2006 Vol.46 No.3 pp.573-576 DOI:

First-Principle Calculations for Thermodynamic Properties of LiBC Under High Temperature and High Pressure

LIU Zhong-Li, CHENG Yan, TAN Ni-Na, and GOU Qing-Quan

Institute of Atomic and Molecular Physics, Sichuan University, Chengdu 610065, China
(Received: 2005-12-5; Revised:)

Abstract: The thermodynamic properties of LiBC are investigated by using the full-potential linearized muffin-tin orbital method (FP-LMTO) within the frame of density functional theory (DFT) and using the quasi-harmonic Debye model. The dependencies of the normalized lattice parameters a/a_0 and c/c_0, the ratio $(c/a)/2$, the normalized primitive volume V/V_0 on pressure and temperature are successfully obtained. It is found that the interlayer covalent interactions (Li-B bonds or Li-C bonds) are more sensitive to temperature and pressure than intralayer ones (B-C bonds), as gives rise to the extreme lattice anisotropy in the bulk hcp LiBC.

PACS: 71.15.Mb, 65.40.-b, 62.50.+p
Key words: thermal expansion, heat capacity, compressibility, LiBC, full-potential linearized muffin-tin orbital

[Full text: PDF]

Close