Understanding Mechanisms of Superconductivity and Design of Advanced Superconductors

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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….


BCS Theory

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.

S. Redner

Basic Energy Sciences

BES Report on Basic Research Needs for Superconductivity
http://www.sc.doe.gov/bes/reports/abstracts.html#SC
the superconductor tsumani (late 1986)


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
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

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

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BES Report on Basic Research Needs for Superconductivity
http://www.sc.doe.gov/bes/reports/abstracts.html#SC
Publication activity in HTS remains prodigious

It is essential to sustain the progress in HTS and the associated fundamental understanding and materials expertise that is accumulating.
20th Anniversary of High $T_c$

**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

\[ \Sigma(\omega) = \stackrel{\text{d}}{\longrightarrow}, \quad \Delta \Gamma = \text{\textbullet} \]

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

Possibility: there is too much data to decide between mechanisms

Is “mechanism” the question…?
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?
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 \( \text{CuO}_2 \) 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
  \( \sim 55^4 \sim 10 \text{ million quaternaries} \)

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 \( \rightarrow \)
  higher critical current

- BSCCO \( > 100 \)
- YBCO \( 7 \)
- target \( 1 \)

Basic Energy Sciences
Workshop on Superconductivity  May 8-11, 2006
**Additional Developments in hTS Materials**

\[ hTS \equiv \text{unexpectedly high } T_c \]

- 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\(_2\)C\(_3\) -- 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

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**Figure 1.** Left: Calculated phonon dispersion curves in MgB$_2$.
The area of each circle is proportional to the mode $k$. The insets at the bottom show the two $\Gamma$-$A$ $E$ eigenvectors (not normalized), which apply to the lobes at the top of the $\sigma$ bands (bond-orthogonal coefficients) as well as to the optical bond-switching phonons (relative change of bond lengths). Right: $F(q)$ (full curve and bottom scale) $\alpha F(q)$ (isoheats) and $\alpha^2 F(q)$ (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)

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

$[T_c(\text{La}_2C_3) = 11$ K]
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

Lithium

Nesting function in three planes

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 \( T_c = 4-5 \) K

\[
\begin{pmatrix}
Y^{3+}_{1/9}TaS_2 \\
La^{3+}_{1/9}TaS_2 \\
Mn^{2+}_{1/6}TaS_2
\end{pmatrix}
\Rightarrow Ta^{+3\frac{2}{3}}
**Li_{1-x}NbO_2: 5 years after HTS**
*(Stacy group, 1991)*

- 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

\[ T_c = 5.5 \, K \]
$\text{Na}_{1-x}\text{CoO}_2$, the Dehydrated Superconductor [add water!]

Triangular lattice
Hole-doped from 
$\text{Co}^{3+}$ semiconductor
Octahedral $\text{CoO}_6$

Edge-sharing $\text{CoO}_6$ octahedra

Superconducting around $x \sim 0.3$

$T_c = 4.5$ K

$\text{Na}_{1-x}\text{CoO}_2 \cdot y\text{H}_2\text{O}$

Jorgensen et al. (2003)

Takada et al., Nature \textbf{422}, 53 (2003);
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 $T_c = 4.2$K at $x = 0.08$
Synopsis: $T_c$ in 2D Triangular Oxides/Chalcogenides

Triangle Lattice Transition Metal Chalcogenides

All $T_c$'s hover around 5 K
**Alkali-doped $A_xZrNCl$ (15 K) & $A_xHfNCl$ (25 K)**

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

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

- In-plane d band holds the carriers

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

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$_2$O (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 = Temperature Composition 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
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

Electron BZ

MgB$_2$

Fermi Surface

Phonon BZ

MgB$_2$

Kohn Anomaly Surface
Database driven design/search

Example: Design of Li$_2$B$_2$ (“MgB$_2$”).
Considered several structures.
Checked stability. Calc’d phonons.

Rational Design/Search for new hTS

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

$T_c \sim 15$ K calculated
Superconductivity - Pasteur’s Science

- Mechanism of superconductivity
- Superconductors by design
- Dynamics of Vortex matter
- New materials

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

Higher critical currents
Simpler architectures
Transform the power grid

- phenomena, performance, applications strongly linked
- breakthroughs in one area drive breakthroughs in others

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