Compton Profile Study of Aluminium Nitride

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In this paper we report the *ab-initio* theoretical Compton profiles of aluminium nitride (AlN) in the framework of the Hartree-Fock, density functional theory and hybridization of Hartree-Fock to density functional theories using the CRYSTAL03 code. To compare our first ever theoretical data, we have also measured the isotropic Compton profile of AlN, using 59.54 keV γ-rays. The Hartree-Fock scheme-based Compton profile agrees better with the experiment than the other theories. The energy bands, density of states and Mulliken's population analysis, using the CRYSTAL03 code, are also reported. Our band structure calculations show a large band gap, while Mulliken's population analysis shows the ionic nature of bonding in AlN.

Key words: X-Ray Scattering; Band Structure Calculation; Density Functional Theory; III-V Semiconductor.

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