

# A combined LDA, GGA, GGA+U, mBJ study on semiconducting Scandium Nitride

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## Abstract

Scandium nitride (ScN) has been studied with respect to its electronic band structure using full-potential linear augmented plane wave (FP-LAPW) method under the Local density approximation, generalised gradient approximation (GGA), GGA+U and modified Becke Johnson approximation (mBJ) to illustrate band gap in the material. It has been found that ScN was stable in rock-salt structure in non-magnetic phase. We have estimated its lattice parameter and bulk modulus in this structure, which were found in good agreement with the experimental values. ScN has intriguing nature in different approximations, nevertheless experimentally it had semiconducting nature. In this paper by using the mBJ under the Wien2k code, ScN showed semiconducting nature in its electronic band structure.

**Keywords:** ScN, Electronic structure, DFT calculation, GGA+U

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## 1. Introduction

There has been increasing interest in the materials with respect to their structural, electronic, magnetic, mechanical, thermal and transport properties. These properties in the materials are being investigated both experimentally [1-3] and theoretically [4]. Earlier days when experimental and theoretical approaches were not available good amount of research couldn't be accounted. With development of various new theoretical modelling and high speed computing, complex problem of the materials can be solved. These involves from tight binding to empirical methods to ab initio theories. The density functional theory (DFT) among ab initio theories plays an important role to solve many electron problem. Based on the DFT many codes have been developed till date. Transition metal compounds have always been remarkable due to their outstanding applications in hard coating for cutting tools [5,6], diffusion batteries, Mechanical strength [2,3,7] and thermoelectric devices [8,9]. As far as studies on ScN, which is one of the transition metal compounds, is concerned extensive studies have been reported []. ScN is experimentally known to have semiconducting nature with narrow band gap of 0.90 eV to 1.3 eV [2,10]. Nevertheless, earlier various theories on ScN show its metallic nature [11-13]. Later on Green's function quasi particle and other theories [14-17] found its character as semiconductor with indirect band gap of 0.54 eV to 1.7 eV. The energy band gap estimation had been a subject of problem using first principles theories. Now-a-days using new approximations with valid mathematical treatment to the old theories such problem has been solved to some extent. DFT+U, where 'U'

represents supplementary Coulomb energy or termed as Hubbard parameter, has been one of the successful formalisms to resolve band gap problem.

In the present paper, we have shown improvement in band gap of ScN from to zero to by using different approximations from LDA to mBJ in support of DFT. In Section 2 we have given method to obtain electronic band structure. On the other hand, in Section 3 we have discussed estimation of energy band gap in ScN, while in Section 4 results were concluded.

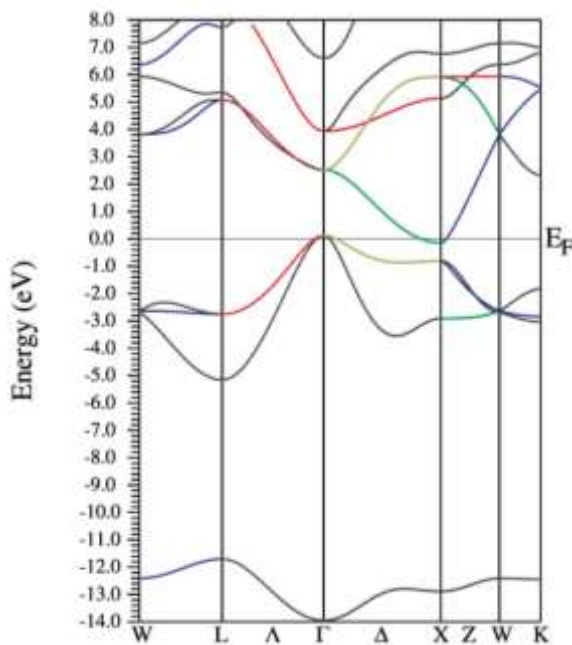
## 2. Method of calculation

Experimentally ScN crystallised in rock-salt structure (Fm-3m, 225 space group) [18]. Total energy calculations have been performed for ScN using full potential augmented plane wave method (FP-LAPW) method [19-21] in the Wien2k [22] code. ScN has been viewed in electronic structure using systematic LDA, GGA, GGA+U and mBJ approximations. According to total energy calculations we found its lower energy in rock-salt structure in non-magnetic phase. For energy convergence  $R_{MT}K_{max}$  was set to 7, where  $R_{MT}$  is the muffin tin radius and  $K_{max}$  is largest wave vector in plane-wave progression. The total energy of the system converges by considering stability of total energy within 0.001 Ry and for charge it was 0.001e/a.u.<sup>3</sup> per unit cell. 1000  $K$ -points were used in Brillouin zone and the tetrahedral method [23] was employed to estimate density of states.

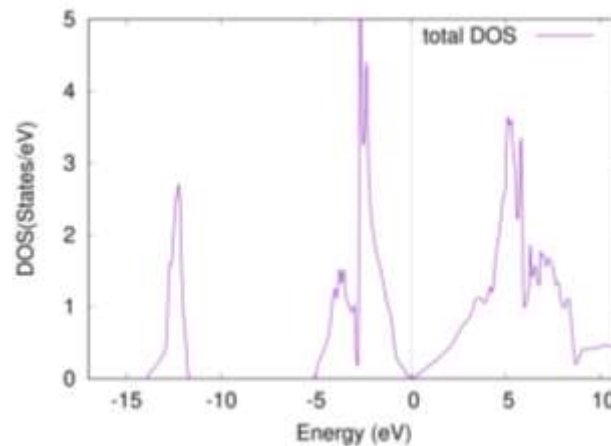
## 3. Results and discussion

As mentioned above ScN crystalized in rock-salt structure with lattice parameter [LP] value of 4.44 Å [18]. The optimization of structure in NaCl-type using LDA-FP-LAPW method calculates its volume to 146.5 a.u.<sup>3</sup> and corresponding lattice parameter to 4.428 Å, which is underestimated by experimental value [18]. LDA calculates bulk modulus and first order pressure derivative to 226 GPa and 4.19, respectively. The experimentally observed value of bulk modulus was 186 GPa [2]. However, in the same way GGA-FP-LAPW method calculates its volume to 155.08 a.u.<sup>3</sup> and corresponding lattice parameter to 4.513 Å, which is little over estimated by the experimental value [18]. Bulk modulus and first order pressure derivative are calculated to 201 GPa and 3.72, respectively. GGA however over estimated LP but modulus is also near to experimental value As it is evident that LDA underestimates LP, while GGA overestimates is true.

In order to clearly understand its electronic structure or more precisely its metallic, semiconducting, semimetallic nature, we have plotted E-K diagram along the high symmetry directions. In Fig 1, we have depicted electronic band structure of ScN using local density approximation (LDA) where one can notice cross over of 'Sc-d' states at 'X' point making it metallic in nature. The band structure diagram can be understood by looking density of states plot as shown in Fig.2 the sharp peak near Fermi level in energy range 0-3 eV is due to 'N-p' states and while broad peak near 0 to 9 eV is due to 'Sc-d', which crosses bit Fermi level, as clearly depicted in Fig. 1.

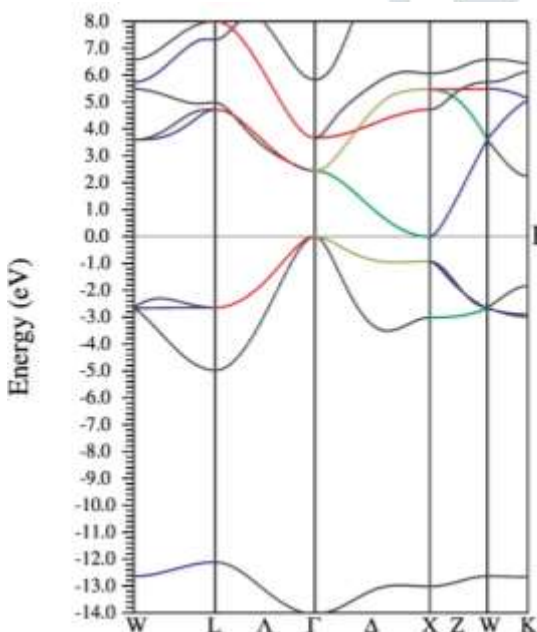


**Fig.1** Band structure of ScN along high symmetry directions using LDA

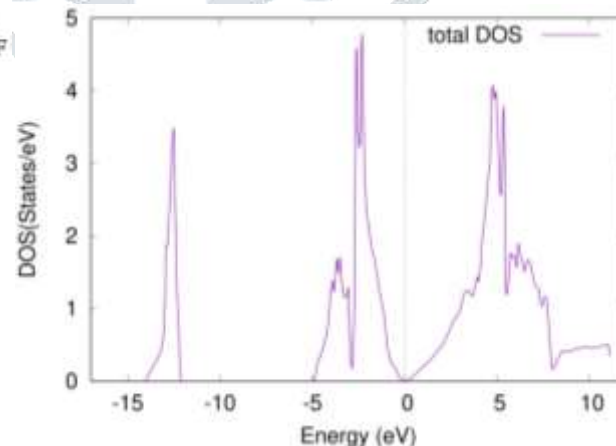


**Fig.2** Density of states of ScN using LDA

In Fig. 3, we have plotted band structure under GGA scheme where we can notice ScN shows semimetallic nature with zero indirect band gap (in direction of 'Γ-X'). The lowest lying band near to -12 and -13 eV is due to 'N-p' states and in GGA it shifted towards little lower side of energy. In Fig. 4 we have plotted DOS for ScN in GGA scheme where at Fermi level bands are exactly touching. A sharp peak in DOS diagram near to -12 and -13 eV representing 'Np-s' states.



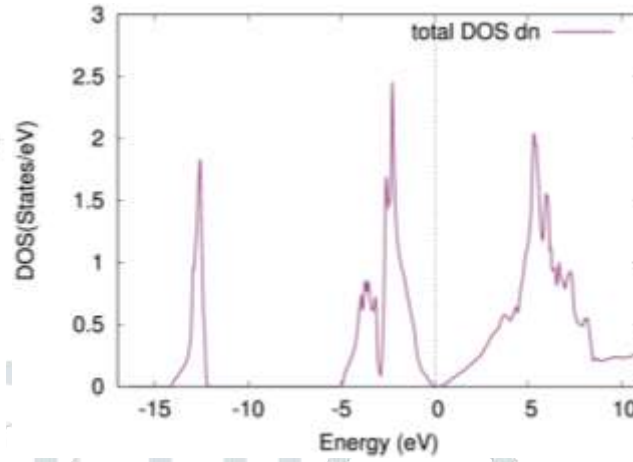
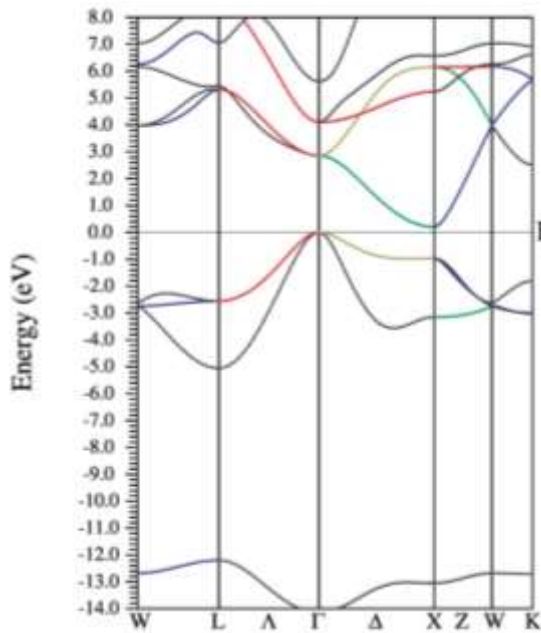
**Fig.3** Band structure of ScN along high symmetry directions using GGA



**Fig.4** Density of states of ScN using GGA

Further we have plotted band structure and density of states for ScN using GGA+U scheme, where  $U = 3.5$  eV was taken. In its band structure diagram it was found that clear narrow energy gap is appearing in the direction of 'Γ-X'. The value of indirect band gap is calculated to 0.20 eV. Such little shiftment in band can also be seen

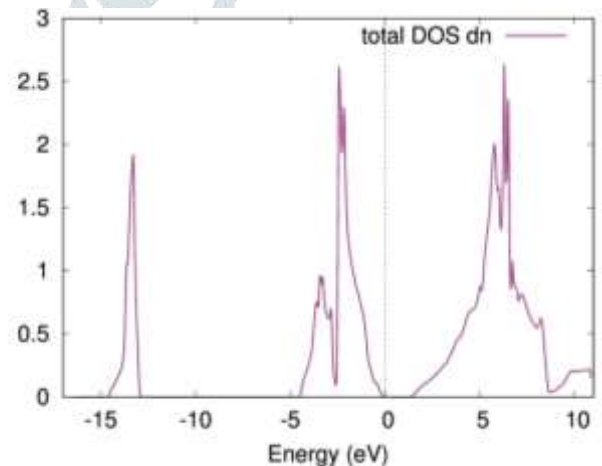
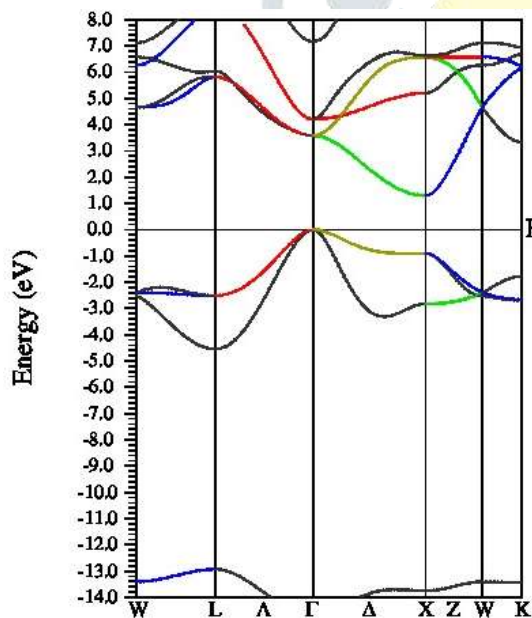
in density of states diagram, which is plotted in Fig. 6. Thus ScN is showing semiconducting behaviour, which is in accordance with the experimental outcomes. ScN is similar like other nitrides of transition metal. YN is also a similar kind of materials, which exhibit similar kind of behaviour upon changing scheme from LDA to GGA. ScN is similar to GaN also, which has many industrial applications.



**Fig.5** Band structure of ScN along high symmetry directions using GGA+U

**Fig.6** Density of states of ScN using GGA+U

In the modified Beckhe Johnson (mBJ) approximation ‘Sc-d’ states are splitted more and such indirect band gap is found more. In Fig. 7 we have plotted band structure diagram with mBJ where such energy gap is



estimated

to 1.3

0

eV, which is reflected in DOS diagram (Fig. 8).

**Fig.7** Band structure of ScN along high symmetry directions using mBJ

**Fig.8** Density of states of ScN using mBJ



#### 4. Conclusion

ScN has been studied with respect to its electronic structure and it has been found that it showed different behaviour in different approximations. It was found in FP-LAPW method, LDA treatment was given to ScN, it behaves like a metal. While it showed semimetallic in GGA approximation. It started turning to semiconducting nature when GGA+U scheme was used. For a particular  $U=3.5$  eV it showed semiconducting nature with indirect band gap of 0.20 eV, which further increased to 1.30 eV in mBJ approximation. Our calculated lattice parameter, bulk modulus and band gaps are in accordance with the experimental and other available results.

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