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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.
{\it 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, {\it et al.}, Scientific Reports {\bf 5}, 8446 (2015).

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