# First-principles calculations to investigate optical properties of $B_yAl_xIn_{1-x-y}N$ alloys for optoelectronic devices


## Abstract

First-principles density-functional theory of Full-Potential Linear Augmented Plane Wave (FP-LAPW) within local density approximation (LDA) of the optical properties of $B_yAl_xIn_{1-x-y}N$ systems (with x = 0.187 and y = 0.062, 0.125 and 0.187) has been performed. Substitutional atoms of Boron induced in small amounts into the ($Al_xIn_{1-x}$)-cationic sublattice of AlInN affects the energy gap of BAlInN. The higher band gap of $Al_{0.375}In_{0.625}N$ alloy can form a useful quantum well (QW) laser structure. A best choice of B-content, $B_yAl_xIn_{1-x-y}N$ could be an alternative to $Al_xIn_{1-x}N$. The results of accurate calculations of the band structures and optical properties show the better performance characteristics belong to the structure containing B-content (y) of 12.5%. The NaCl metallic $B_yAl_{0.1875}In_{0.8125-y}N$ has a direct character for y = 12.5%. The imaginary part of dielectric function, reflectivity, refractive index, absorption coefficient and optical conductivity are investigated well and provide reasonable results for optoelectronic devices applications.