

Theoretical Investigation of Structural and Electronic Properties of AlBi

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Abstract : The purpose of this work is to provide some additional information to the existing data on the physical properties of AlBi with state-of-the-art first-principles method of the full potential linear augmented plane wave (FPLAPW). Additionally to the structural properties, the electronic properties have also been investigated. The dependence of the volume, the bulk modulus, the variation of the thermal expansion α , as well as the Debye temperature are successfully obtained in the whole range from 0 to 30 GPa and temperature range from 0 to 1200 K. The latter are the basis of solid-state science and industrial applications and their study is of importance to extend our knowledge on their specific behaviour when undergoing severe constraints of high pressure and high temperature environments.

Keywords : AlBi, FP-LAPW, structural properties, electronic properties

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