Predicting the Superconducting Transition Temperature for LiBC
Introduction

• Transition Temperature, $T_c$
• High Transition Temperature of MgB$_2$, 39K
• Similarity in Structure of MgB$_2$ and LiBC

• Lack of Success in Formulating Superconducting LiBC

BCS Theory of Superconductivity

• Bardeen, Cooper, and Schrieffer (1972)
• Effect of Phonon Vibrational Modes on Electrons
  – Electrons as Fermions: Half Spin (1/2, 3/2, etc.)
  – Coupled Electrons as Bosons: Integral Spin
• Allen-Dynes Equation: $T_c \uparrow: \omega_{ln} \uparrow, \lambda \uparrow$
Electron Band Structure

- Hybridization of Atomic Energy Levels from Bonding
- Picture of Allowed Levels but not Probabilities
  - Multiple Locations with Same Energy Level
  - Slope of Bands
  - Density of States (DOS)
Example of Energy Bands
Electron Band Structure

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Energy Band Structure for LiBC
Phonon Dispersion

• Graphs Similar to Electron Band and DOS Plots
• Vibrational Frequencies for Energy Levels
Dispersion Curve
Computations

- **BICON – CEDiT**
  - Martin Brändle, Ruedi Rytz, and Gion Calzaferri, Department of Chemistry and Biochemistry, University of Berne
  - Electron Band Structure

- **Unisoft**
  - P. Elter and G. Eckold, Institut for Physical Chemistry, University of Göttingen
  - Phonon Dispersion Curve
Unisoft

Enter Crystal Structure
- Lattice Constants
- Atom Positions
- Atom Masses

→

Enter Wave Vectors
Like a Mesh for Integration

→

Choose Interaction Model
Ideal Springs
Determination of Spring Constants

- BICON – CEDiT for Total Energy
- Displacements along Lines between Atom Pairs
- Equation from Classical Mechanics: \( E = \frac{1}{2} k x^2 \)
- Inaccuracy
  - Other Atoms in Structure
  - ABINIT a common project of the Université Catholique de Louvain, Corning Incorporated, and other contributors (http://www.abinit.org)
Figures

Calculations and Results

• High and Low Values of $\lambda$ (Doping)
  – The Effect of Doping ($\lambda = 0.5$ and 1.0)
  – DOS Peak near Fermi Level

• Logarithmically Averaged Frequency, $\omega_{\text{ln}}$

• Values of $T_c$: 16 K and 45.4 K
Calculations and Results

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Conclusions

• $T_c$ Lower than Expected
  – Effect of Doping on $\omega_{ln}$
  – Anharmonicity

• Range Still High