Modified Becke-Johnson potential investigation of InAsxSb1-x semiconductors

A. Bentayeb1,2,a, F. Saadaoui2, N. Marbouh2, K. Bouhafs1,2, F. Driss-Khodja2, O. Arbouche3

1Laboratoire de Technologies des Communications, Université de Saïda, 20000 Saïda, Algérie

2 Laboratoire d'Etudes Physico-Chimiques, Université de Saïda, 20000 Saïda, Algérie

3 Laboratoire de Physico-Chimie des Matériaux Avancés, Université de Sidi-Bel-Abbes, 22000 Sidi-Bel-Abbes, Algérie

kaderbentayeb@gmail.com

Abstract

In this paper we have investigated structural, electronic, and thermodynamic properties of ternary InAsxSb1-x semiconductors within the full potential-linearized augmented plane wave (FP-LAPW) method based on the density functional theory (DFT). We used the quasi-harmonic Debye model when calculating thermodynamic properties. We treated the exchange-correlation effects with the Tran-Blaha modified Becke-Johnson + local density approximation (TB-mBJLDA) potential. The obtained results are reported, discussed, and compared with previous data.

Keywords: Semiconductors; FP-LAPW; mBJ-LDA; structural properties; thermodynamic parameters; electronic structure.