The Energy Band Gap of ScN in the Rocksalt Phase Obtained with LDA/GGA+U^{SIC} Approximations in FP-LAPW Method

M. S. Abu Jafar, A.M. Abu Labdeh & Musa El Hasan

Physics Department, An-Najah University, Nablus, Palestine

Abstract:

The structural properties of ScN compound in the rocksalt phase (RS) have been calculated using the full potential linearized augmented plane wave (FP-LAPW) method within the local density (LDA), Predew-Burke- Ernzerhof (PBE-GGA),WU- Cohen (WC-GGA) and Engel –Vosko (EV-GGA) approximations.The influecce of electron correlation, has also been considerd in calculating the electronic struture of RS-ScN within LDA+U^{SIC}, PBE-GGA+U^{SIC},WC-GGA+U^{SIC} and EV-GGA+U^{SIC} approximation. For the system of interest, the calculations, show that EV-GGA and PBE-GGA approximations give more accurate values for lattice parameter (a_0) and Bulk modulus (B_0) than LDA and WC-GGA approximations. The calculations also show that EV-GGA+U^{SIC}approach improves the description of electronic structure of RS-ScN than LDA+U^{SIC}, WC-GGA and PBE-GGA methods.

The energy band gap of RS-ScN within EV-GGA+U^{SIC} scheme is found to be 1.09 eV. This value is in excellent agreement with experimental value of 0.8-1.6 eV.

Email addresses
melhasan@najah.edu