Engineering room-temperature superconductors via ab-initio calculations

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US ONR support is acknowledged
RTS needs no special introduction:

- Institutes, schools
- Articles, books
- Manifestos...
- New materials
- Theoretical explorations
- Government programs
- Projects...
- Still lack of understanding
- How to use predictive power of ab-initio calculations?

Superconductivity

Chairs: Stuart Parkin, IBM Research - Almaden
Claudia Felser, MPI - Dresden
October 17 - 18, 2012
Summer School Sessions: October 15 and 16

The successful finding of a material superconducting near room temperature would have enormous technological impact. Such a material could, for example, help to reengineer entire energy production, engineer faster computers, allow for novel memory-storage devices, and enable ultra-sensitive sensors, among many other possibilities.

The Institute will focus on classifications of materials, based on their bonding, structure and chemistry, that might help to identify new superconducting materials with higher transition temperatures.

A series of tutorials on the themes of the Institute will be available for all interested. The school and tutorials are intended for graduate and PhD students. While there is no registration fee for the institute, space in the School and Institute is limited.

For more information: spinaps@us.ibm.com
Predictive power of theory

(history)

BCS, 1957:

\[ T_c \sim \omega_D \exp\left(-\frac{1}{\lambda}\right) \]

Bogolyubov et al., 1958; Eliashberg, 1960; MacMillan, 1968:

\[ T_c \sim \omega_D \exp\left\{ \frac{1.04(1+\lambda)}{\lambda-\mu^*(1+0.62\lambda)} \right\} \]

Little, Ginzburg, 1964:

\( T_c > 300K \)

Cohen, Anderson, 1972:

\( T_c < 10K \)
Importance of $\varepsilon(q, \omega)$

Kirzhnitz, 1976: $\varepsilon(q, \omega=0)<0$

admissible!

Dolgov, Maximov 1979: it is negative!!

Finding $\varepsilon(q, \omega)$ means determining the dynamics of the system

$$\int d\vec{q} \frac{4\pi e^2}{\varepsilon(q, \omega=0)q^2} = \mu - \lambda$$

$$V(q, \omega) = V_{(Coulomb)} + V_{(el-ph)} = \frac{4\pi e^2}{\varepsilon(q, \omega)q^2}$$

$$\frac{1}{\varepsilon(q, \omega)} = \frac{q^2}{q^2 + k_{TF}^2} [1 + \frac{\omega^2}{\omega^2 - \omega_q^2}]$$
Obvious parallels between

Historic suggestions by Little and others

Contemporary ab-initio calculable and experimentally achievable nanostructures
Ab-initio calculations of $\varepsilon(q,\omega)$

• We made use of the Density Functional Theory (DFT) code ABINIT [Gonze et. al (2005) and (2009)] and the add-on Time Dependent Density Functional Theory (TDDFT) code DP [Reining, Olevano, et al. (2008)].

• ABINIT was used to compute the electronic density and band structure. The computed data were then fed into DP to calculate the dielectric function.

• Graphical interface of QuantumWise commercial software was used for acceleration of relaxation studies.
First principle calculations for Aluminum

No negativity of $\text{Re } \varepsilon^{-1}(q, \omega=0)$ in frozen lattice model.

Conclusion:
phonons are important for SC in this material!
However, Ti-decoration delivers the tendency…

\[ V(q, \omega) = \frac{4\pi e^2}{\varepsilon(q, \omega)q^2} \]

The mechanism is purely electronic!
Moreover, for ropes of CNTs: $\varepsilon(q_0, \omega) < 1$!

Negativity of $\varepsilon(q_0, \omega)$ means we can expect SC!

Direct analogy $\Rightarrow$

$$V(q, \omega) = \frac{4\pi e^2}{\varepsilon(q, \omega) q^2} = \frac{4\pi e^2}{q^2 + k_{TF}^2} + \frac{4\pi e^2}{q^2 + k_{TF}^2} - \frac{\omega_q^2}{\omega^2}$$
On the agenda: $\varepsilon(q,\omega)$ for YBCO

Just single layer of Cu-O

Young collaborators are welcome to join us:
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Thank you!