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Ab INITIO STUDY OF STRUCTURAL, ELECTRONIC, OPTICAL, AND ELASTIC PROPERTIES OF YN_xBi_{1-x} AND YAs_xBi_{1-x} ALLOYS FOR INFRARED AND VISIBLE OPTOELECTRONIC APPLICATIONS

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This paper presents a pioneering first-principles investigation into the structural, elastic, electronic, and optical properties of novel ternary alloys YN_xBi_{1-x} and YAs_xBi_{1-x} which are considered promising candidates for advanced photonic and electronic applications. We employed the full-potential linearized augmented plane wave (FP-LAPW) method, based on density functional theory (DFT), as implemented in the WIEN2K simulation code, for compounds crystallizing in the NaCl-type structure. Structural properties, including lattice constants, bulk modulus and elastic properties, such as elastic constants, shear modulus, anisotropy factor, Poisson's ratio, Young's modulus, and the Kleinman parameter were calculated using the generalized gradient approximation (GGA) for the exchange-correlation (XC) potential. Furthermore, the Wu-Cohen generalized gradient approximation (WC-GGA) and the modified Becke and Johnson (mBJ) approaches were applied to examine electronic **(**band structure) and optical (real and imaginary parts of the dielectric function**,** refractive index) properties, respectively. These findings highlight the significant potential of these materials for use in advanced optoelectronic technologies, opening new avenues for future innovation.

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