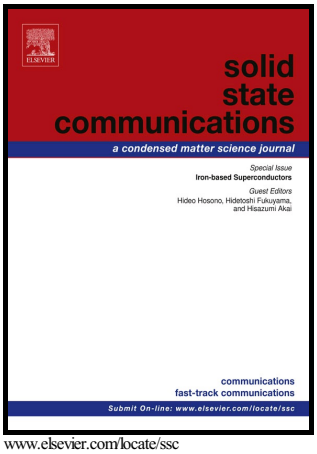

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PII: S0038-1098(17)30245-4
DOI: http://dx.doi.org/10.1016/j.ssc.2017.08.007
Reference: SSC13252

To appear in: *Solid State Communications*

Received date: 9 June 2017
Revised date: 12 August 2017
Accepted date: 16 August 2017

Cite this article as: Nikita Acharya and Sankar P Sanyal, Structural Phase Transition, Electronic and Superconducting Properties of ScBi and YBi, *Solid State Communications,* http://dx.doi.org/10.1016/j.ssc.2017.08.007

Structural Phase Transition, Electronic and Superconducting Properties of ScBi and YBi

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Abstract

The structural, electronic, lattice dynamic and superconducting properties of ScBi and YBi compounds are investigated using density functional theory. The calculated values of structural phase transition pressure from NaCl-type (B_1) to CsCl-type (B_2) phase and ground state properties such as lattice constant (a_0), bulk modulus (B) and its pressure derivative (B′) are compared with the available theoretical data. The electronic and bonding properties are discussed in terms of band structure, density of states and charge density difference plots. The phonon dispersion curves and phonon density of states are also discussed for both the compounds and calculated for the first time for ScBi compound. The phonon frequencies are positive at ambient and high pressure throughout the Brillouin zone in rock-salt structure revealing the stability in that phase. Eliashberg spectral function, electron-phonon coupling constant and superconducting transition temperature of ScBi and YBi are discussed in detail. The values of T_c are 0.97K for ScBi and 1.29K for YBi at ambient pressure.

Keywords: A. Superconductivity; C. Phase transition; D. Electronic structure; D. Electron-phonon interaction.

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