Известия НАН Армении, Физика, т.61, №1, с.31–32 (2026)
DOI: 10.54503/0002-3035-2025-61.1-31

FIRST-PRINCIPLES STUDY OF $B_{1-x}Ga_xP_yBi_{1-y}$ QUATERNARY ALLOYS FOR NEAR-INFRARED OPTOELECTRONIC, SPECTROSCOPIC AND SENSING APPLICATIONS

S. Touam[1,2*], N. Mounis[3], F. Guenfoud[1], I .Bendjedide[1], S. Chelli[1,2], F. Z. Khelifati[1], D. Lamrous[1,4], O. Belaidi[5], S. Ghemid[2], H. Meradji[2]

[1]Physico-Chemistry of Materials Laboratory (LPCM), Department of Physics, Faculty of Science and Technology, Chadli Bendjedid University (UCBET), El Tarf 36000, Algeria

[2]Radiation Physics Laboratory (LPR), Department of Physics, Faculty of Sciences, Badji Mokhtar University, Annaba 23000, Algeria

[3]Department of Physics, Faculty of Exact Sciences, Sidi Bel Abbés University,22000 Algeria

[4]Laboratory of Magnetism and Solid Spectroscopy, Badji Mokhtar University, Faculty of Sciences, Department of Physics, Annaba 23000, Algeria

[5]Physico-Chemistry of Materials Laboratory (LPCM), Chemistry Department, Faculty of Science and Technology, Chadli Bendjedid University (UCBET), El Tarf 36000, Algeria

[*]e-mail: touam-selma@univ-eltarf.dz

(Поступила в редакцию 7 января 2026 г.)

We realized an exhaustive study about structural, electronic and optical properties of the quaternary alloys $B_{1-x}Ga_xP_yBi_{1-y}$ in zinc blend phase by applying the full-potential augmented plane wave method FP-LAPW within the scope of density functional theory DFT. Potentials were determined using modified generalized gradient GGA and Becke-Johnson approximations. We analyzed the effects of the compositions (*x, y*) on the lattice parameters, bulk modulus, and band gap energy, revealing a non linear dependence of these quantities. We also investigated several optical constants, including the real and imaginary parts of the dielectric function, the absorption coefficient α(ω), the refractive index n(ω), and the reflectivity. Our obtained results about lattice parameters, energetic gaps and optical constants for the binary compounds are in well correspondence with the provided experimental and theoretical values. However, for alloys, differences were observed against linearity for lattice constants and bulk modulus. Moreover, we examined the energy band of zinc-based quaternary alloys $B_{1-x}Ga_xP_yBi_{1-y}$ those corresponding to ZnS lattice. It is worth mentioning that this study represents an innovative contribution in the domain of quaternary alloys, since it is the first theoretical analysis about these alloys.

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