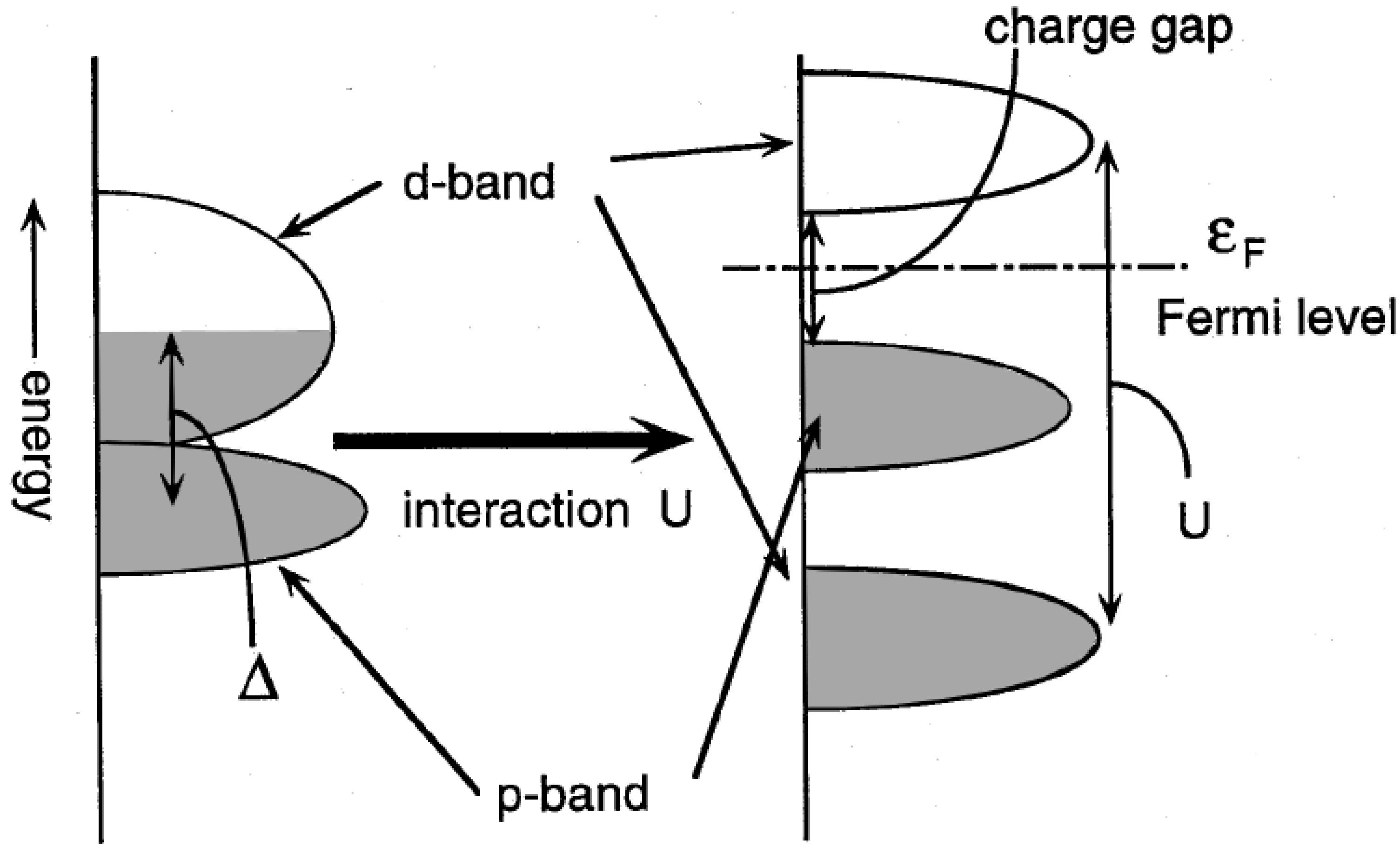
$$kT_N \sim 4t^2 / S^2 U$$

DFT & (LDA + U)

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

- Implemented in LMTO by Anisimov, et al, JPCM 2, 3973 (1990)
  - Applied to NiO, MnO, FeO, CoO and La_2CuO_4
- 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

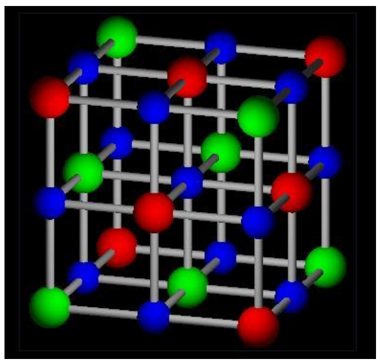
Charge Transfer Insulator



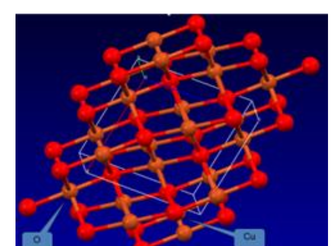
After Imada, et al, RMP 70, 1039 (1998)

Cubic Rocksalt Divalent TMOs

TMO	3d Config	Properties
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	**XX *Doesn't Exist!***

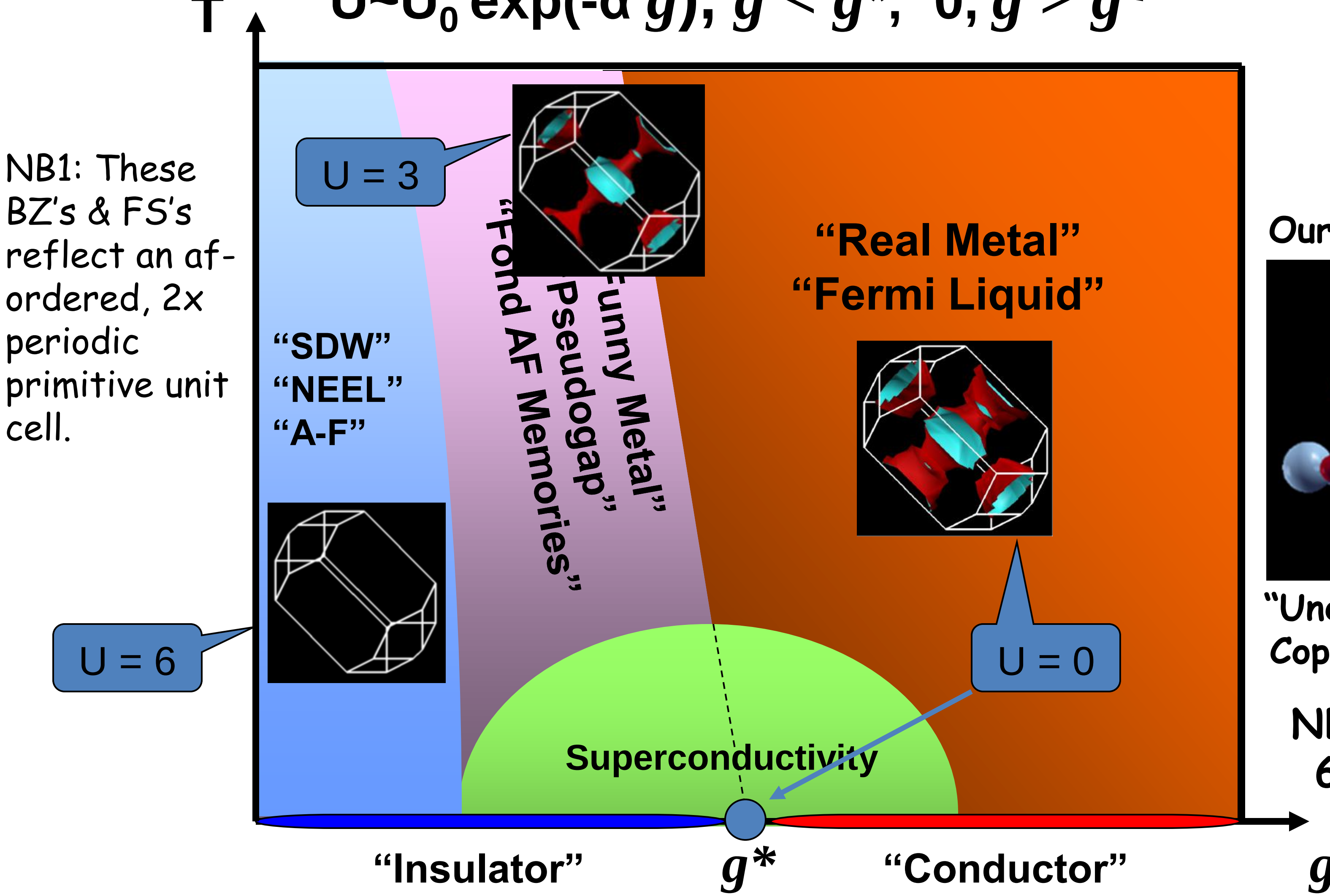


Tennorite

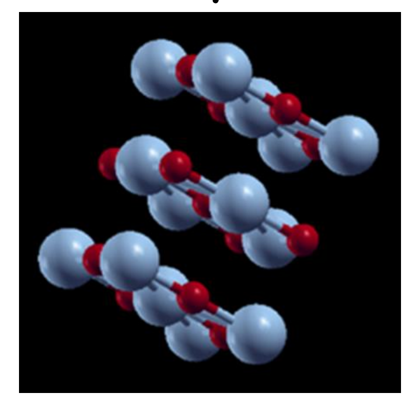


The Colossal Quantum Conundrum

$U \sim U_0 \exp(-\alpha\, g),\ g < g^*;\ \ 0,\ g > g^*$



Our Proxy HTSC!

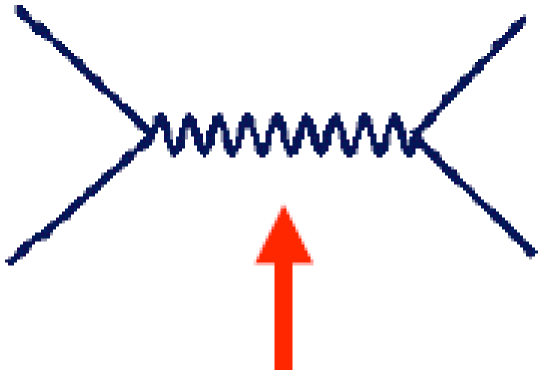


"Undoped Rocksalt Copper Monoxide"

NB2: For U < 6 eV, it's a **metal**!

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

IOW, What's theFermion-Boson Interaction That Leads to HTSC?



Insert your favorite "on" here

(phonon, magnon, exciton, plasmon, anyon, moron …)

"Put-on !"

The Pairing Glue

"Alex says it's phonons"

OK, OK...J-T polarons and/or bipolarons (after Chakravarty/Hoest)

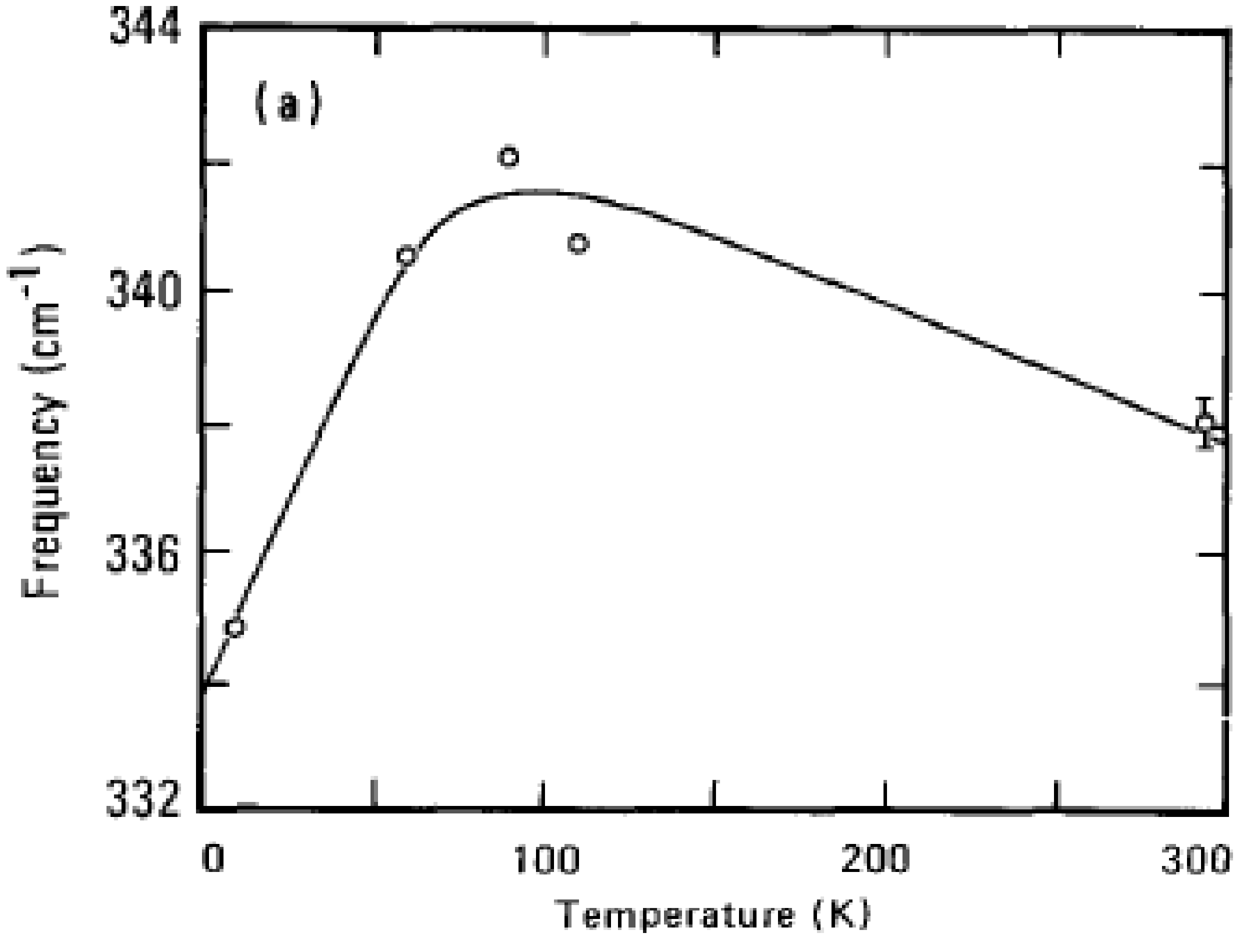
Could he be right after all?

Hey! Maybe, they're there!

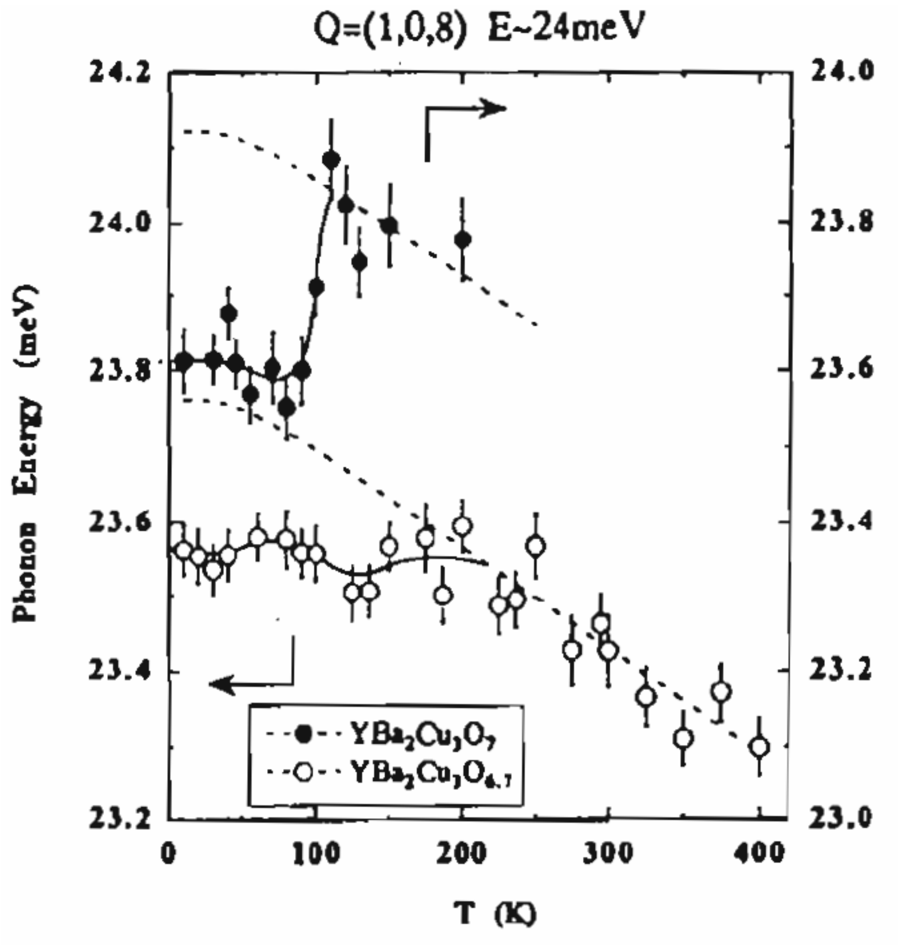
Macfarlane, Rosen, Seki, SSC 63, 831 (1987)

(These data were taken in early March, 1987, a week before "Woodstock")

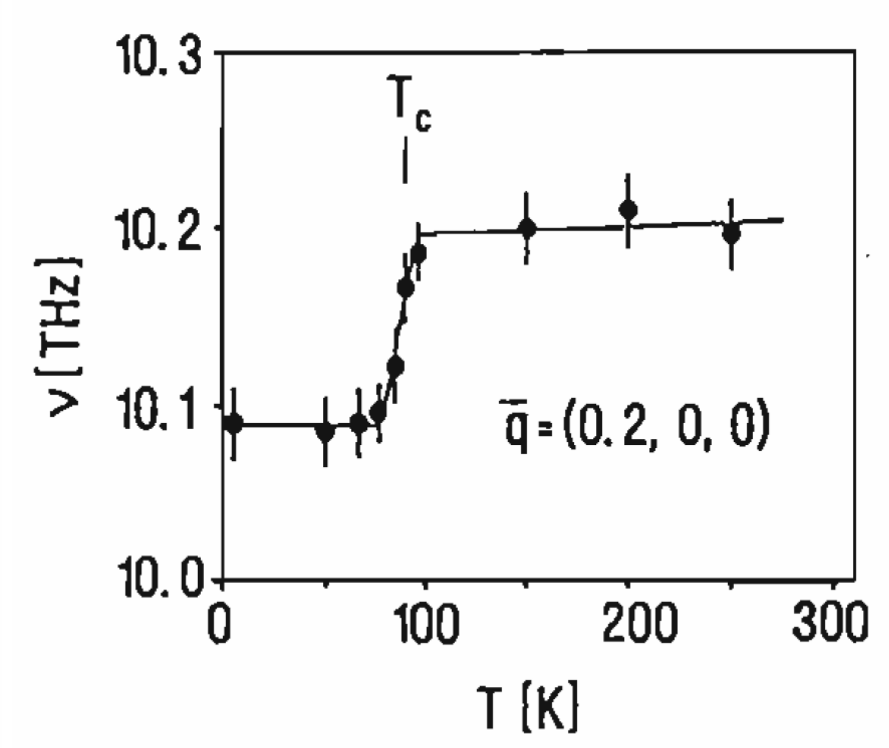
Raman Spectroscopy of YBCO



More Phonon Phootprints!



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

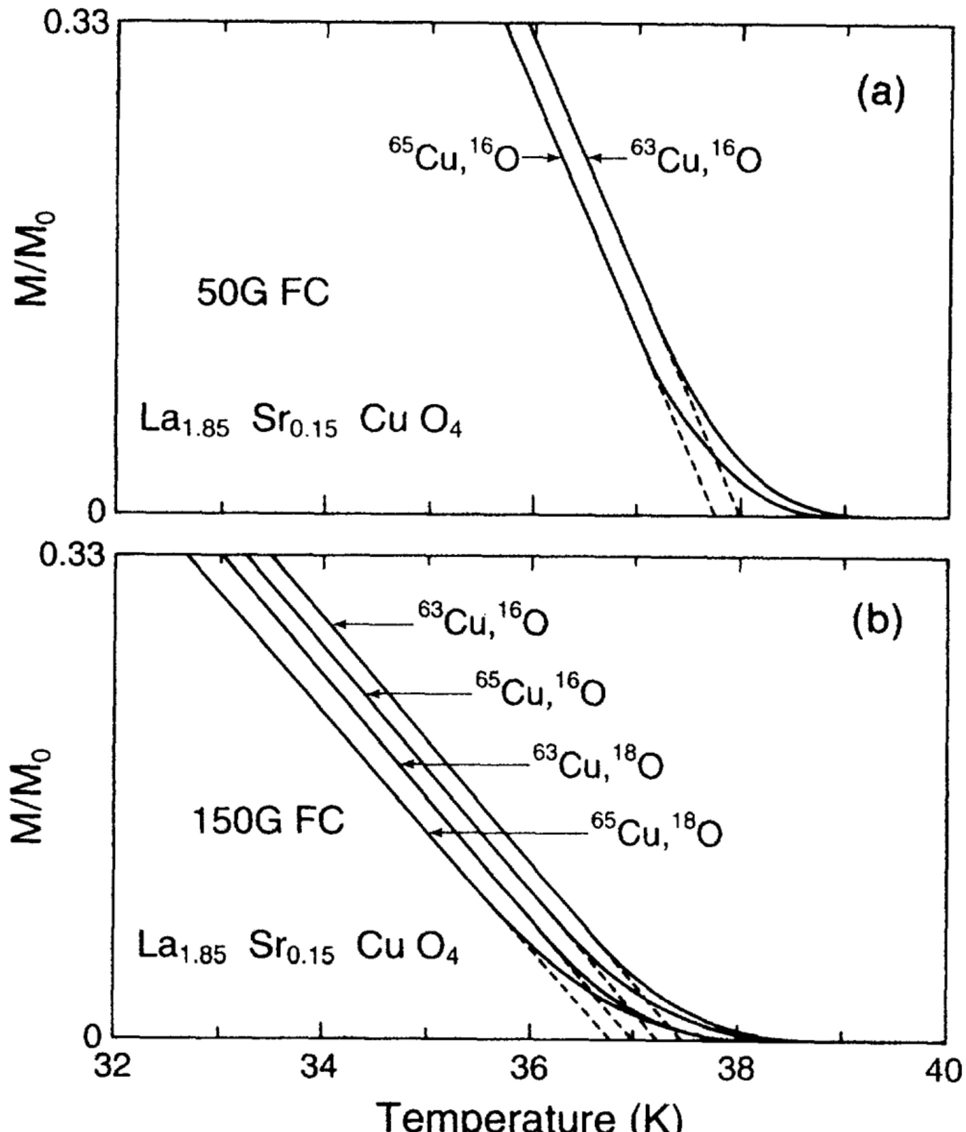


Pyka, et al., PRL 70, 1457, (1993)

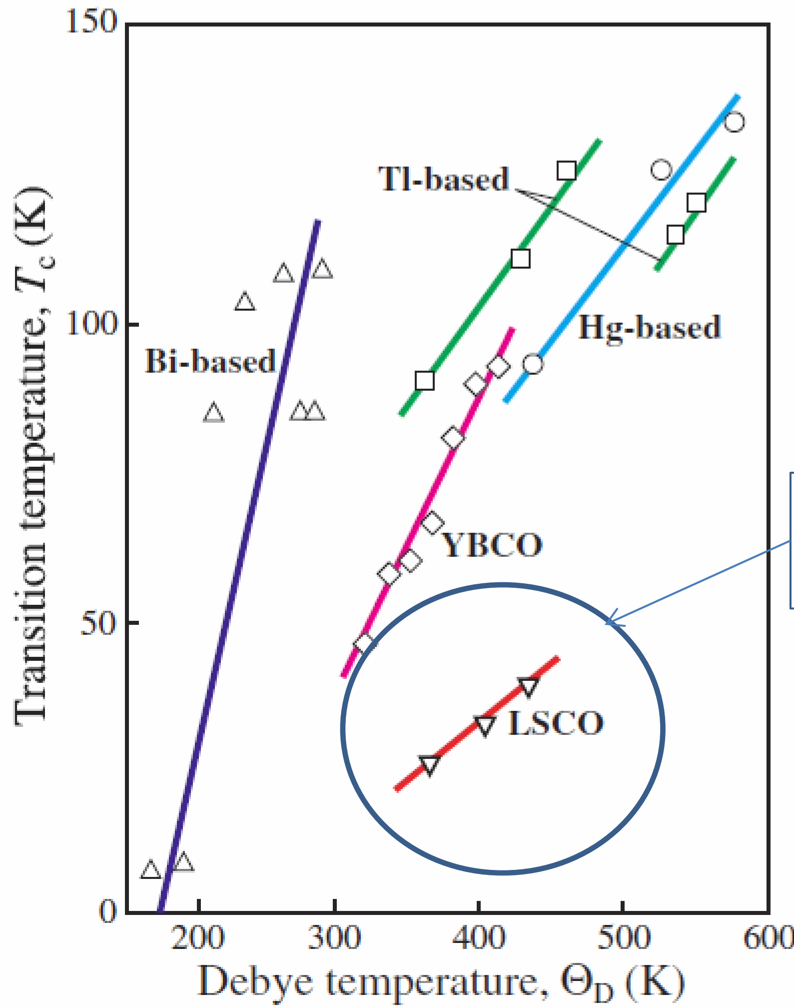
...and More!

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

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



Finally, T_C scales (roughly) with Θ_D!



Nota Bene!
"S" denotes Ca, Sr, Ba

Ledbetter, Physica C 235, 1325 (1994)

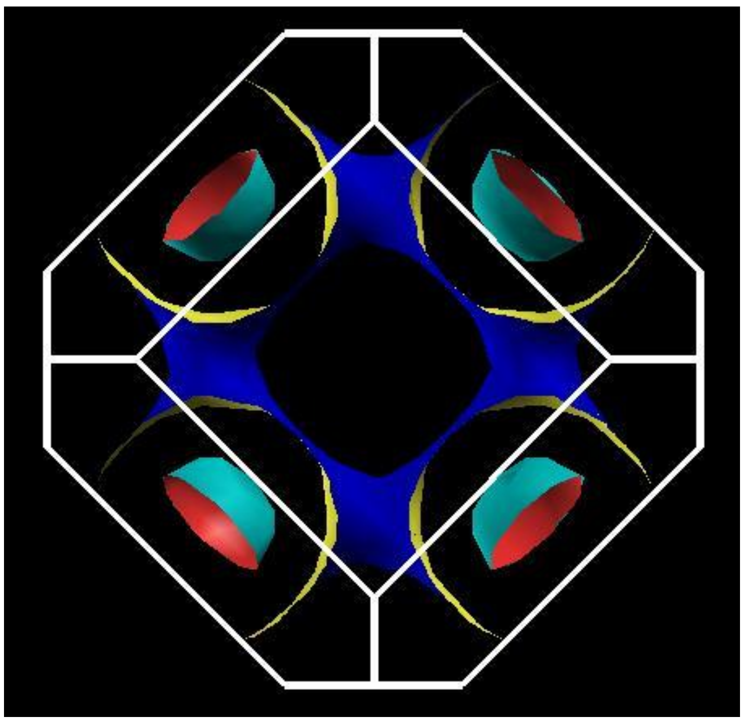
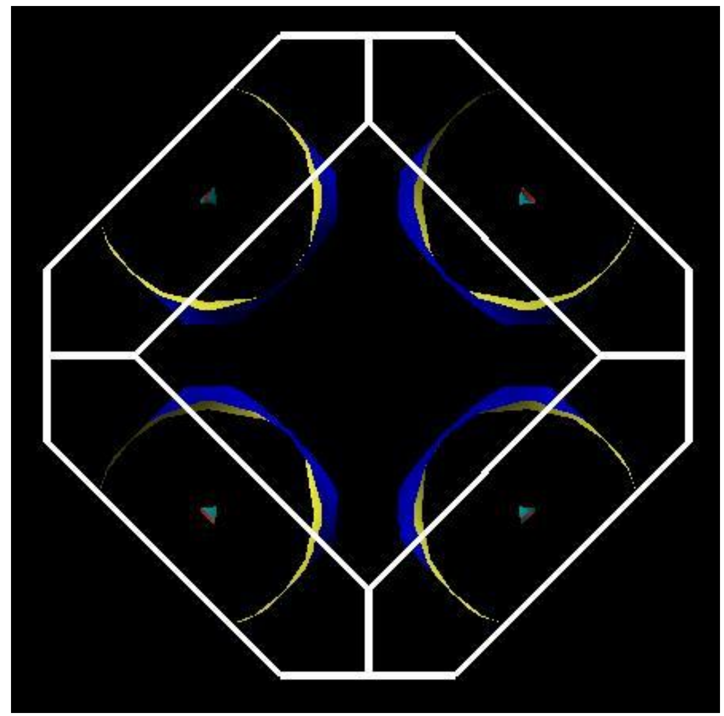
What Can DFT(LDA+U) Along With Eliashberg-McMillan-Allen-Dynes (EMAD) Formalism Tell Us About e-p Mediated Pairing in the Copper Oxide Perovskites?

- Assume the simplest and highest symmetry possible Cu-monoxide to model (e.g. cubic or tetragonal rocksalt CuO...see Grant (Proc IOP (2008) and Siemons, et al., PRB (2009)).
- Apply the Quantum-Espresso DFT Package to calculate the eigenspectrum and e-p coupling for these proxy structures, followed by application of EMAD to estimate Tc (Grant, Proc. MRS, to appear).
- Perform the above for both hole and electron doping levels $\pm 0.15|e|/CuO$ under the assumption these levels of carrier densities effectively screen Hubbard U (see "Quantum Conundrum")

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

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

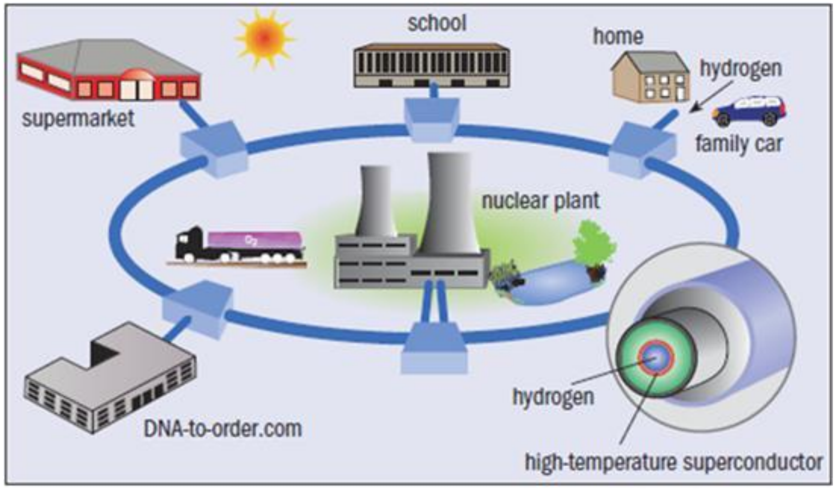
Assumptions: $\Theta_D \approx 440$ °K, $\mu^* \approx 0.01$, a = 3.06 Å, c/a = 1.3 (nmTet cell)

q = 0.15 |e|/CuO (holes)	**q = -0.15 |e|/CuO (electrons)**
	
λ = 1.2	**λ = 0.7**
≈ 43 °K	**≈ 25 °K**

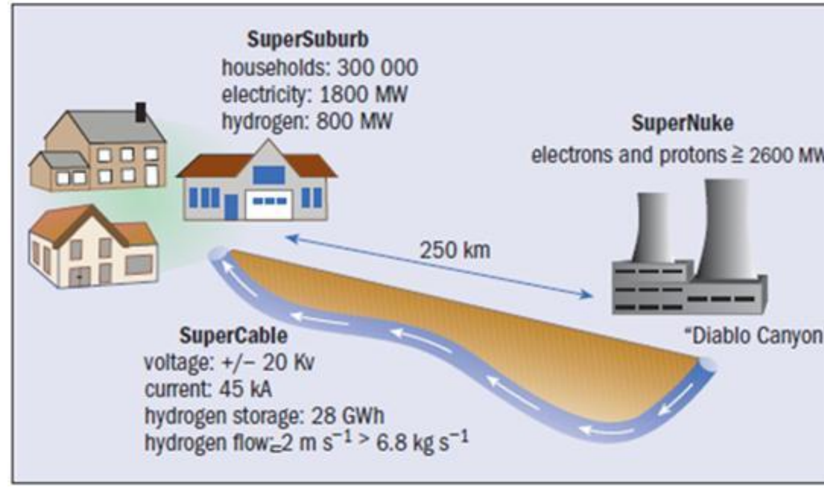
OK…What's Next (Materials-Wise)?

- Force-epi 10 monolayers of tet-CuO
  - Overlay with 2 monolayers of Li as "neighborhood" dopant…look for SC
  - Trying this right now at Stanford!
  - "Topological Metal?" ☺
- Look for explicit "phonon-spinon" coupling:
  - "Paramagnetic Dispersion Measurements at 77.3 °K," C. Starr (MIT). Examines the coupling between spins and phonons in transition metal carbonates and hydrates.
  - Published in Phys. Rev. 60, 241 (1941!)
  - Have such studies been done on the copper oxide perovskites? If not, why not?
- Apparently no DFT(LDA+U) tools yet exist to calculate electron-phonon λ in the presence of a finite Hubbard U…why not?

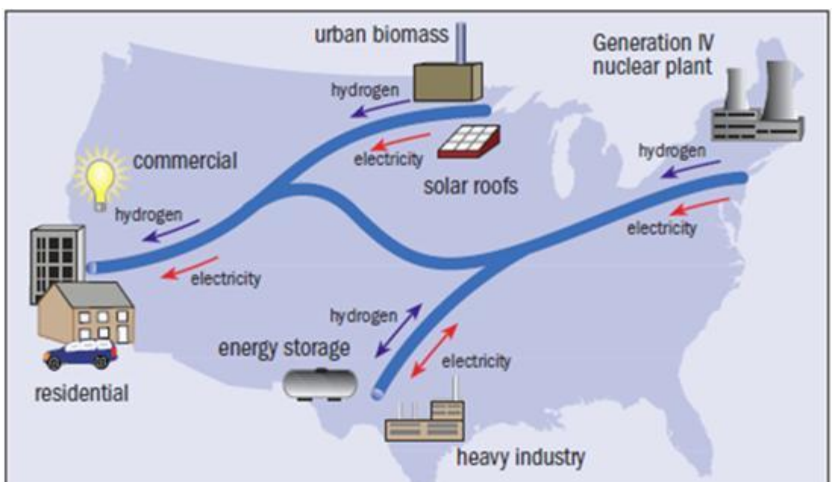
Now for something slightly bigger… by 10^{19} (Exascale!)



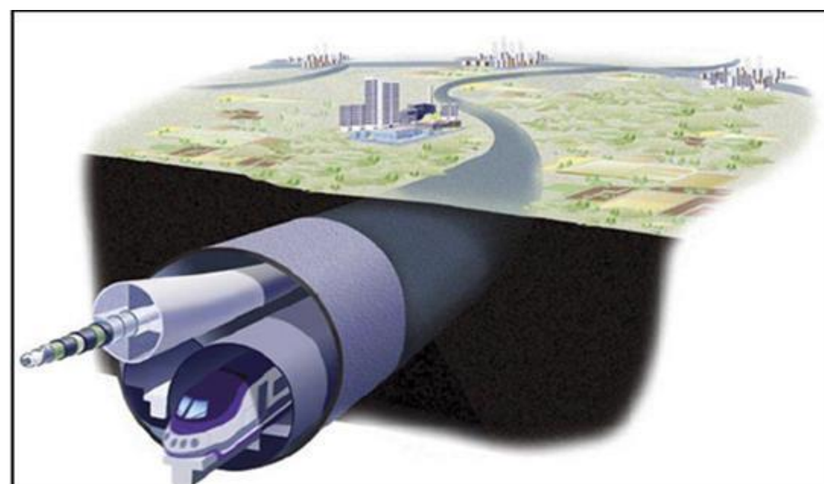
SuperCity



SuperSuburb



SuperGrid

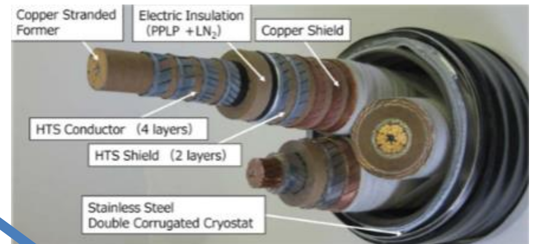


SuperTrain

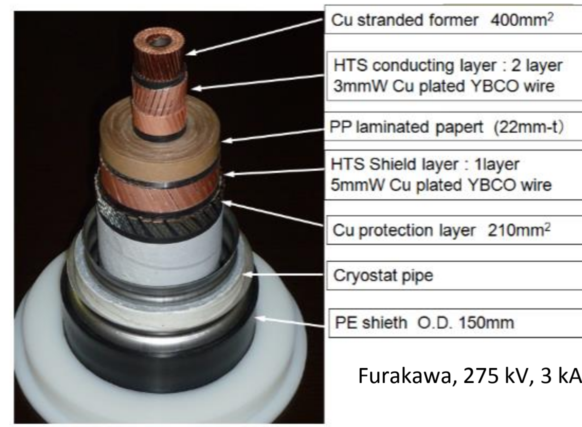
~ 1997

HTSC SuperCables: Past, Present, and...Future?

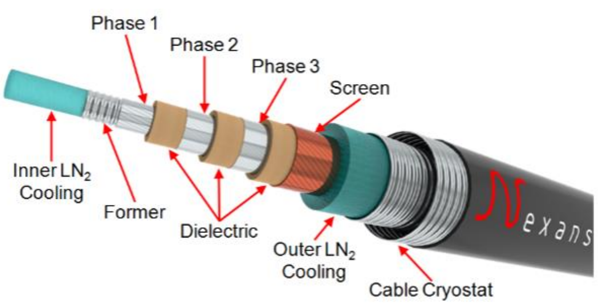
Pirelli

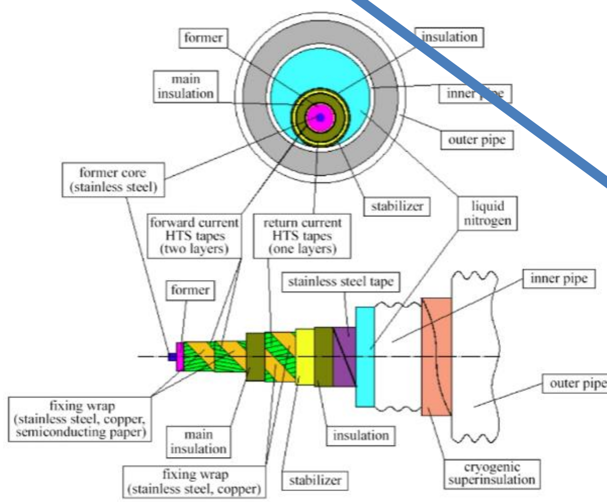


Sumitomo 66 kV 3-in-1

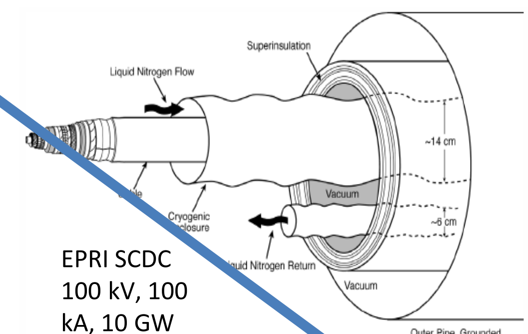


Furakawa, 275 kV, 3 kA





St. Petersburg, Russia



EPRI SCDC 100 kV, 100 kA, 10 GW

~ 2014

Required Reading!
(Thanks to Steve Eckroad, EPRI)

- Two EPRI Reports (available free from epri.com or w2agz.com)
  - (2012) Superconducting Power Equipment; Technology Watch 2012 (1024190)
  - (2013) SIU: Superconductivity for PDA (03002001)
- Bottom Lines:
  - Work continues on wire improvement and power application demonstration, although not at the pace of a decade ago.
  - HTSC materials performance and costs have matured.
  - What's needed is a strong business case for HTSC power applications.
  - So…does there exist a "compelling need," now or in the next decade, to effect a major and continuing deployment of HTSC in the electricity enterprise?

Pacific Intertie

- HVDC, +/- 500 kV, 3.1 kA, 3.1 GW
- 1,362 km
- ~50% of LA Power Consumption
- T&D Losses ~ 10%

Tear down the PI and replace with HTSC underground cables to capture this saving?

Ain't gonna happen, baby! Not a "compelling need!"

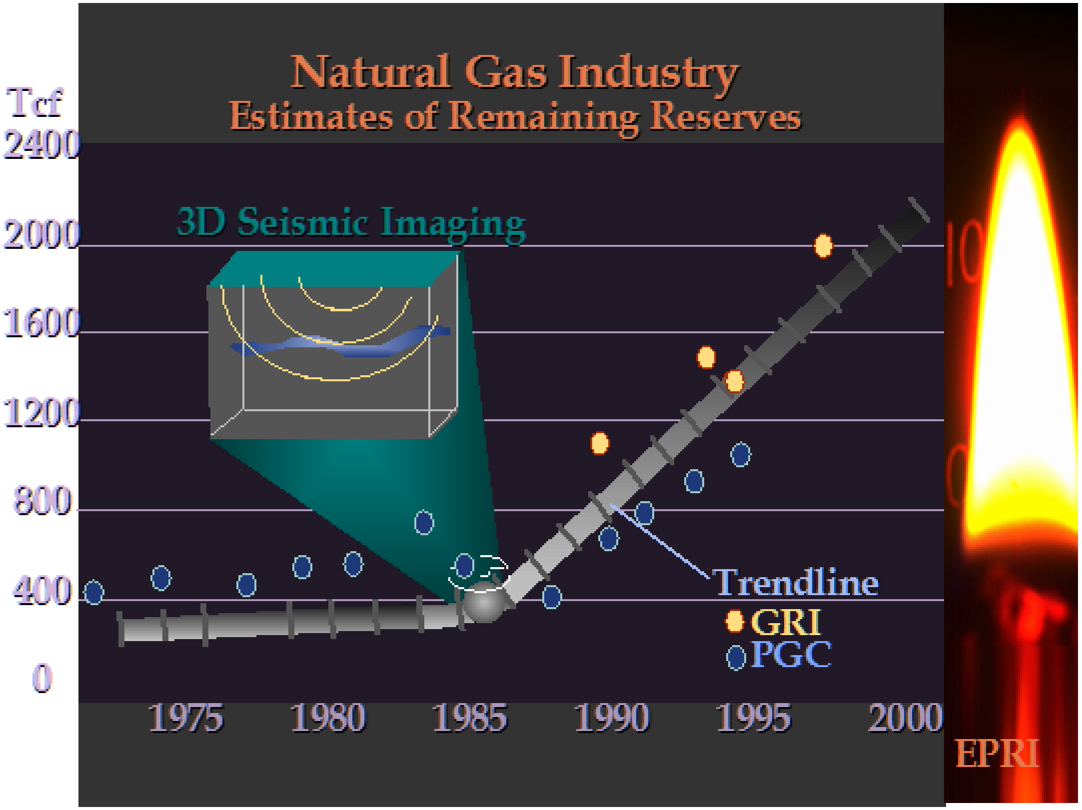
Even should the cost of the wire be zero!

However, do we have a "compelling new opportunity elswhere?"

P.M. Grant, EPRI, 1998

North American CH_4

There's Lots of It



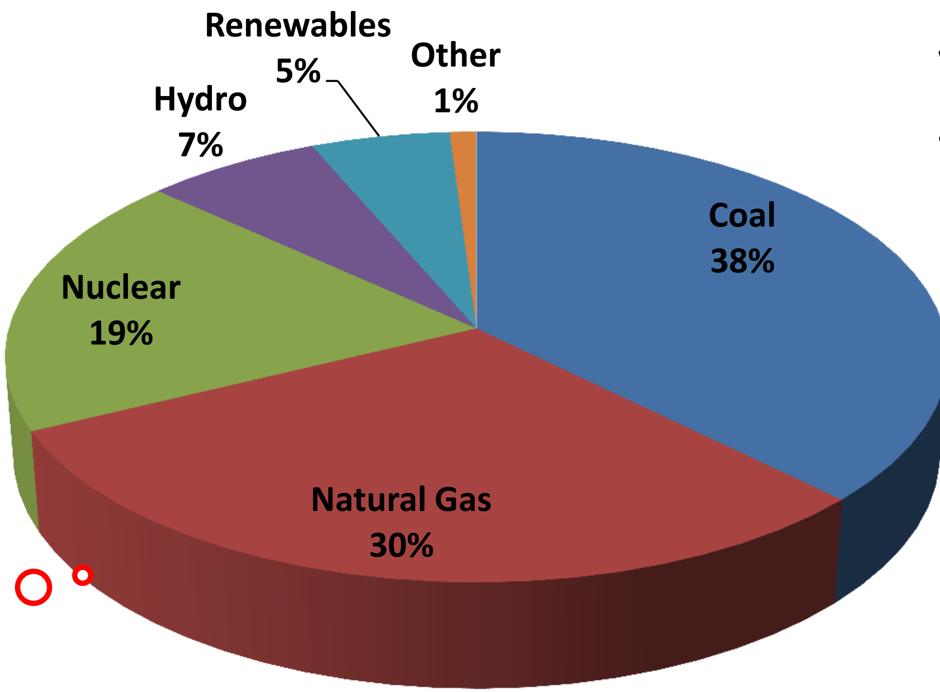
3D Seismic Imaging Plus Directional Drilling

50 Years at '97 Prices!

...& hydraulic fracturing, aka "fracking"

Why not make dual-use of emerging gas pipeline rights-of-way to transport electricity via HTSC cables?

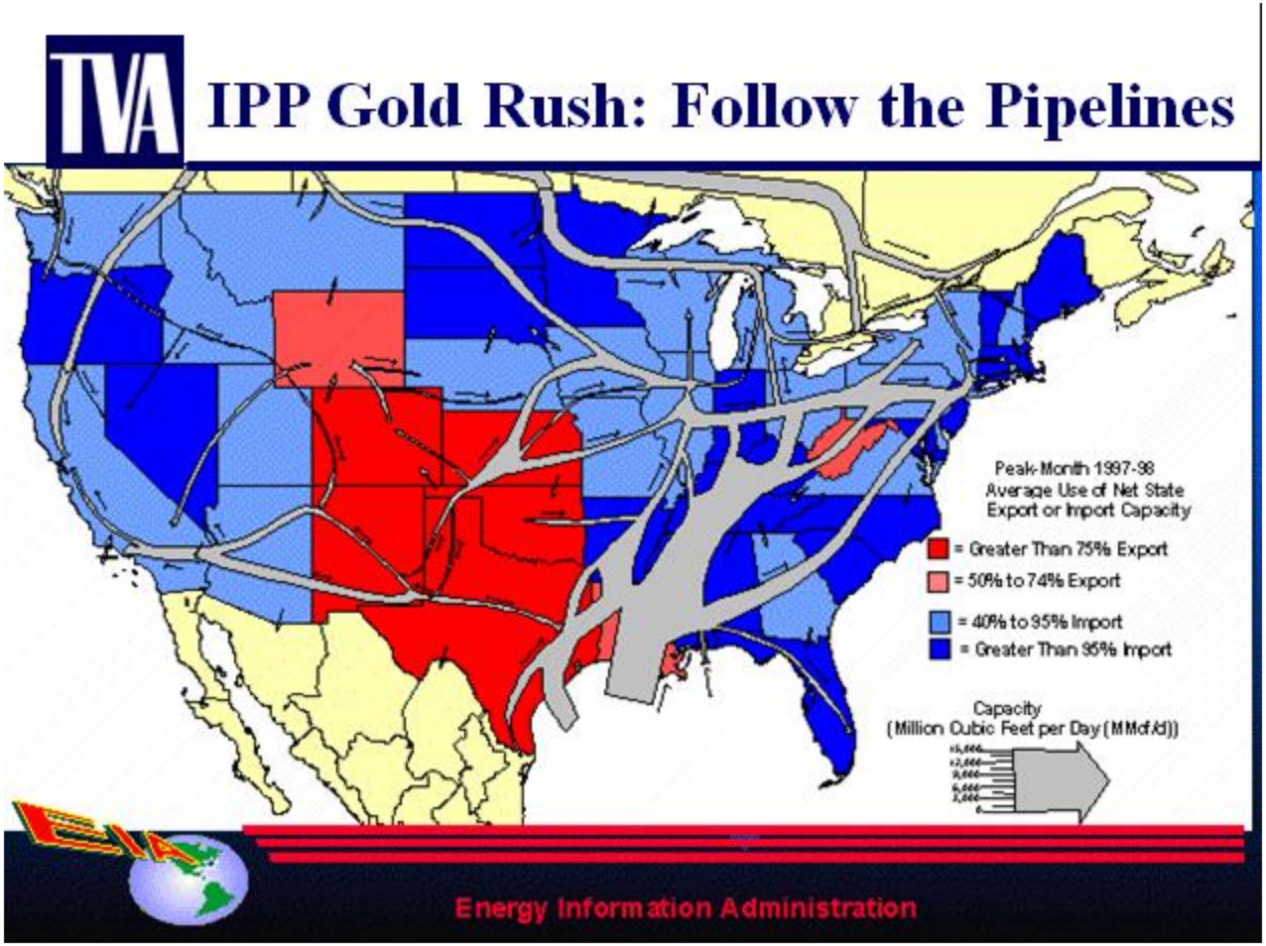
Natural Gas & Electricity!



"Fraternal Twins," Smart Grid News 16 April 2013

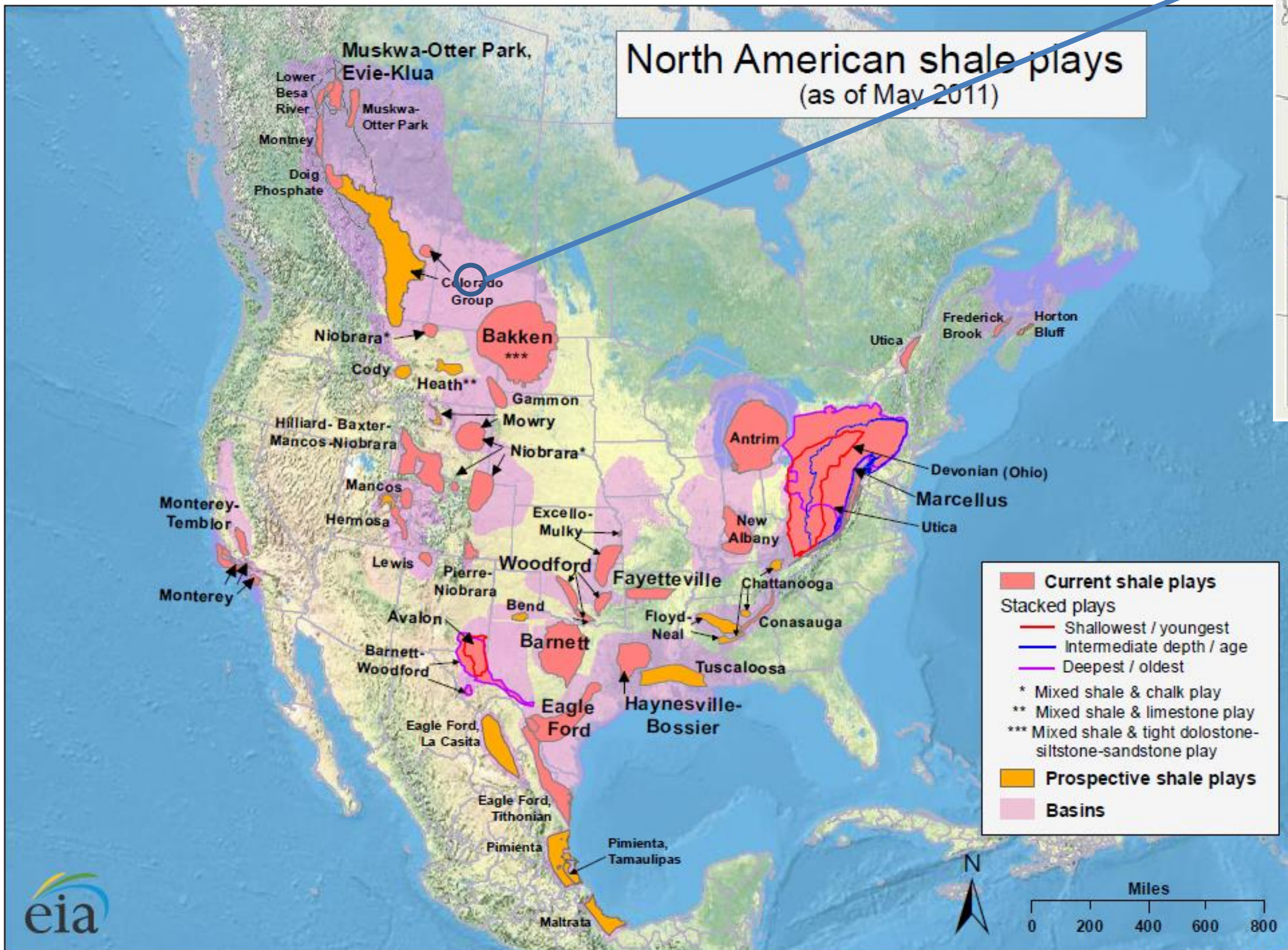
2012 USA Electricity Generation by Primary Fuel Source

Well...Let's Have a Look!



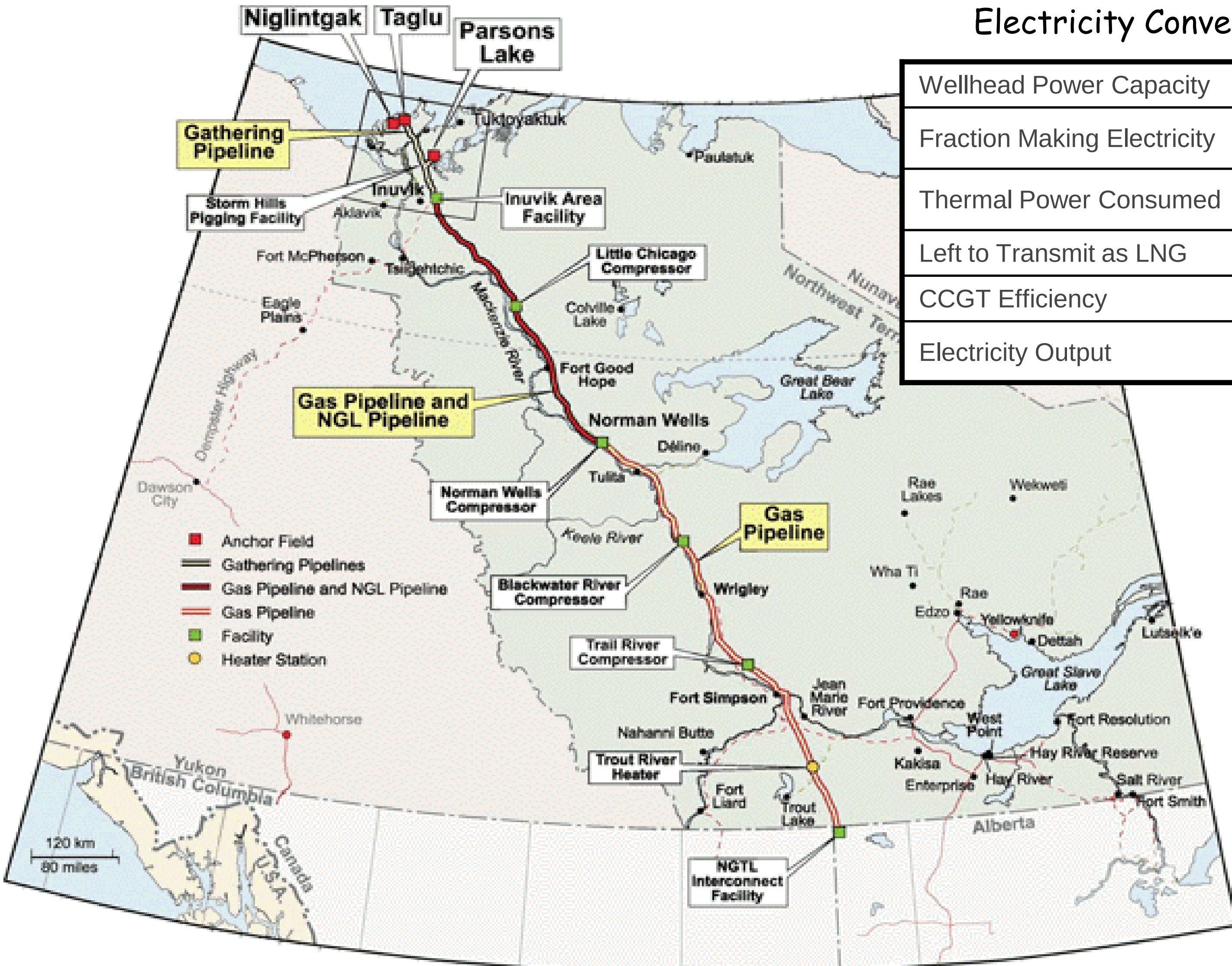
TVA Study...2001

Does "Keystone XL" Provide a "Compelling Opportunity" to "Raise Our Fraternal Twins?"



Let's encourage DOE to enlist EPRI, GTI, EIPC, INGAA,...in a collaboration to conduct an "engineering economy" study focused on the dual-use ROW concept.

...and in the long term...



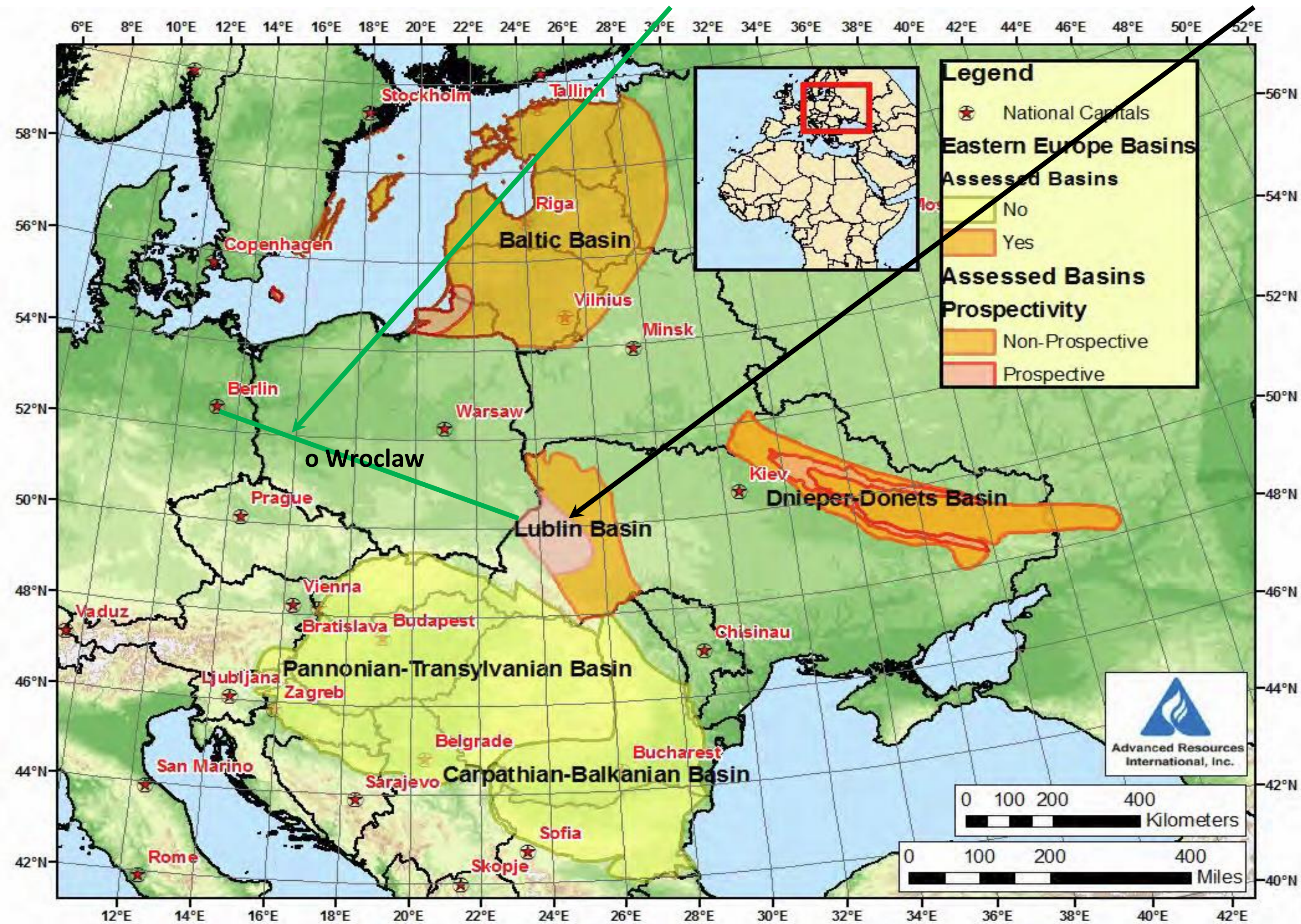
Electricity Conversion Assumptions

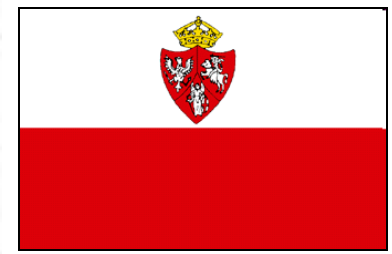
Wellhead Power Capacity	18 GW (HHV)
Fraction Making Electricity	33%
Thermal Power Consumed	6 GW (HHV)
Left to Transmit as LNG	12 GW (HHV)
CCGT Efficiency	60%
Electricity Output	3.6 GW (+/- 18 kV, 100 kA)

"Cryodelivery Systems for the Cotransmission of Chemical and Electric Power,"
P.M. Grant, AIP Conf. Proc. 823, 291 (2006).

Let's Not Forget Europe!

The Wola Obszańska (<u>Lublin</u>) 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 ($1\times10^9 m^3$). "Dual-Pipe" to Berlin?



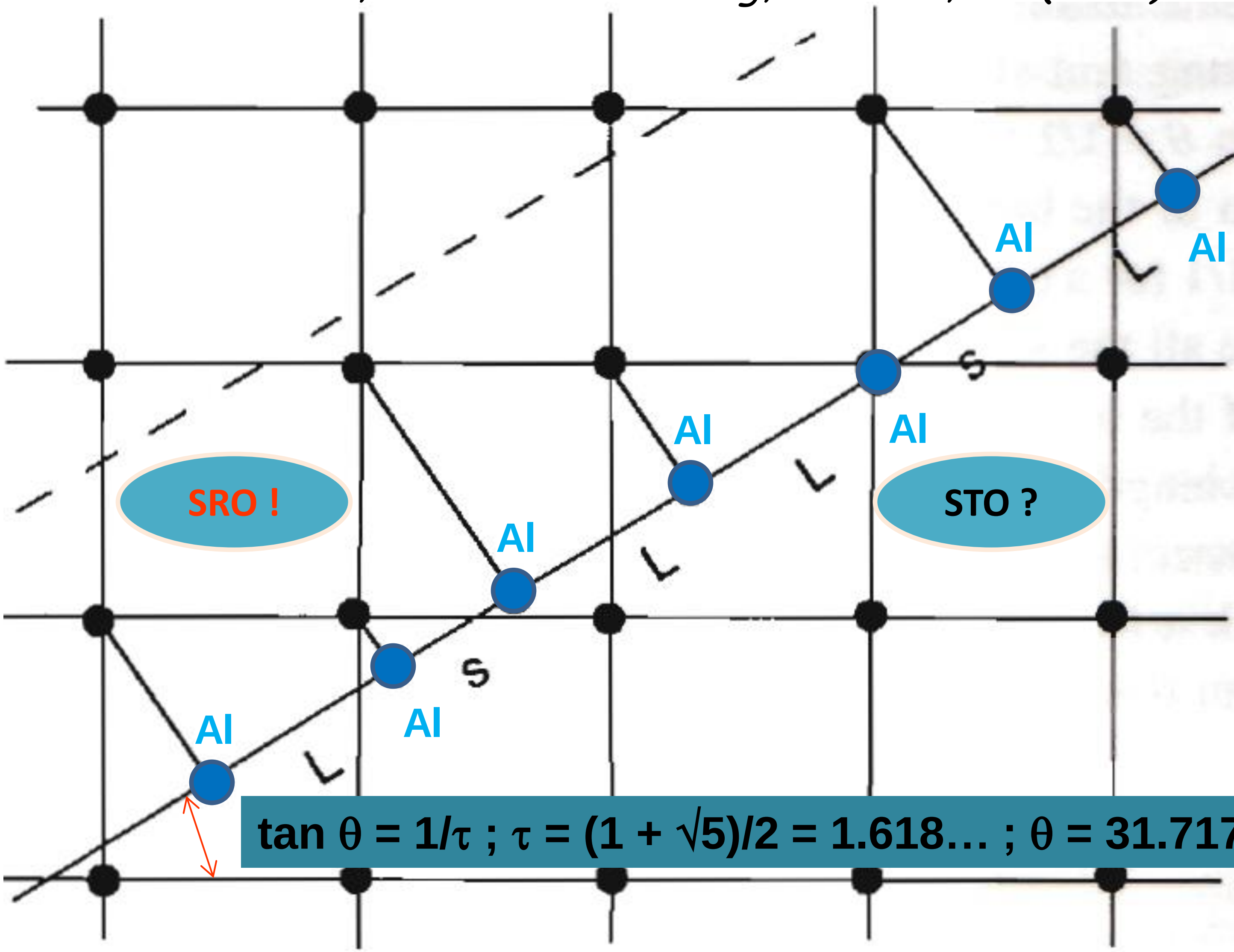


Back to the Future (of Nanoscale!)

- The Grand Challenge of Materials Science: Can we make a room temperature superconductor?
  - Bill Little says "yes" (1963)...simply surround a 1D metal chain with polarizable molecules and use "excitons" as the "pairing boson."
  - Problem: Periodic 1D metals are unstable and want to became insulators (dimerization).
- Solution:
  - Create a 1D Fibonacci (quasiperiodic) chain of "metal" atoms that resists CDW and dimerization "gapping" instabilies on a suitable "polarizable" substrate.
  - How? "Decorate" a dislocation line on the [100] surface of STO, SRO, Si...

A Fibonacci "Dislocation Line"

From P.M. Grant, APS March Meeting, Portland, OR (2010)



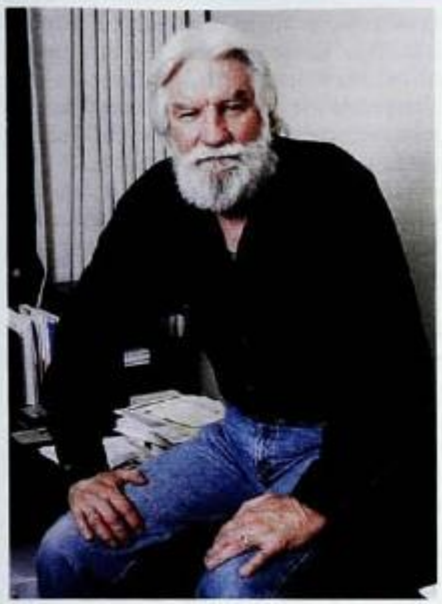
tan θ = 1/τ ; τ = (1 + √5)/2 = 1.618… ; θ = 31.717…°

L = 4.058 Å (fcc edge)

s = 2.869 Å (fcc diag)

Does the DA VINCI CODE Hold the Key to Room Temperature Superconductivity?

PHYSICS TOMORROW: ESSAY CONTEST WINNER



RESEARCHERS FIND EXTRAORDINARILY HIGH TEMPERATURE SUPERCONDUCTIVITY IN BIO-INSPIRED NANOPOLYMER

Paul M. Grant
May 2028

50th Anniversary of Physics Today, May 1998

Lessons from “Four Aging British Philosophers”

...for engineers and physicists under 50...

“You can’t always get what you want…”

"…you get what you need!"