Influence of hydrostatic pressure on the structural, electronic, and optical properties of $B_xAl_yGa_{1-x-y}N$ quaternary alloys: a first-principle study

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To investigate the effects of Al-doping on the structural, electronic, and optical properties of $B_xAl_yGa_{1-x-y}N$ quaternary alloys in the zinc-blende (ZB) phase, first-principle total-energy calculations were performed using the full-potential linearized augmented plane wave (FP-LAPW) technique as implemented in the WIEN2k code, which is based on density functional theory (DFT). Different exchange correlation energy approximations were used, such as the local density approximation (LDA) and the generalized gradient approximation within the Perdew–Burke–Ernzerh (PBE-GGA) parameterization. We also used the Tran-Blaha modified Becke–Johnson (TB-mBJ) approach to determine the band structures with great precision. Under hydrostatic pressure ($P = 0$ to 30 GPa), the pressure dependency of the $B_xAl_yGa_{1-x-y}N$ with different concentrations $(x, y) = [(0.25, 0.25), (0.25, 0.50)$, and $(0.50, 0.25)]$ for electronic and $B_{0.50}Al_{0.25}Ga_{0.25}N$ for optical properties was also investigated. In addition, we discovered that $B_xAl_yGa_{1-x-y}N$ retains its direct band-gap energy semiconductor. Using this value range, we can get the appropriate optical characteristics for several technical applications. When these quaternary alloys are subjected to hydrostatic pressure, we notice that all energy gaps widen as the pressure rises, while the nature of the fundamental gap remains unchanged for all quaternary compounds.

Keywords: density functional theory (DFT), electronic band-structure, optical properties, semiconductors, quaternary alloys.

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