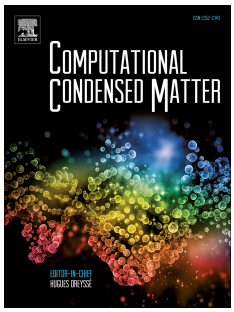
Accepted Manuscript



Ab initio study of novel III–V nitride alloys $B_{1-x}Tl_xN$ for optoelectronic applications

M. Belabbas, O. Arbouche, M. Zemouli, Y. Benallou, M. Benchehima, M. Ameri

PII: S2352-2143(18)30118-7

DOI: 10.1016/j.cocom.2018.e00309

Reference: COCOM 309

To appear in: *Computational Condensed Matter*

Received Date: 13 April 2018

Accepted Date: 25 May 2018

Please cite this article as: M. Belabbas, O. Arbouche, M. Zemouli, Y. Benallou, M. Benchehima, M. Ameri, Ab initio study of novel III–V nitride alloys $B_{1-x}Tl_xN$ for optoelectronic applications, *Computational Condensed Matter* (2018), doi: 10.1016/j.cocom.2018.e00309.

Ab initio study of novel III–V nitride alloys $B_{1-x}Tl_xN$ for optoelectronic applications

M. Belabbas[1*], O. Arbouche[2], M. Zemouli[3], Y.Benallou[1], M.Benchehima[4], and M. Ameri[2]

1. — Laboratory of Technology of Communications, Faculty of Technology, University of Saïda Dr Tahar Moulay, P. O. Box 20000, Saïda, Algeria

2. — Laboratory of physico-chemistry of advanced materials, Faculty of Sciences, University of Djillali Liabes, P. O. Box 22000, Sidi Bel Abbes, Algeria

3. — Laboratory of physico-chemical studies, Faculty of Sciences, University of Dr Tahar Moulay, Saïda P. O. Box 20000, Saïda, Algeria

4. — Applied Material laboratory University of Djillali Liabes, P. O. Box 22000, Sidi Bel Abbes, Algeria

Corresponding author: arbouche_omar@yahoo.fr

Abstract:

In this study, we propose the cubic $B_{1-x}Tl_xN$ ternary alloy as a promising infrared material. We used the full potential-linearized augmented plane wave (FP-LAPW) method within the Density Functional Theory (DFT) to predict the structural, electronic and optical properties of the $B_{1-x}Tl_xN$ ternary alloys. The structural properties such as the equilibrium lattice parameter, bulk modulus and its pressure derivative are investigated with the effect of the concentration variation of Tl atom, x (x=0, 0.25, 0.50, 0.75, and 1). We note that, because of existence of heavy elements in our alloys, spin-orbit coupling (SOC) is incorporated for electronic and optical calculations in order test the effect of spin-orbit interaction on these properties. Our results show the direct nature of the energy band gap of the ternary $B_{1-x}Tl_xN$ alloy for all composition of Tl-substitution. Furthermore, investigation of the dielectric function and refractive index shows that our materials are active in infrared and visible energy regions. We found that the spin-orbit effects opens up a very small gap at concentrations x = (0.75 and 1), resulting in a nearly metallic behavior of its optical response (imaginary part of dielectric function).

Keywords: III-nitrides; III-V;FP-LAPW; GGA-PBEsol, TB-mBJ, Spin-Orbit Coupling; electronic structure; optical properties;