

Electron-phonon driven superconductivity of LiBi

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LiBi is a very intriguing material, as it is built up from the heaviest and the lightest nonradioactive metals in the periodic table. Bismuth is a semimetal with interesting Dirac-like electronic states, while lithium contains only one valence electron and has nearly free-electron Fermi surface.

LiBi superconducts below $T_c = 2.45$ K and its crystal structure is tetragonal and can be seen as bcc structure distorted along z -axis.

In this work, theoretical and experimental studies of LiBi are presented. The experimental part consists of magnetic susceptibility and heat capacity measurements.

Ab initio calculations of the electronic structure, phonons and the electron-phonon interaction function were done. On this basis two important features of superconductivity are calculated, the transition temperature and electron-phonon coupling constant.

The band structure of LiBi is affected by structural distortion and is an interesting interplay between dominating p -states of Bi and states of Li, while phonons reflect the huge mass difference of these two elements. Superconductivity of this material is driven by the electron-phonon coupling with moderate magnitude.

Finally, our results are confronted with properties of NaBi, superconductor with $T_c = 2.15$ K, which is isostructural and isoelectronic with LiBi and whose bandstructure was reported to show a topological character [1].

Refs

[1] R. Li, *et al.*, Scientific Reports **5**, 8446 (2015).

Primary authors: GUTOWSKA, Sylwia (AGH University of Science and Technology, Cracow, Poland); GÓRNICKA, Karolina (Gdansk University of Technology, Gdansk, Poland); WINIARSKI, Michał (Gdansk University of Technology, Gdansk, Poland); XIE, Weiwei (Department of Chemistry, Louisiana State University, Baton Rouge, USA); CAVA, Robert (Department of Chemistry, Princeton University, Princeton, USA); KLIMCZUK, Tomasz (Gdansk University of Technology, Gdansk, Poland); WIENDŁOCHA, Bartłomiej (AGH University of Science and Technology, Cracow, Poland)

Presenter: GUTOWSKA, Sylwia (AGH University of Science and Technology, Cracow, Poland)