# Ab-initio calculations of Optoelectronic Properties of $Al_xGa_{1-x}N$ semiconductors

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**Abstract.** This paper communicates structural and optoelectronic properties of $Al_xGa_{1-x}N$ ($x$ = 0, 0.25, 0.5, 0.75, and 1) alloys, this properties have been calculated using the full-potential augmented plane wave FP-LAPW method based on the density functional theory DFT, within the generalized gradient approximation GGA-PBEsol. The calculated lattice parameters are in good agreement with the previous experimental and theoretical results. The modified beck-Johnson potential TB-mBJ is used to investigate the electronic and optical properties. Direct bandgap change to indirect bandgap with increasing in Al concentrations was found for this material. Furthmore, the dielectric function, reflectivity, absorption coefficient and refractive index are presented and discussed in detail. The peak in the imaginary part of the dielectric function and the absorption edge are found to have a remarkable blue-shift with the increase of Aluminum concentration. These theoretical studies predict that this compound could be efficient material for optoelectronic applications and need further experimental and theoretical studies.

Keywords**:** semiconductors, $Al_xGa_{1-x}N$ alloys, DFT, optoelectronic properties, structural properties.