A Comparative study for structural and electronic properties of ScN compound

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Abstract:

A comparative study by FP-LAPW calculations based on DFT within LDA, PBE- GGA, PW-EV-GGA, and EV-GGA schemes is introduced for the structural and Electronic properties of ScN in RS, ZB, WZ, and CsCl phases. According to all Approximations used in this work, the RS phase is the stable ground state structure and makes a transition to CsCl phase at high transition pressure. While PBE-GGA and PW-EV-GGA's have provided better structural features such as equilibrium lattice constant and bulk modulus, only PW-EV-GGA and EV-GGA's have given the non zero, positive indirect energy gap for RS-ScN, comparable with the Experimental ones. The indirect band gap of RS-ScN may be enlarged to the measured value by PW-EV-GGA calculations corrected with an on-site and angular dependent Coulomb potential approximation (U^{SIC}). The PW-EV-GGA calculations have also provided good results for the structural and electronic features of ScN in ZB, WZ, and CsCl phases comparable with the theoretical data available in the literature.
PW-EV-GGA and PW-EV-GGA+U^{SIC} schemes are considered to be the best ones among the others when the structural and electronic features of ScN are aimed to be calculated by the same exchange - correlation energy approximations.