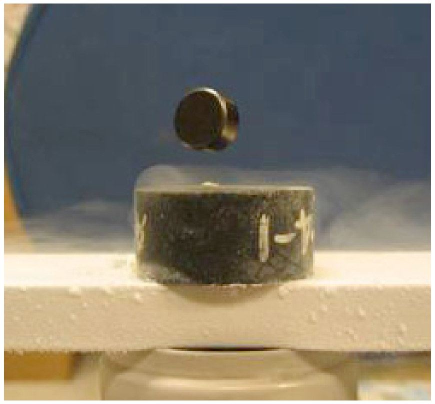
Understanding Mechanisms of Superconductivity and Design of Advanced Superconductors

Warren E. Pickett (UCDavis)

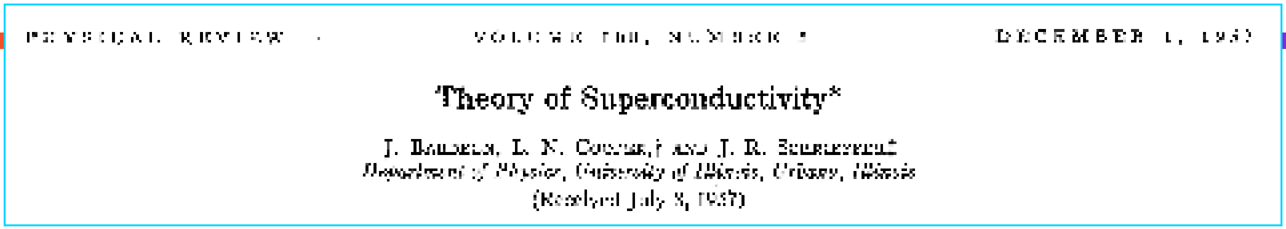
Based in part on 2006
DOE/BES Report



Outline:
- history, mechanisms of HTS
- perspective: requirements of a theory of HTS
- outstanding challenges in mechanisms (non-HTS) stimulated by new materials discoveries
- design of new, advanced superconductors

In the beginning….. Phys. Rev. 108, 1175-1204 (1957)

BCS Theory


PHYSICAL REVIEW VOLUME 108, NUMBER 5 DECEMBER 1, 1957

Theory of Superconductivity*

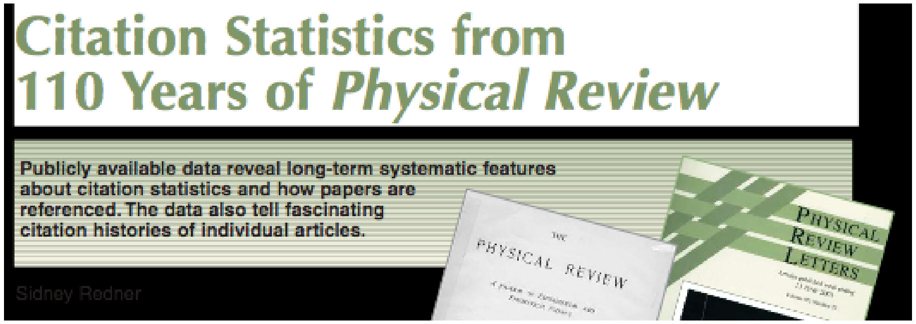
J. Bardeen, L. N. Cooper,† and J. R. Schrieffer‡
Department of Physics, University of Illinois, Urbana, Illinois
(Received July 8, 1957)

John Bardeen
Leon Cooper
J. Robert Schrieffer

50th anniversary of the BCS paper

1360 citations as of 2003
5th most of any in PR/PRX/PRL/RMP

S. Redner,
Physics Today,
2005


Citation Statistics from
110 Years of *Physical Review*

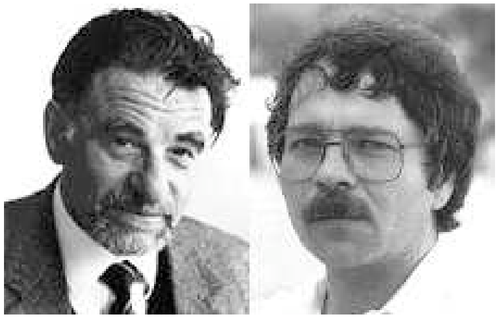
Publicly available data reveal long-term systematic features about citation statistics and how papers are referenced. The data also tell fascinating citation histories of individual articles.

Sidney Redner

the superconductor tsumani (late 1986)

30 K onset

Z. Phys. B - Condensed Matter 64, 189-193 (1986)



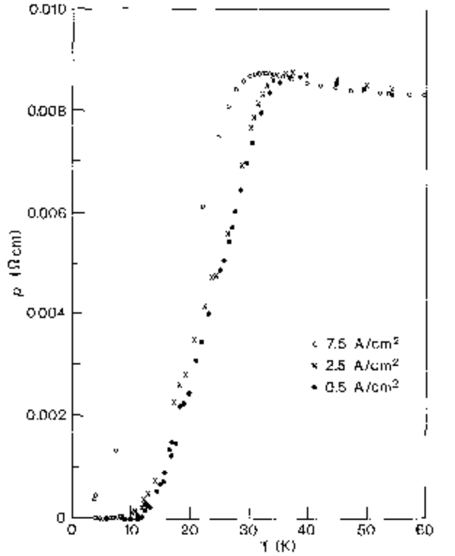


Fig. 3. Low-temperature resistivity of a sample with x(Ba) = 0.75, recorded for different current densities

Possible High T_c Superconductivity in the Ba – La – Cu – O System

J.G. Bednorz and K.A. Müller
IBM Zürich Research Laboratory, Rüschlikon, Switzerland

Received April 17, 1986

20th Anniversary

Nobel Prize in Physics, 1987

HTS Superconductivity

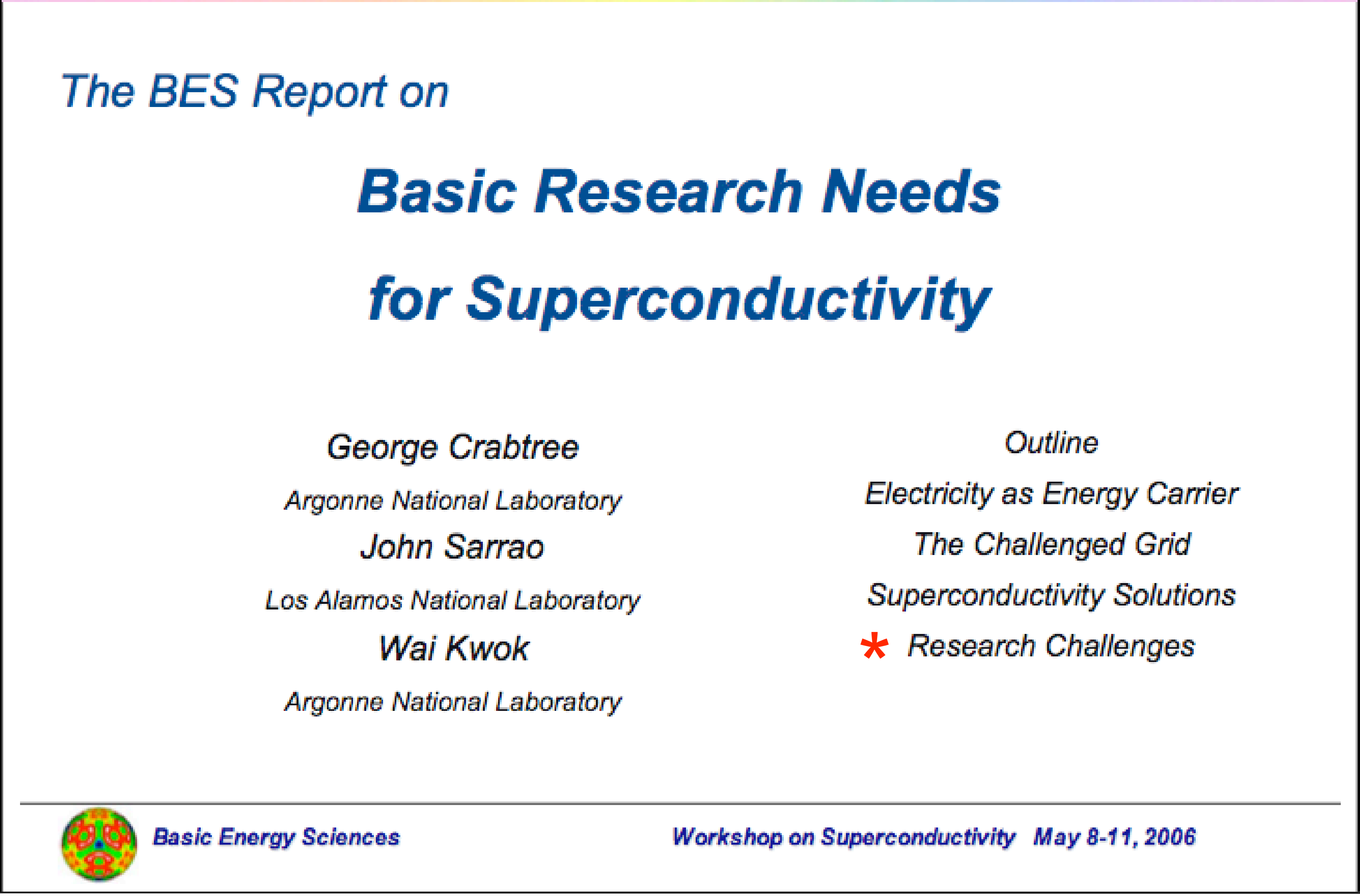
Session B1 (yesterday): 20th anniversary of
High T_c Superconductivity 'Woodstock Session'

6th anniversary of MgB2 mini-Woodstock

54 sessions at this meeting with
"supercond" in the title

This continues a 20 year tradition of
numerous superconductivity sessions at the
APS March Meeting.

DOE Workshop, May 2006



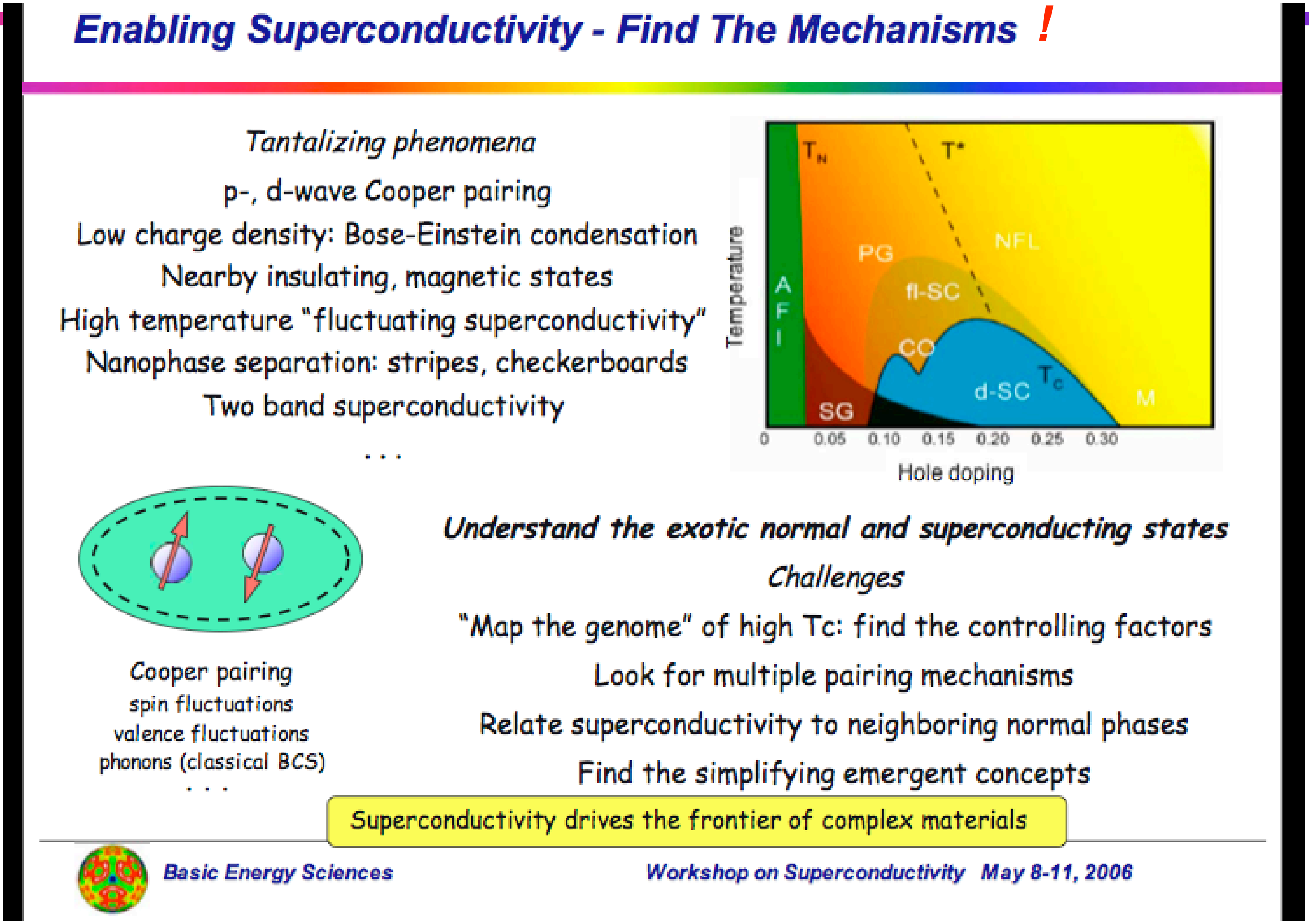
The BES Report on

Basic Research Needs for Superconductivity

George Crabtree
Argonne National Laboratory
John Sarrao
Los Alamos National Laboratory
Wai Kwok
Argonne National Laboratory

Outline
- Electricity as Energy Carrier
- The Challenged Grid
- Superconductivity Solutions
- * Research Challenges

Basic Energy Sciences Workshop on Superconductivity May 8-11, 2006



Enabling Superconductivity - Find The Mechanisms !

Tantalizing phenomena

p-, d-wave Cooper pairing

Low charge density: Bose-Einstein condensation

Nearby insulating, magnetic states

High temperature "fluctuating superconductivity"

Nanophase separation: stripes, checkerboards

Two band superconductivity

. . .

Cooper pairing

spin fluctuations

valence fluctuations

phonons (classical BCS)

. . .

Understand the exotic normal and superconducting states

Challenges

"Map the genome" of high Tc: find the controlling factors

Look for multiple pairing mechanisms

Relate superconductivity to neighboring normal phases

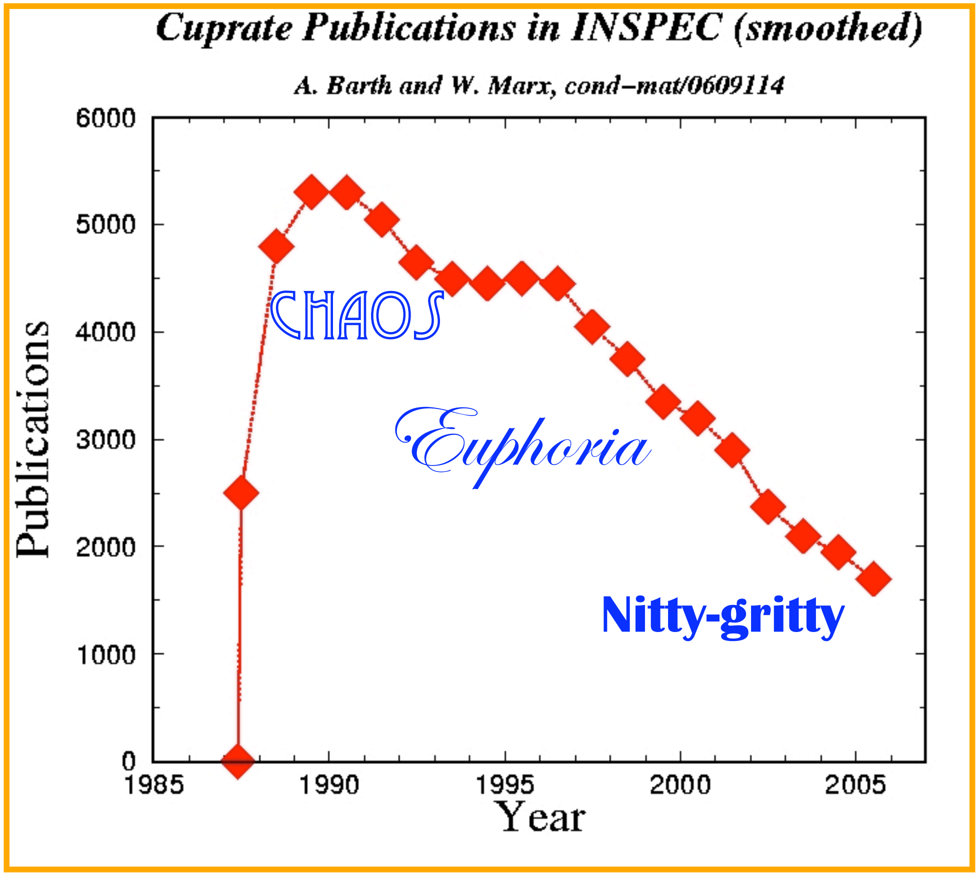
Find the simplifying emergent concepts

Superconductivity drives the frontier of complex materials

Basic Energy Sciences

Workshop on Superconductivity May 8-11, 2006

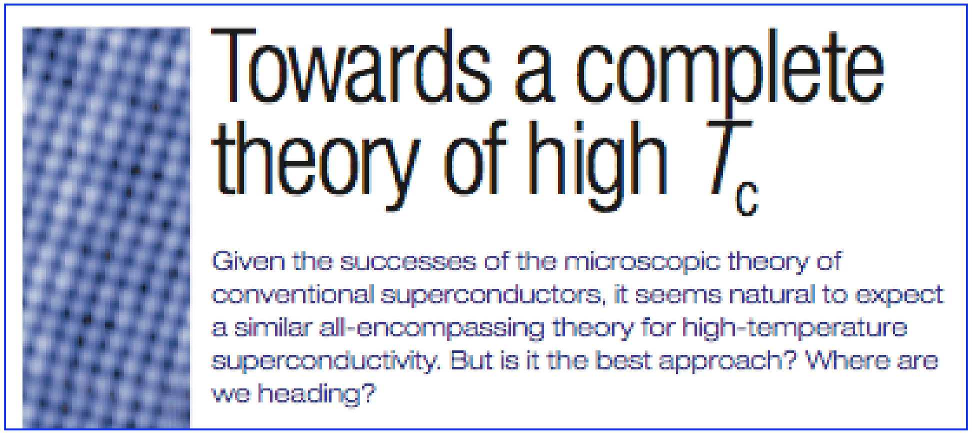
Publication activity in HTS remains prodigious



It is essential to sustain the progress in HTS and the associated fundamental understanding and materials expertise that that is accumulating

20th Anniversary of High T_c

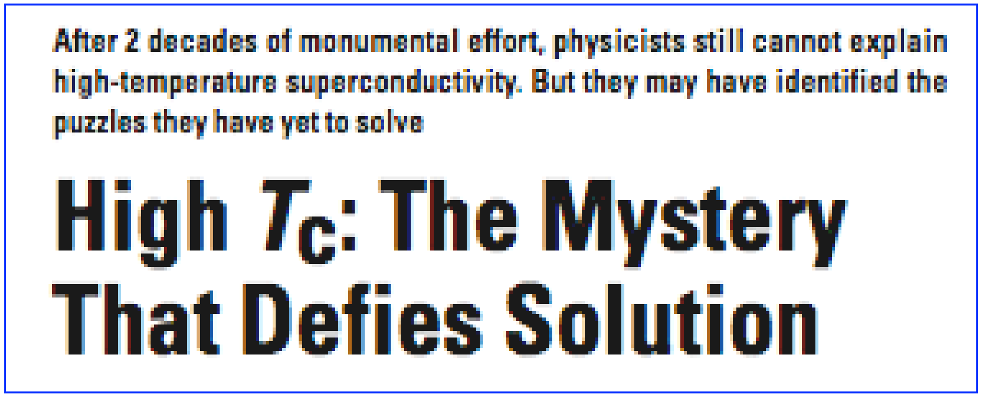
Nature
March 2006



Towards a complete theory of high T_c

Given the successes of the microscopic theory of conventional superconductors, it seems natural to expect a similar all-encompassing theory for high-temperature superconductivity. But is it the best approach? Where are we heading?

Science
Nov 2006



After 2 decades of monumental effort, physicists still cannot explain high-temperature superconductivity. But they may have identified the puzzles they have yet to solve

High T_C: The Mystery That Defies Solution

Synopsis: elaboration and acceptance of the **mechanism** of HTS mechanism is not imminent

Proposed Mechanisms of HTS Superconductivity

[from D. J. Scalapino, gleaned from presentations at M2S-HTS, Dresden, July 2006]

- Jahn-Teller bipolarons
- stripes (role of inhomogeneities)
- RVB-Gutzwiller projected BCS
- electron-phonon + U
- spin fluctuations
- charge fluctuations
- electric quadrupole fluctuations
- loop current fluctuations
- d-DW, d-CDW
- quantum critical point fluctuations
- competing phases
- Pomeranchuk instabilities
- d-to-d electronic excitations

DJS: there is plenty of data available to decide between mechansims

Possibility: there is *too much* data to decide between mechanisms

Is “mechanism” the question…?

What is needed to constitute ……..

A Faithful and Convincing Mechanism of HTS

Faithful theory

- *(semi)quantitative explanation of the observations that are central to optimally doped HTS (focus!)*
- *no spurious predictions*

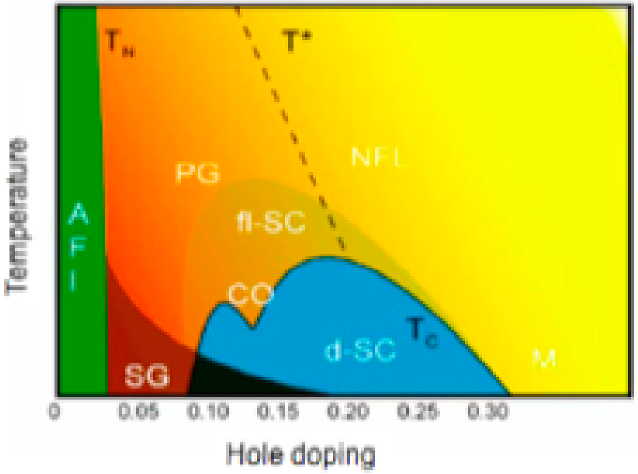
Convincing theory

- *majority of workers in the field accept the theory*
- *there are no seriously competing theories*
- *no `reasonably objective' person can disbelieve its general applicability*

I.e. "BCS-like in its convincibility." Is this a plausible goal?

What is needed to constitute ……..

A Faithful and Convincing Theory of HTS

*

***In principle**, to discover the mechanism*
- ** focus on optimally doped region*
- ** analogy: mag. impurities in BCS sc'or*

***In practice**: entire phase diagram needs to be understood*
- ** majority of workers seem to accept this*
- ** this is a much broader goal than `the mechanism', it is `the theory'*

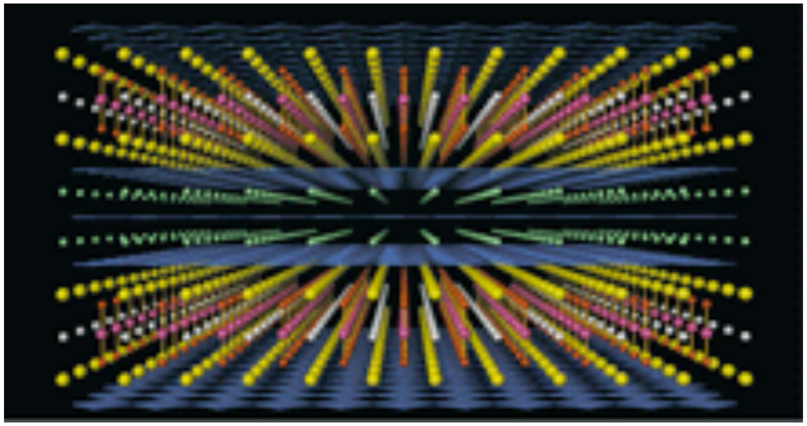
Complication: there are other similar phase diagrams in low-Tc systems

What are the broadest issues for ……

A Faithful and Convincing Theory of HTS

First address the broadest issues

Hg2223



- *SAMENESS: why layered cuprates and only cuprates?*
  - ** all HTS have CuO_2 planes; no others are HTS*
  - ** there are other quasi-2D doped insulating antiferromagnets;*
    why only cuprates?
- *VARIATION: why so much; what is the essence; what does it tell us?*

What may be needed to comprise ……

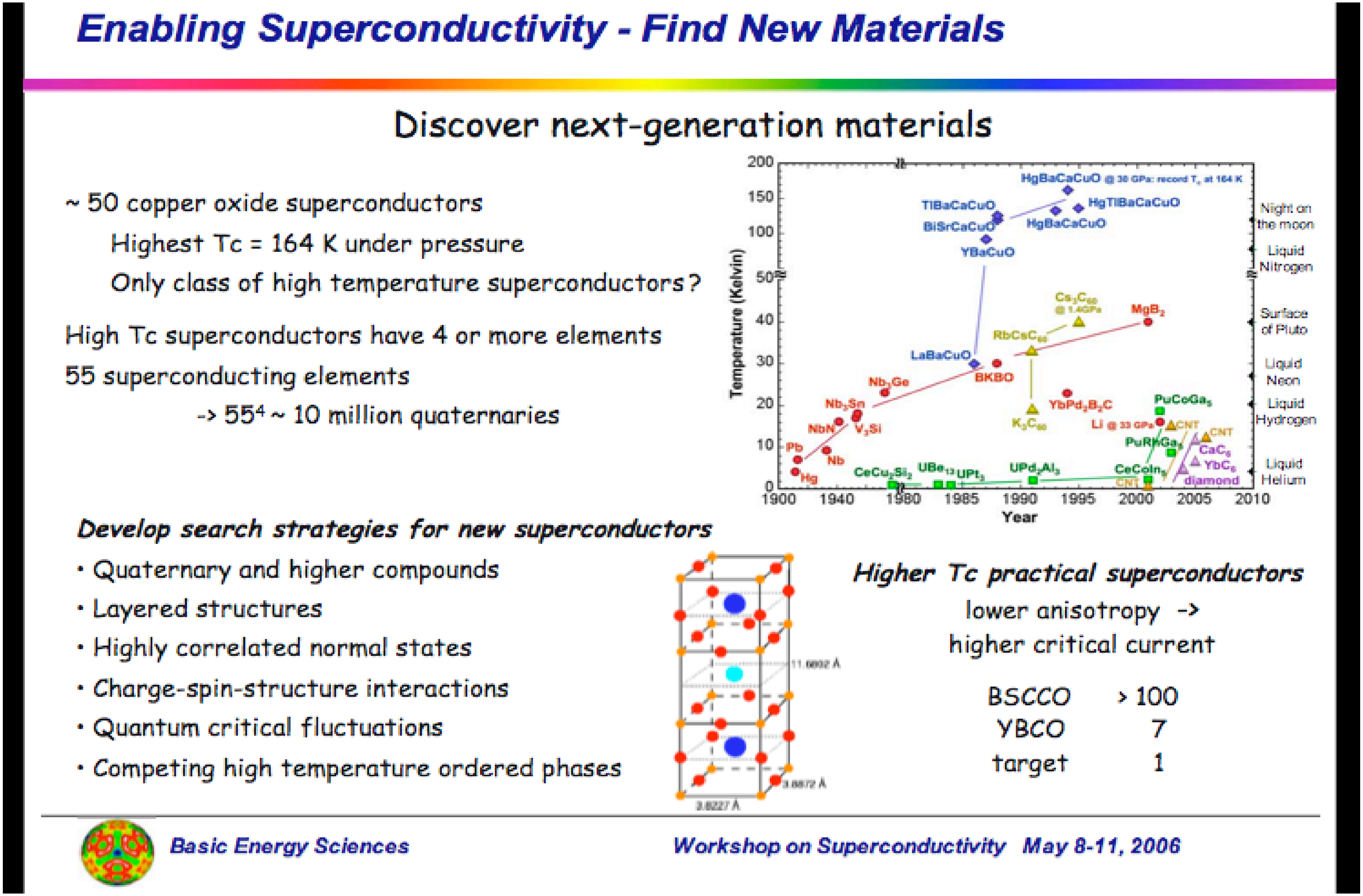
A Faithful and Convincing Theory of HTS

Several proposed mechanisms unify certain aspects of HTS

Big issue: what distinctions need to be explained? Some propositions:

- *Shape of Fermi surface (system dependent); effect on mechanism*
- *Value of T_c (within factor of two, with correct trends)*
- *Symmetry of superconducting order parameter*
- *Low E excitations: 1-particle; magnetic; phononic; other collective*
- *Inhomogeneities: patterns, connections to other phenomena*
- *Trend of T_c in cuprate classes: [Bi] < [Tl] < [Hg]*
- *Trend of T_c with number of CuO_2 layers (maximum at 3 layers)*
- *Pressure dependence of T_c: theory must work at any volume*
- *(many, many more related to the entire HTS phase diagram)*

Theory of the entire phase diagram is a huge issue (an attractive one)



Enabling Superconductivity - Find New Materials

Discover next-generation materials

~ 50 copper oxide superconductors

Highest Tc = 164 K under pressure

Only class of high temperature superconductors?

High Tc superconductors have 4 or more elements

55 superconducting elements

-> 55^4 ~ 10 million quaternaries

Develop search strategies for new superconductors

- Quaternary and higher compounds
- Layered structures
- Highly correlated normal states
- Charge-spin-structure interactions
- Quantum critical fluctuations
- Competing high temperature ordered phases

Higher Tc practical superconductors

lower anisotropy ->
higher critical current

BSCCO	> 100
YBCO	7
target	1

Basic Energy Sciences

Workshop on Superconductivity May 8-11, 2006

Additional Developments in hTS Materials

[hTS == unexpectedly high T_c]

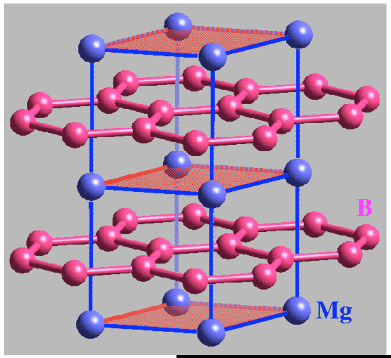
- 40: MgB_2
- 40: Alkali-doped fullerenes
- 35: $(Ba,K)BiO_3$ [BKBO] (discovered in 1986)
- 25: Alkali-doped HfNCl, ZrNCl
- 25: Elemental metals under pressure
- 19: $PuCoGa_5$ a novel heavy fermion sc'or
- 18: Y_2C_3 -- who ordered this one?

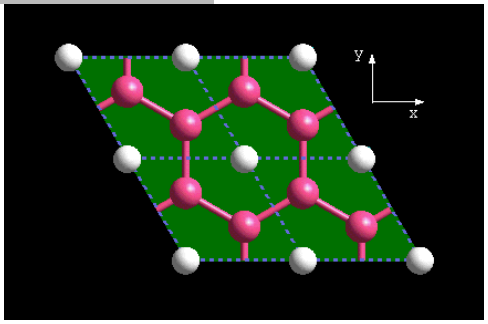
- 2D triangular lattice oxides & chalcogenides

MgB$_2$ is the champ (Akimitsu group, 2001)

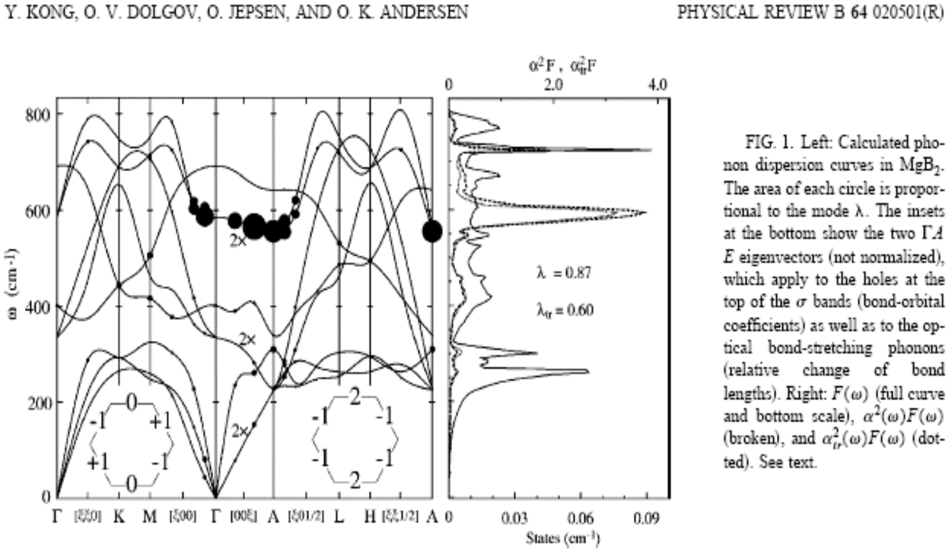
1. MgB$_2$: covalent bonds become metallic
2. Deformation potential D=13 eV/A
   (amazingly large, especially for a metal)
3. 2D (cylinder) Fermi surfaces focus strength
4. Yet structure remains stable: intrinsic covalency

J. M. An and WEP, Phys. Rev. Lett. (2001)
J. Kortus et al., Phys. Rev. Lett. (2001)
Y. Kong et al., Phys. Rev. B (2001)
K.-P. Bohnen et al., Phys. Rev. Lett. (2001)
……..more…….





T. Yildirim (NIST)



Y. KONG, O. V. DOLGOV, O. JEPSEN, AND O. K. ANDERSEN PHYSICAL REVIEW B 64 020501(R)

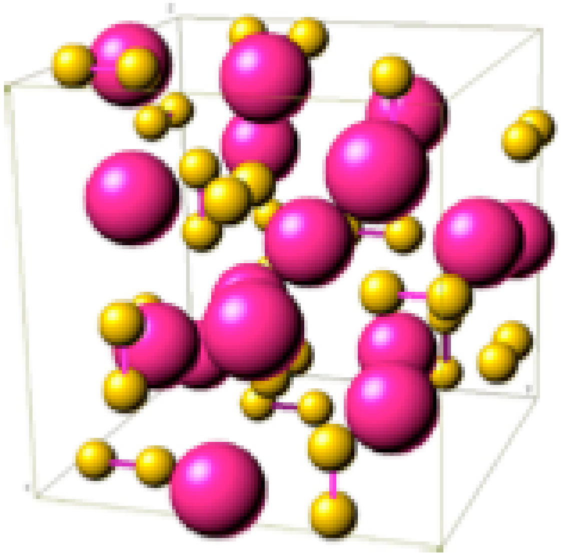
FIG. 1. Left: Calculated phonon dispersion curves in MgB$_2$. The area of each circle is proportional to the mode λ. The insets at the bottom show the two ΓA E eigenvectors (not normalized), which apply to the holes at the top of the σ bands (bond-orbital coefficients) as well as to the optical bond-stretching phonons (relative change of bond lengths). Right: $F(\omega)$ (full curve and bottom scale), $\alpha^2(\omega)F(\omega)$ (broken), and $\alpha^2_{tr}(\omega)F(\omega)$ (dotted). See text.

Yttrium Sesquicarbide Y_2C_3

Coupling to high frequencies?

Simple cubic Bravais lattice
of Y_8C_{12} primitive cells

Distinctive feature:
triply-bonded C_2 dimers



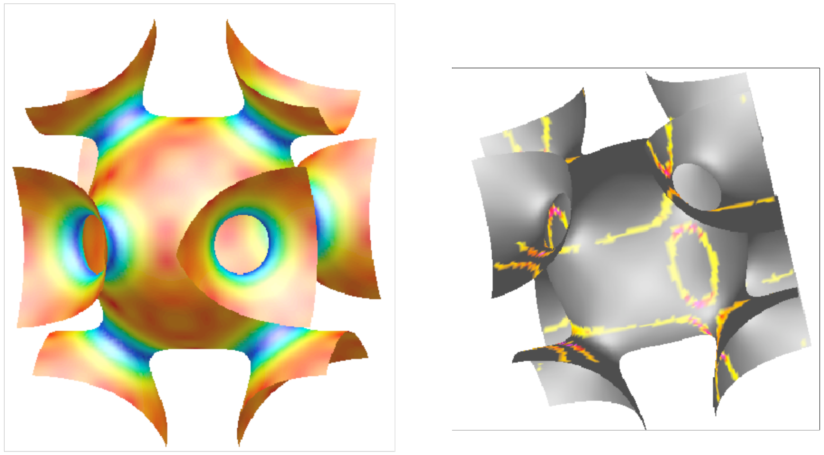
Singh & Mazin, 2004
C_2 dimer state near E_F
A_g modes: 120 K, 1000 K

T_c = 18 K (Akimitsu group)

[$T_c(La_2C_3)$ = 11 K]

Coupling to hard C_2 mode
may be important for the `high' T_c

Pressure as a Tool to Produce Superconductors: Elemental Metals under Pressure: T_c=20-25K

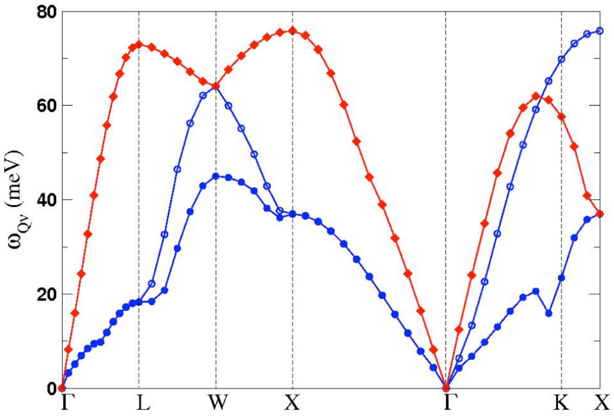


Li: T_c up to 20 K

Y: T_c up to 20 K

Ca: T_c up to 25 K

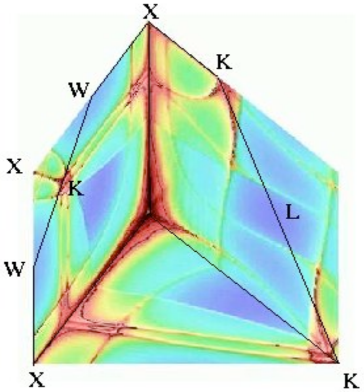
!



fcc Li: strong coupling,
phonon anomalies,
instabilities under pressure

Nesting function
in three planes

Lithium



$$\xi_{\vec{Q}} = \sum_{k} \delta(\varepsilon_k)\delta(\varepsilon_{k+Q}) = V_c \int_{\mathcal{L}} \frac{d\mathcal{L}(k,Q)}{|\vec{v}_k \times \vec{v}_{k+Q}|}$$

Eliashberg theory: UCDavis
DFT for superconductors: Berlin, Gross et al.

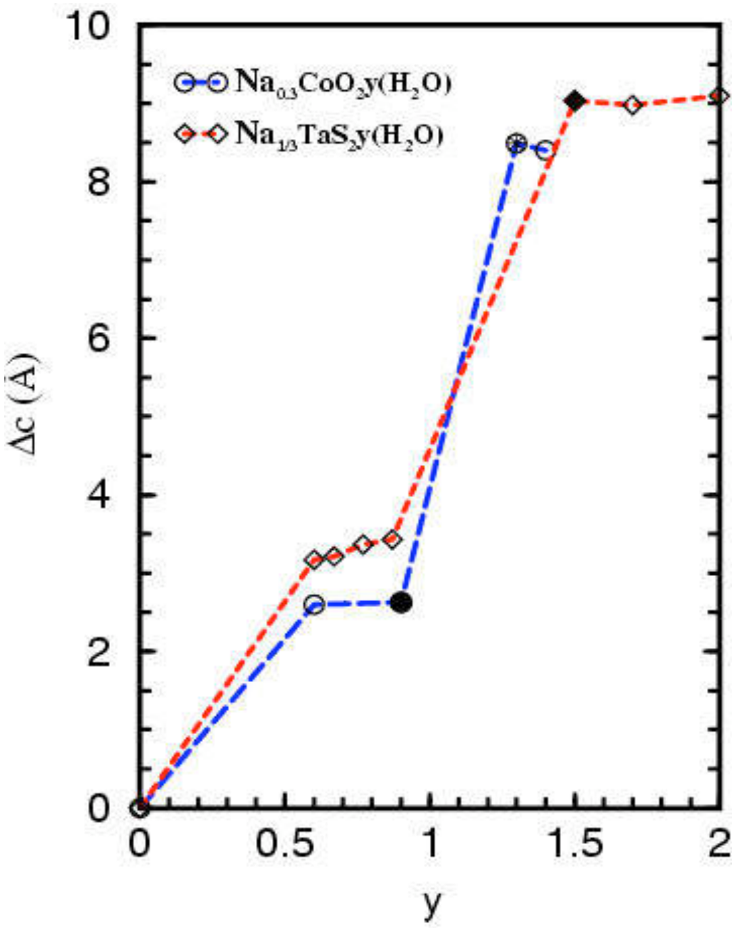
Observations about Carrier-doped Layered Transition Metal 'Oxides'

- Electron-doped TaS_2
- Hole-doped $LiNbO_2$
- Hole-doped $NaCoO_2$ (hydrated)
- Electron-doped $TiSe_2$

Observation about Carrier-doped Layered Transition Metal Nitride

- Electron-doped ZrNCl, HfNCl

Co-Intercalated Layered Dichalcogenides
(D. C. Johnston et al., 1983-4)



Several distinct phases
y=0, 2/3, 0.8, 3/2, 2

$$Na_{1/3}TaS_2 \cdot yH_2O$$

All have $T_c = 4\text{-}5$ K

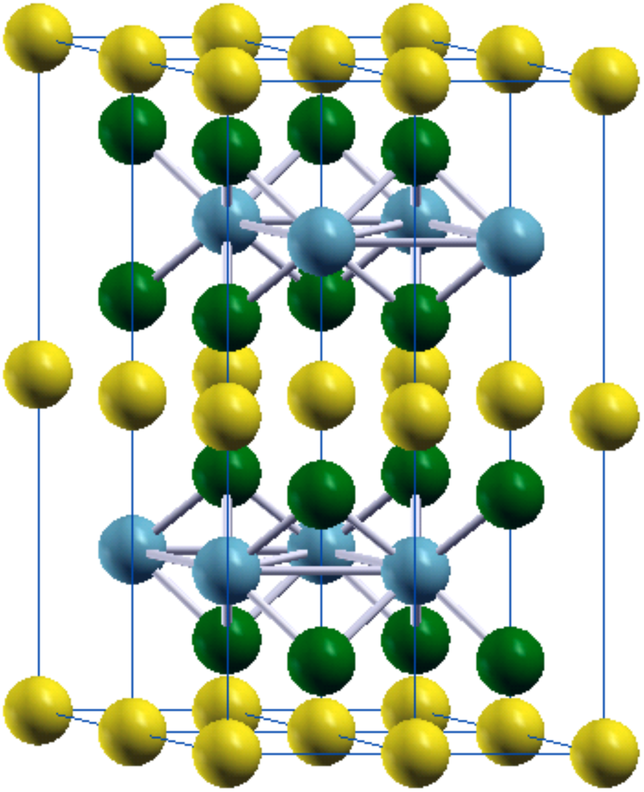
$$\begin{bmatrix} Y^{3+}_{1/9}TaS_2 \\ La^{3+}_{1/9}TaS_2 \\ Mn^{2+}_{1/6}TaS_2 \end{bmatrix} \Rightarrow \quad Ta^{+3\frac{2}{3}}$$

$Li_{1-x}NbO_2$: 5 years after HTS (Stacy group, 1991)

$T_c = 5.5$ K

- Layered TM oxide
- Trigonal-prismatic coordination
- Triangular lattice
- Nb d^{1+x} configuration
- Single $d(z^2)$ band is occupied
- Hole-doped from semiconductor

- Single-band triangular lattice system
- Superconducting in a wide range around x ~ 0.5



$Na_{1-x}CoO_2$, the Dehydrated Superconductor [add water!]

$T_c = 4.5$ K

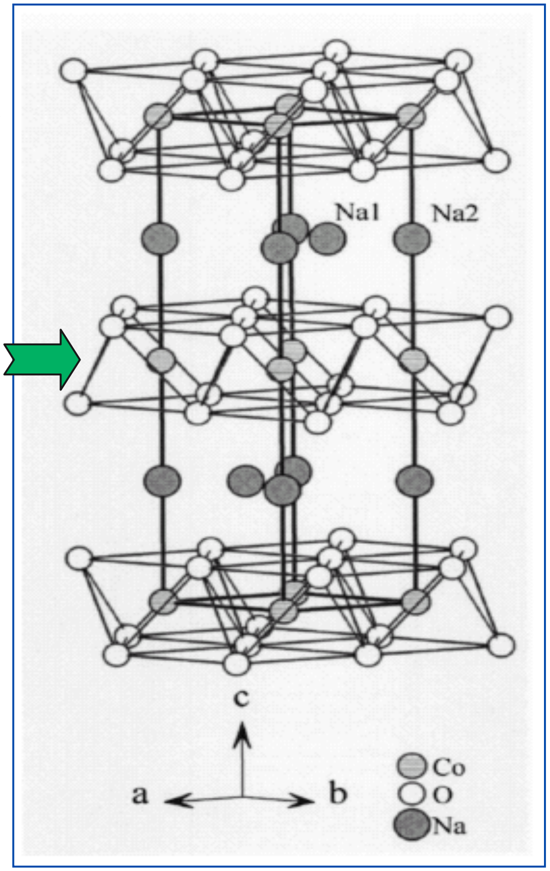
Triangular lattice

Hole-doped from
Co^{3+} semiconductor

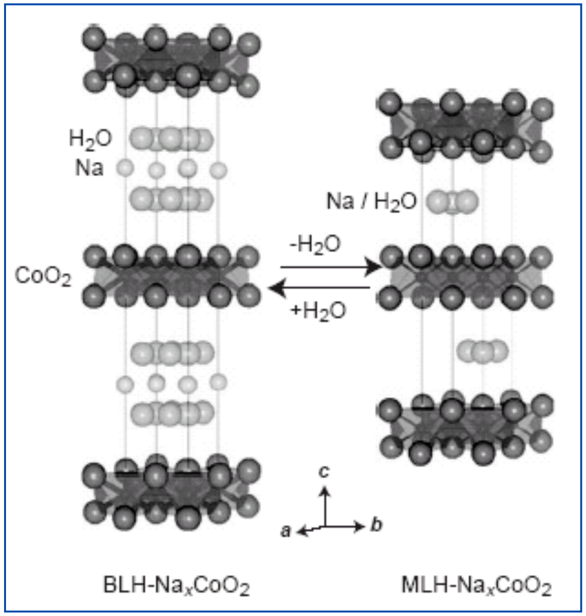
Octahedral CoO_6

Edge-sharing CoO_6 octahedra

Superconducting around x ~ 0.3



Jorgensen et al. (2003)



$$Na_{1-x}CoO_2 * yH_2O$$

Takada et al., Nature 422, 53 (2003);

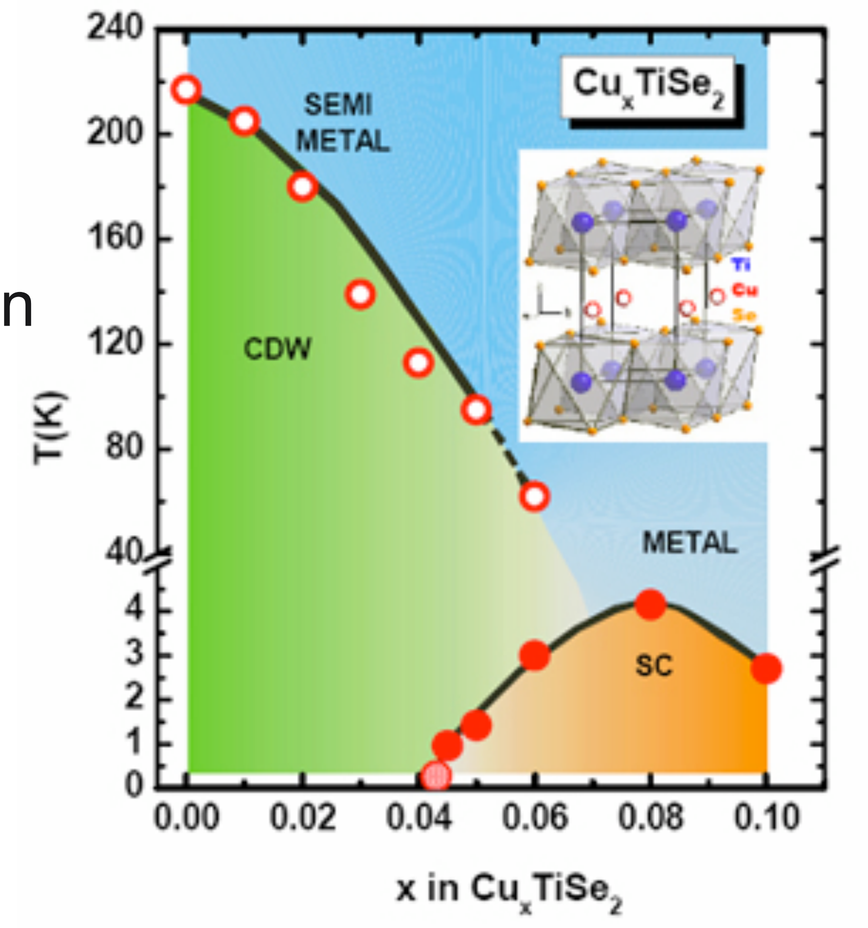
Adv. Mater. 16, 1901 (2004)

Cu_xTiSe_2: CDW--> Superconductivity

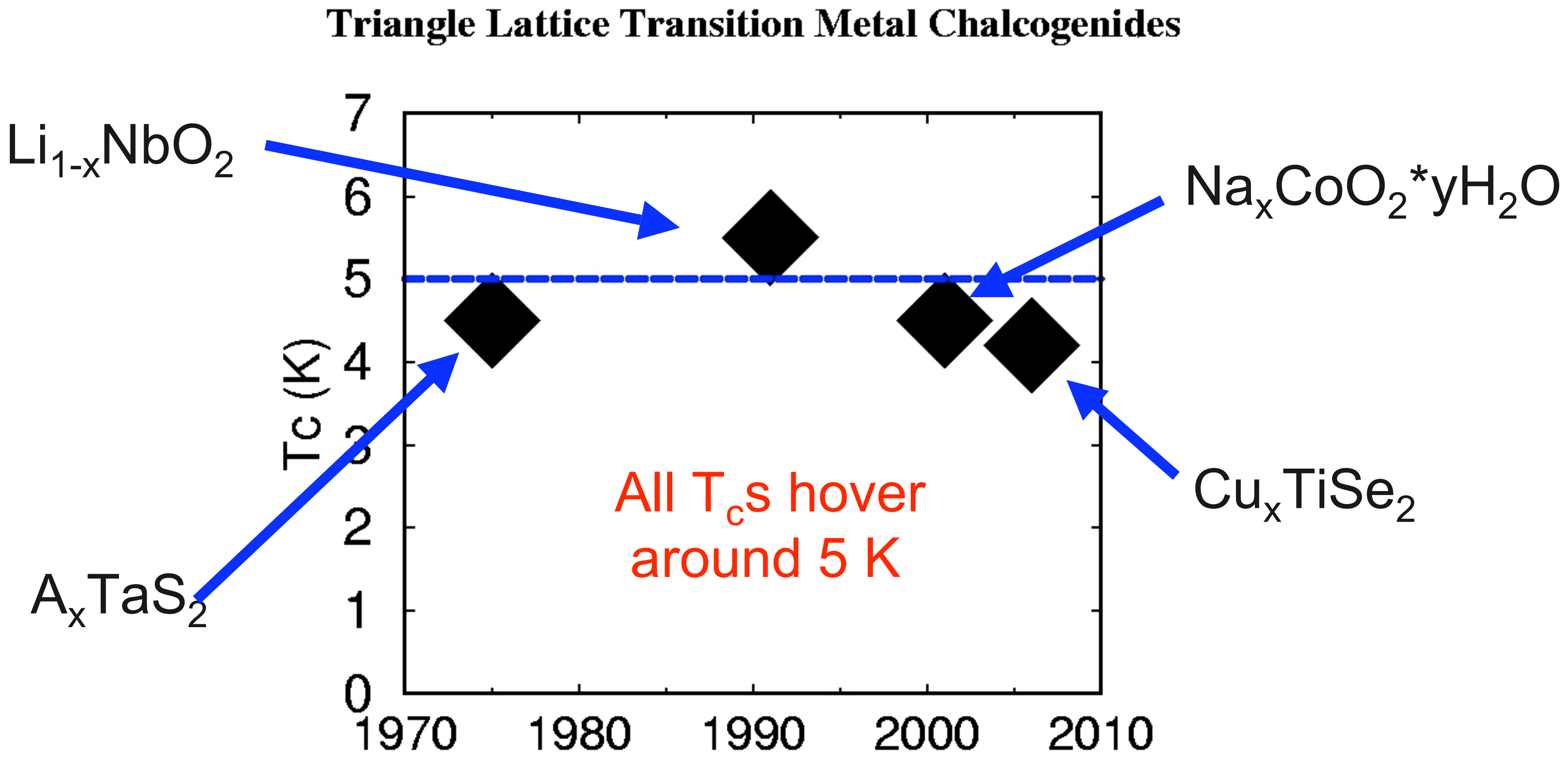
Morosan et al. (2005)

- Layered 2D TM chalcogenide
- Triangular lattice system
- Trigonal-prismatic coordination
- CDW has long been studied
- Nominal d^0 Ti configuration
- Electron-doped --> sc'y

Maximum T_c=4.2K at x=0.08



Synopsis: T_c in 2D Triangular Oxides/Chalcogenides



Triangle Lattice Transition Metal Chalcogenides

$Li_{1-x}NbO_2$

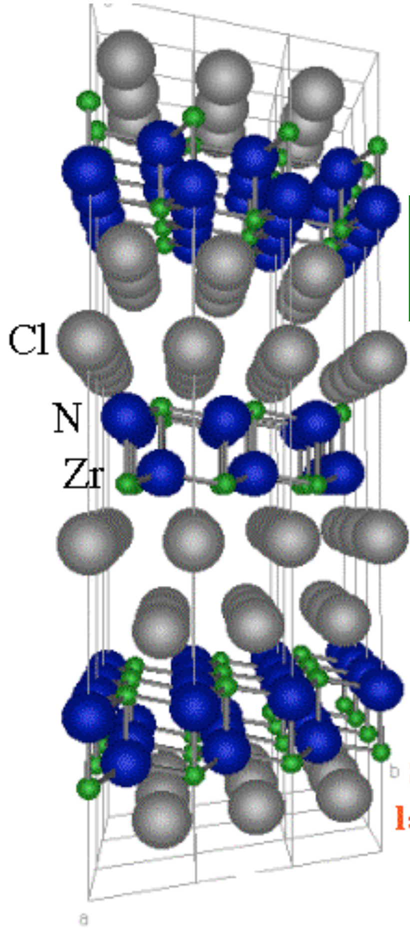
$Na_xCoO_2{*}yH_2O$

A_xTaS_2

Cu_xTiSe_2

All T_cs hover around 5 K

Alkali-doped A_xZrNCl (15 K) & A_xHfNCl (25 K)

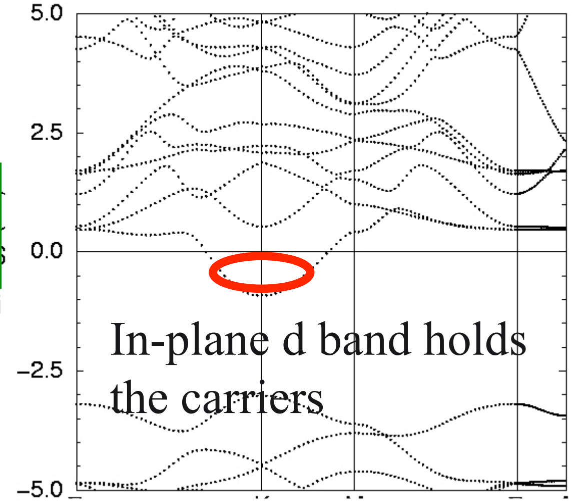


SmSI type layer structure

Structure is somewhat MgB2-like; so is it electron-phonon?

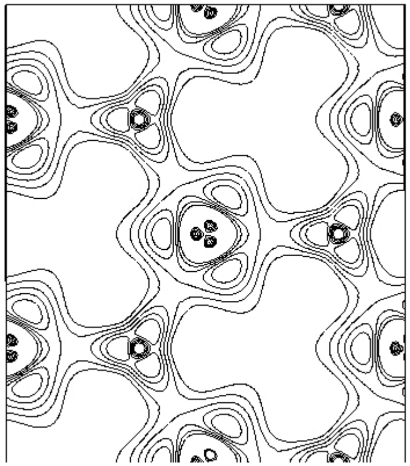
Heid & Bohnen (2006) el-ph coupling strength is not large enough

Bill et al. (2003) Coupling to/ screening by low energy plasmons may be important



In-plane d band holds the carriers

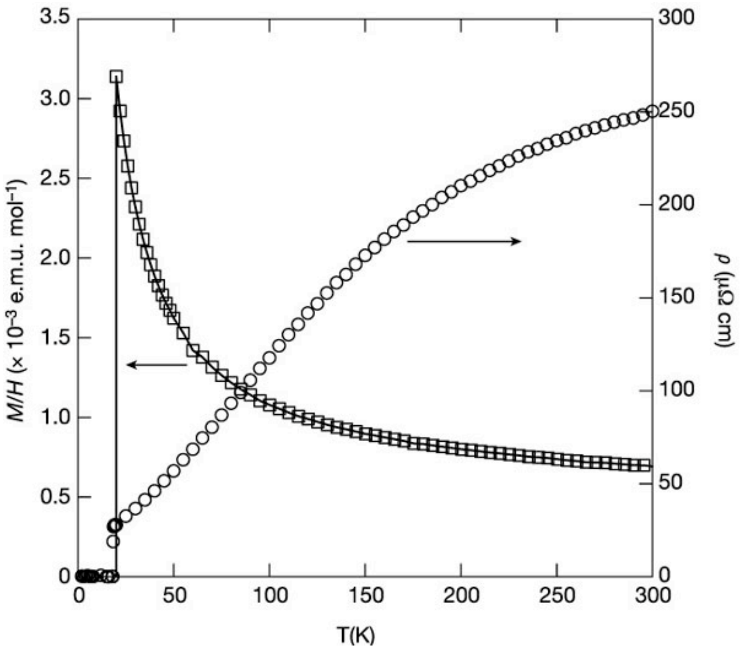
- Double Zr-N layer, corrugated graphitic
- Strongly 2D bands
- Electron-doped
- Inverse ‘isotope shift’

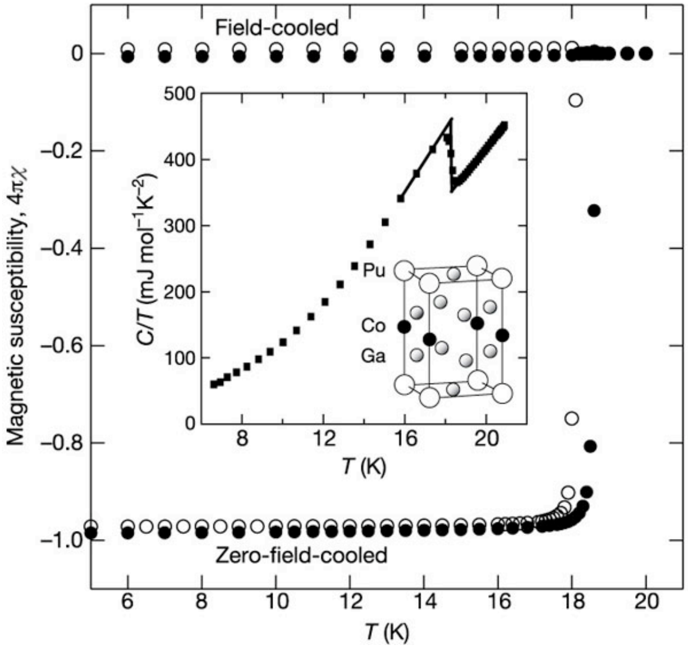


Superconductor-insulator transition at x=0.06

$PuCoGa_5$: 18.5 K (Sarrao et al. 2002)

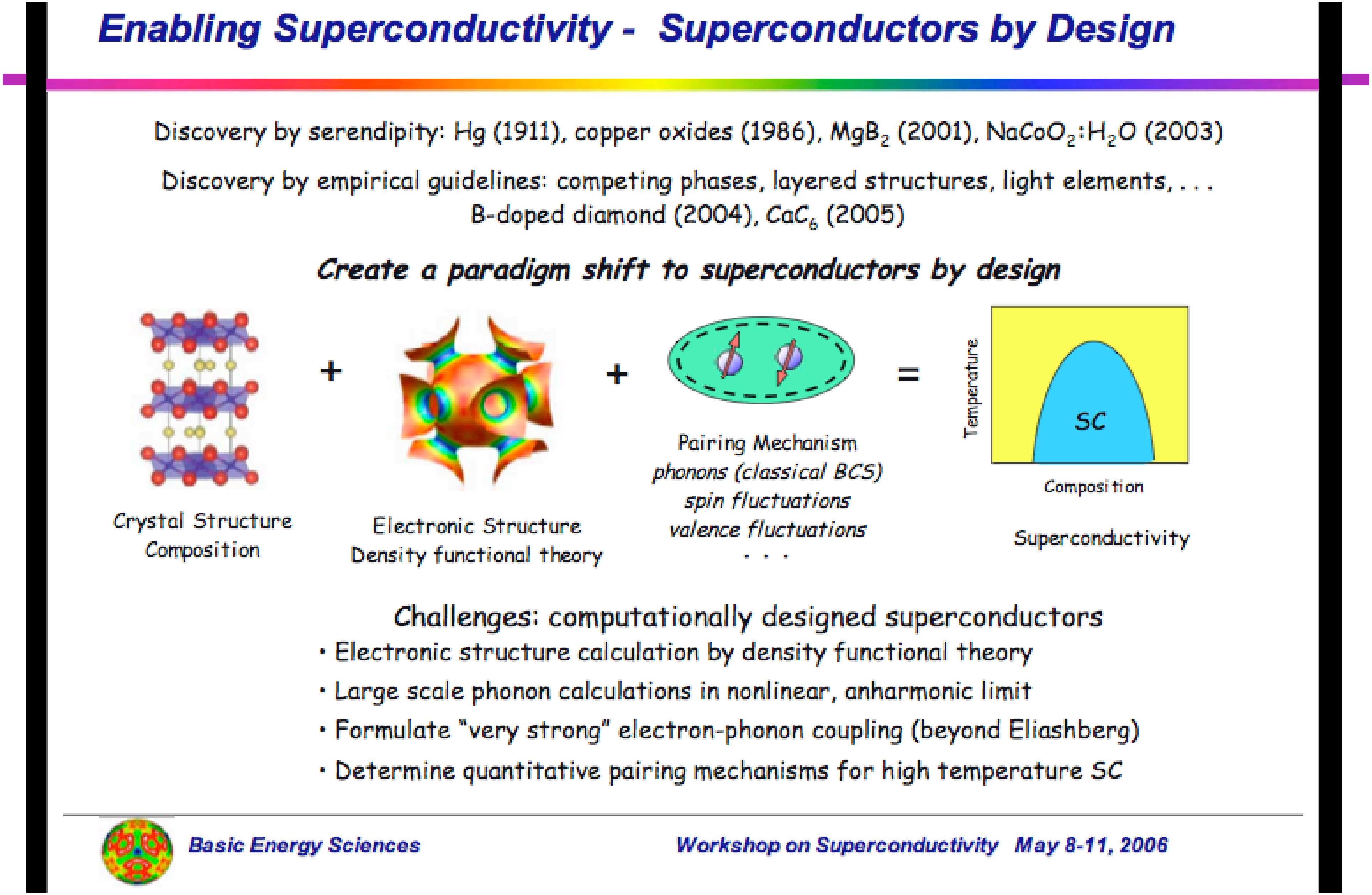
Order of magnitude higher than previous heavy fermion sc'y





Other heavy fermion superconductors: $T_c < 2$ K

$PuCoGa_5$ may provide the key to HF sc'y mechanism



Enabling Superconductivity - Superconductors by Design

Discovery by serendipity: Hg (1911), copper oxides (1986), MgB_2 (2001), $NaCoO_2$:H_2O (2003)

Discovery by empirical guidelines: competing phases, layered structures, light elements, . . .
B-doped diamond (2004), CaC_6 (2005)

Create a paradigm shift to superconductors by design

Crystal Structure
Composition

+

Electronic Structure
Density functional theory

+

Pairing Mechanism
phonons (classical BCS)
spin fluctuations
valence fluctuations
. . .

=

Superconductivity

Challenges: computationally designed superconductors

- Electronic structure calculation by density functional theory
- Large scale phonon calculations in nonlinear, anharmonic limit
- Formulate "very strong" electron-phonon coupling (beyond Eliashberg)
- Determine quantitative pairing mechanisms for high temperature SC

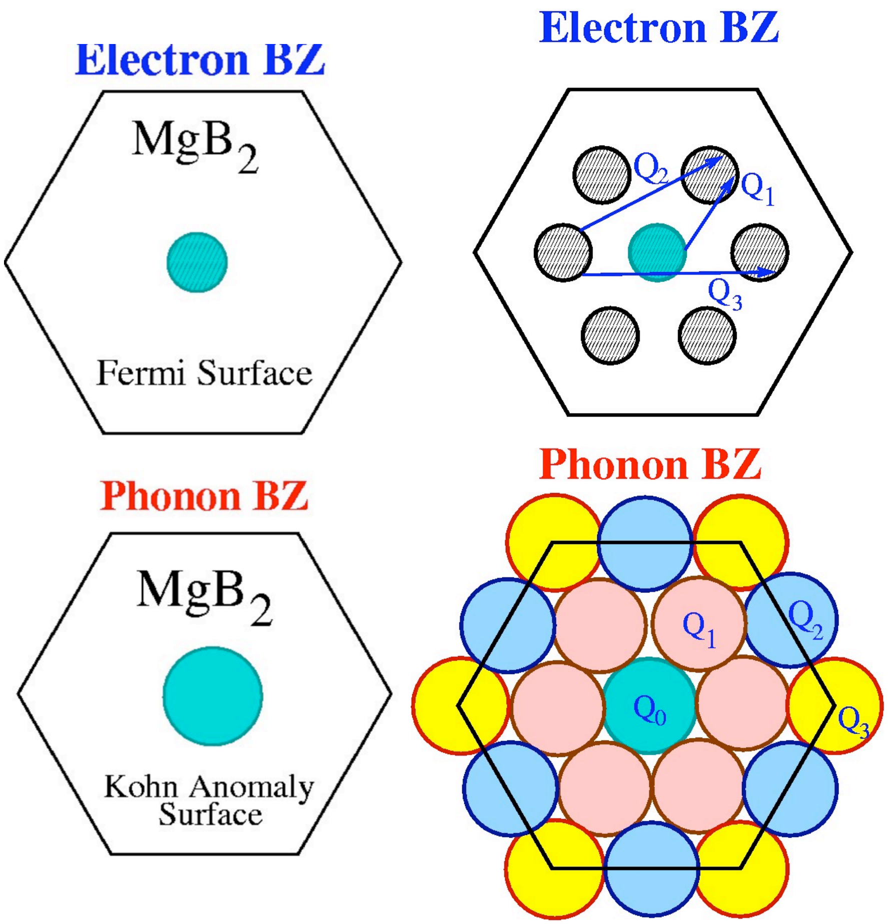
Basic Energy Sciences *Workshop on Superconductivity May 8-11, 2006*

Design of new superconductors: is it viable?

Rational Design/Search for new hTS

Example of one design criterion, enabled by understanding of mechanism

Select band structure to enable the phonons to use more of the Brillouin zone



Database driven design/search

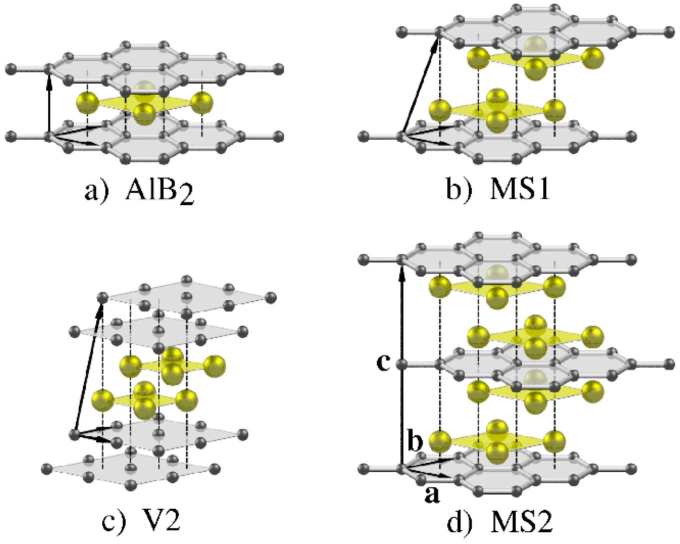
……..imposing phase stability.

Example: Design of Li_2B_2 (“MgB_2”).
Considered several structures.
Checked stability. Calc’d phonons.

Rational Design/Search for new hTS

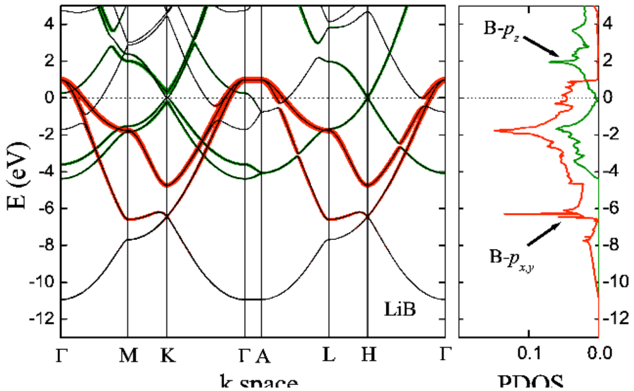
Kolmogorov, Curtarolo, Calandra
cond-mat/0603304, 0701199

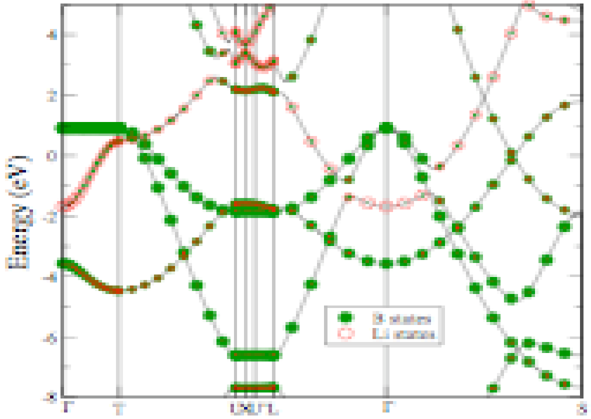
T_c ~ 15 K calculated

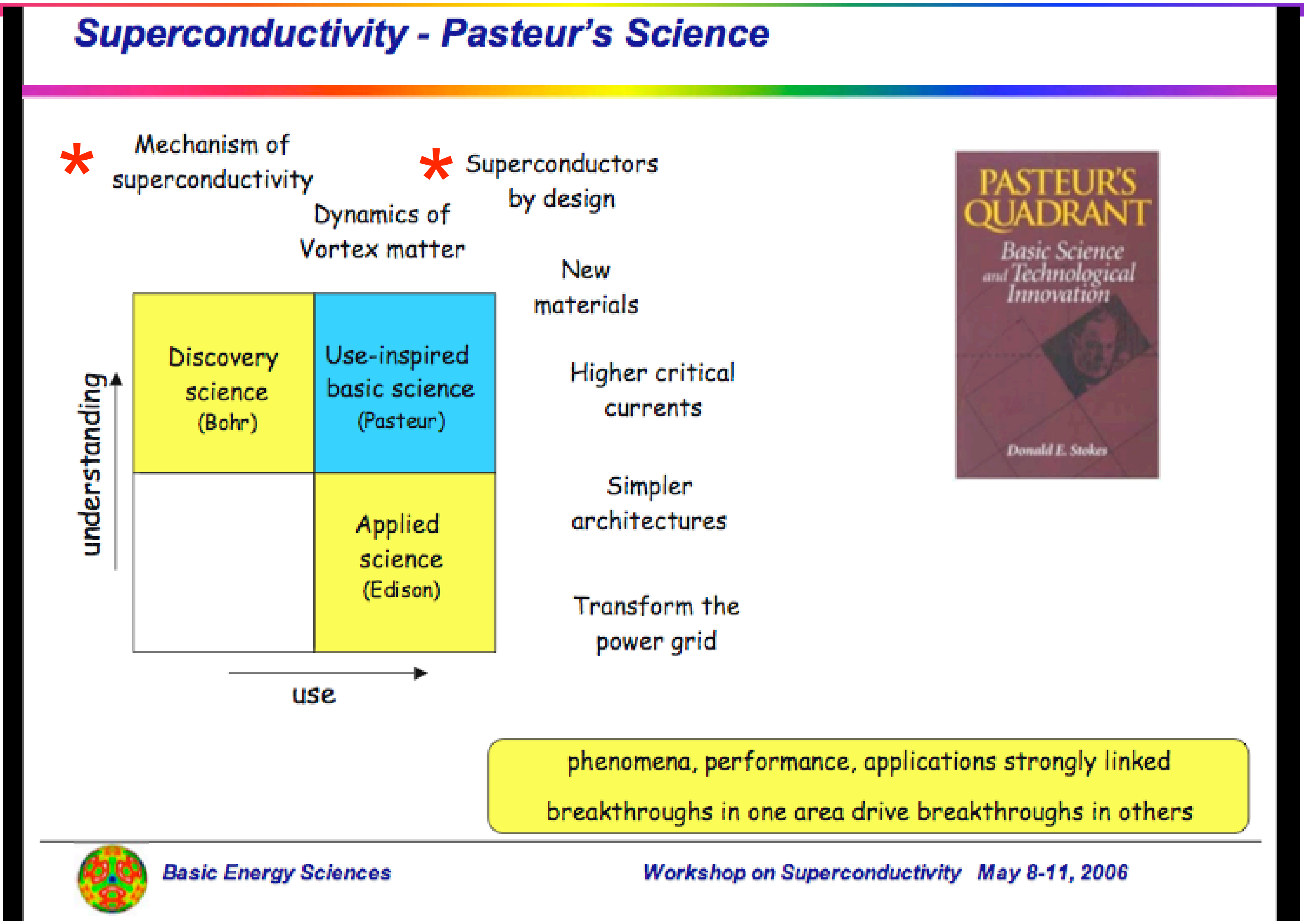


a) AlB_2 b) MS1

c) V2 d) MS2







Superconductivity - Pasteur's Science

* Mechanism of superconductivity

Dynamics of Vortex matter

* Superconductors by design

New materials

Higher critical currents

Simpler architectures

Transform the power grid

Discovery science (Bohr)	Use-inspired basic science (Pasteur)
	Applied science (Edison)

phenomena, performance, applications strongly linked

breakthroughs in one area drive breakthroughs in others

Basic Energy Sciences **Workshop on Superconductivity May 8-11, 2006**