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A theoretical study of Structural and electronic properties of $Al_{0,125}B_{0,125}Ga_{0,75}N$; optoelectronic applications

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Abstract **–** Semiconductor materials are highly valued in the electronics industry. Gallium nitride (GaN) from the family of these compounds is particularly important due to its use in various applications, including P-N junction diodes, transistors, and laser components. Our study focused on the effect of doping GaN with aluminum and boron simultaneously, using density functional theory (DFT) calculations with the Gradient Generalized Approximation (GGA-PBE) implemented in the CASTEP code. Our results showed that the volume of the primitive cell within the hexagonal wurtzite structure was 44.62$A^{\circ 3}$, and a bulk modulus of 163.07 GPa. In analyzing of the band structure, we found that the energy gap of $Al_{0,125}B_{0,125}Ga_{0,75}N$ was 3.75 eV, higher than the band gap of GaN, which was 3.40 eV.

Keywords – $Al_{0,125}B_{0,125}Ga_{0,75}N$; DFT; CASTEP; Band Gap