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Theoretical Study of the Electronic Properties of YN using Density Functional Theory

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Abstract

We present the results on electronic and semi-conducting properties of YN in rocksalt and zinc-blende structure by using FP-LAPW method as implemented in the Wien2k code. By performing the volume optimization method, a theoretical lattice constant is obtained which is used for performing our calculations. Results on density of states (DOS) and energy bands of YN are presented. It is found that YN acts as a semi-conducting behaviour in both the NaCl and ZB structures.

Keywords: DFT, GGA, FP-LAPW, DOS, BAND STRUCTURE.
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Introduction

YN belongs to transition metal nitrides group which has a wide spectrum of interesting physical properties. It is a material of fundamental importance in the semiconductor industry [1]. It has important technological applications like electric contact, magnetic storage device, optical switching devices, diffusion barriers, buffer layer etc [2]. In future these compounds possibly will be used as the electronically active layers in diodes and transistors. Therefore, transition metal nitrides represent a novel and probably technologically important group of semiconductor materials.

Several authors have presented results of electronic-structure calculations for YN from different view points. Mancera *et al.* [3] have done the first principles calculations of the ground state properties and structural phase transformation of YN. They have shown the possibility of phase transformation to a CsCl structure when pressure is applied to a system. Stampft *et al*. [4] investigated the bulk electronic and physical properties of 4d-transition-metal-nitrides like YN, ZrN, NbN in the rocksalt phase. Ghimire *et al*. [5] also calculated the electronic properties of YN in ZB phase and calculated its dielectric functions using Lindhard dielectric model.

In this report, we present the DOS and the band structure results of YN in NaCl and ZB phase. FP-LAPW method will be applied by implementing the Wien2k code [6].

Computational details

The calculations are performed in the frame work of density functional theory (DFT) as stated by Hohenberg *et al.*[7]. The exchange and correlation effects were treated using the generalized gradient approximation (GGA) [8], where the total Coulomb and orbital potential will be taken into consideration.

The crystal structure of YN is rock-salt and ZB with four atoms per unit cell. The full space group is Fm3m and F43m respectively. In the calculation, 393 LAPW basis functions were used for the expansion of the charge density and the potential in the interstitial region and lattice harmonics up to *lmax* = 10 for the expansion inside the muffin-tin spheres. In our calculations, core states were treated fully relativistically and the valence states were treated semi-relativistically. A satisfactory degree of convergence was achieved by considering a number of FP-LAPW basis functions up to $R_{MT} * K_{MAX} = 8$, (where R_{MT} is the average radius of the muffin-tin spheres and K_{MAX} is the maximum value of the wave vector) and $G_{max} = 12$. The number of k-points in the BZ is 172 with muffin-tin radii 1.058 Å and 0.89 Å for Y and N atoms respectively. Self-consistency is achieved by setting the convergence of both the total energy and eigen values to be smaller than 10^{-6} eV.

The Y atom is located at the origin and the N atom at (1/2, 1/2, 1/2) sites for NaCl structures, and (1/4, 1/4, 1/4) sites for ZB structures respectively. An energy cut-off of -122.4 eV is taken to separate the core states from the valence states. The experimental lattice constants a = 4.877 Å [9] is used in Murnaghan equation of state [10] to get equilibrium lattice constant.

Results and Discussions

Knowledge of the electronic properties is crucial to the understanding of the stability of the different structures. The energy bands are affected by factors like nearest-neighbor distances and changes in symmetry. These factors influence the overlaps of bands, bandwidths and also the p-d hybridization as well as band-repulsion.

The equilibrium lattice constants obtained is a = 4.927 Å for NaCl and a = 5.19 Å for ZB structure respectively as shown in Table 1. The obtained lattice constants are used to calculate the DOS and band structures.

Figs.1 shows the total DOS for YN, Y and N in NaCl phase. It can be predicted that DOS contribution above Fermi level is due to Y- d state electrons. Three main regions can be observed in the total DOS of YN : one below −11.4 eV due to N-2s electrons, another between −3 eV and the Fermi level due to N-2p electrons with a small contribution from Y-4d electrons, and the last one in the empty states at 6.5 eV with high contribution from Y-4d electrons and and some N-p electrons. Fig. 2 supplements the contribution of electrons from the d- states of Y in the conduction region, which decomposes into d_{eg} and d-t_{2g} states. The contribution from Y-d_{eg} in the

valence band near the Fermi level is higher than d-t_{2g} while in the conduction region; the main contribution to the bonding states is due to d-t_{2g} states of Y.

Fig. 3 shows the band structure results to supplement the DOS profiles of YN. From the band structure plot it can be seen that lowest energy bands due to 2s states of N lies in the core region at -12.9 eV from E_F at the symmetry point Γ. So there is no contribution to the bonding states of YN. A direct transition had been observed at E_F at X point with a gap of 0.4 eV. The maximum of the valence bands lies at Γ and the minimum of conduction bands lies at X. There is an indirect band gap of 0.15 eV. It can therefore be stated that YN in NaCl phase behaves as a semi-conductor with an indirect band gap of 0.15 eV along (X→Γ).

Fig.4 shows the total DOS for YN, Y and N in ZB phase. The DOS features for YN show close similarity as observed in NaCl phase. From this DOS features we see that the N-p states hybridize strongly with the Y-4d states. Three main regions can be observed in the total DOS of YN : one below −10.8 eV and mainly due to nitrogen 2s electrons, another between −2.6 eV and the Fermi level due to N-2p electrons with a small contribution from Y-4d electrons, and the last one in the empty states region from 2.2 eV – 6.8 eV with high contribution from Y-4d electrons and some from N-2p electrons. Fig. 5 shows the partial DOS for Y-total and Y-d states. From these results it is seen that Y-d state electrons contribute to the bonding states of YN. It can therefore be predicted that the energy region above E_F is dominated by Y-4d state electrons and below E_F is dominated by N-2p state electrons [Fig. 4]. Therefore, the bonding of this material has a covalent-like character as seen by the hybridization of N and Y states, but there is also an ionic component with a charge transfer from the Y atom to the more electronegative nitrogen atom.

The calculated band structures along symmetry directions W→K are shown in Figure 6. It is seen that energy bands transitions is an indirect type with band gap of 2.15 along (Γ→X), and also a small direct transition occurring at the symmetry point X. A large band-gap indicates the semiconductor behaviour of YN in ZB phase.

The band separations of different bands originating from N (2s,2p) and Y-4d states are shown in Figs. 3 and 6 for YN in NaCl and ZB phase. They exhibit different levels originated from atomic states Γ_1 (N-2s), Γ_{15}^{v} (N-2p + Y-4d), Γ_{12} (Y-4d), and Γ_{15}^{c} (N-2p + Y-4d), at the Γ. It is seen that the 4d atomic states of Y are split into the Γ_{12} and Γ_{15} representations at the Γ point. E_g^1 refers to the energy gap between the lower bands Γ_1 and Γ_{15}^{v}, E_g^2, between Γ_{15}^{v} and Γ_{12}, and E_g^3, between Γ_{12} and Γ_{15}^{c}. $E(\Gamma_{15}^{v}- \Gamma_1)$ refers to the energy difference between the Γ_{15}^{v} and Γ_1 levels at the Γ; $E(\Gamma_{12}- \Gamma_{15}^{v})$ and $E(\Gamma_{15}^{c}- \Gamma_{12})$ have analogous meanings. These energy gaps are direct and occur always at the Γ point of the Brillouin zone.

The eigenvalues and the energy gap for the symmetry point Γ from GGA calculation for YN in NaCl and ZB structures are listed in Table 2. All energies are in reference to the Fermi level. The top of the valence bands is at Γ and the bottom of the conduction bands is at X for NaCl structure. Similarly the top of the valence bands lies at X and the bottom of the conduction bands lies at Γ for ZB structure. The calculated minimum gap for the compound is 0.15 eV and 2.15 eV for NaCl and ZB phase respectively. Although there is no availability of experimental gap value for YN

in both phase, our results accords with the SX-LDA as given by Stampfl *et al.* [4] and Mancera *et al.* results [3].

Table 1: The lattice constants and the band gaps of YN in GGA calculations for NaCl and ZB phase.

	a_o (Å)		E_g (eV)	
	Obs	Expt	Obs	Oths.
NaCl	4.927	4.877[(a)]	0.15	0.4[(b)]
ZB	5.19	4.877	2.15	2.25[(c)]

*Compared values: (a) Ref. (10) (b) Ref. (4) (c) Ref. (3)

Table 2: YN eigenvalues and energy gap (in eV) for different energy bands at high symmetry points Γ in GGA calculations.

Energy bands at Γ	NaCl	ZB
Γ_1	-12.9	-12.0
Γ_{15}^{v}	0.0	-1.7
Γ_{12}	2.7	2.15
Γ_{15}^{c}	4.8	5.5
E_g^1	12.9	10.3
E_g^2	2.7	3.8
E_g^3	2.1	3.4

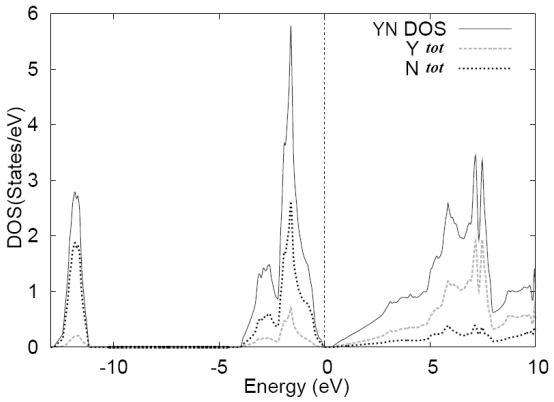

Figure 1: Plot of total density of states for YN, Y and N as a function of energy (eV) calculated by DFT – GGA in rocksalt structure.

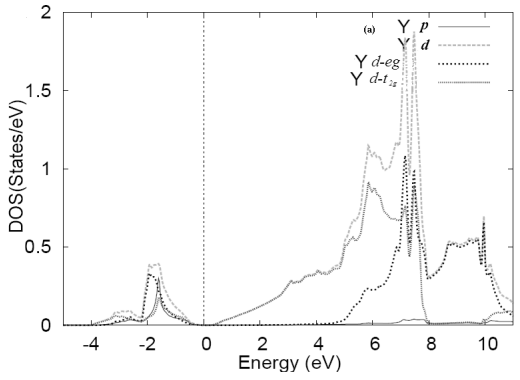

Figure 2: Plot of density of states for Y total, Y-d,eg, t2g as a function of energy (eV) calculated by DFT – GGA in rocksalt structure.

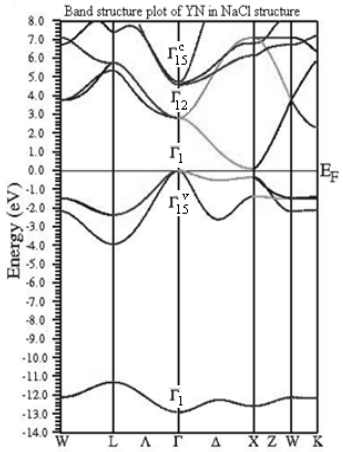

Figure 3: Electronic energy band structures plot of YN obtained by DFT – GGA calculations along principal symmetry directions in rock-salt structure.

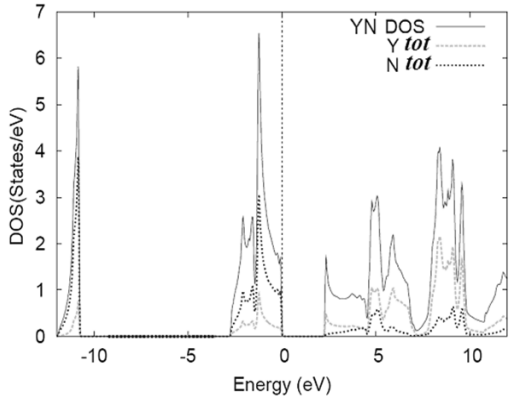

Figure 4: Plot of total density of states for YN, Y and N as a function of energy (eV) calculated by DFT – GGA in zincblende structure.

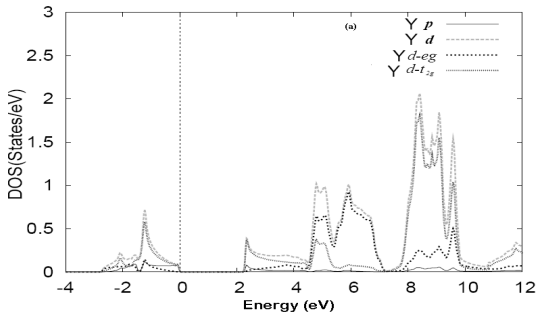

Figure 5: Plot of density of states for Y-p, Y-d, eg and t2g states as a function of energy (eV) calculated by DFT – GGA in zinc-blende structure.

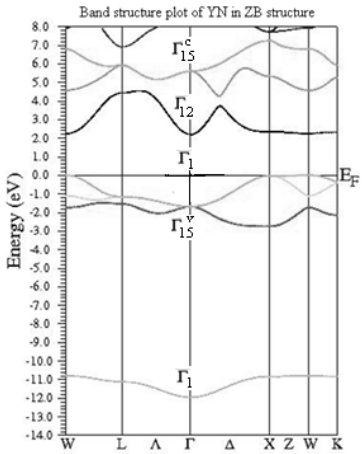

Figure 6: Electronic energy band structures plot of YN obtained by DFT – GGA calculations along principal symmetry directions in zinc-blende structure.

Conclusions

In our calculations we first calculate theoretical lattice constants by using the experimental data as shown in Table 1. We have shown the results of the DOS and band structure of YN in NaCl and ZB structure along with the energy eigenvalues and the energy gap of different bands due to N and Y state electrons [Table 2]. The results of band structures and DOS shows that YN is a semi-conductor with an indirect band gap of 0.15 eV in the NaCl phase and 2.15 eV in ZB phase.

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References

[1] Eck, B., Dronskowski, R., Takahashi, M., and Kikkawa, S., 1999, "Theoretical calculations on the structures, electronic and magnetic properties of binary 3d transition metal nitrides," J. Mat. Chem., 7(9), pp. 1527-1537.

[2] Soto, G. Moreno-Armenta, M. G. and Reyes-Serrato, A., 2008, "First principles study on the formation of yttrium nitride in cubic and hexagonal phases," Comp. Mat. Sc., 42(1), pp. 8-13.

[3] Luis Mancera, Jairo A. Rodriguguez, and Noboru Takeuchi, 2003, "First principles calculations of the ground state properties and structural phase transformation in YN," J. Phys: Condens. Matter., 15 pp. 2625-2633.

[4] Stampfl, C., Mannstadt, W., Asahi, R., and Freeman, A.., 2001, "Surface properties of the refractory metal-nitride semiconductor ScN: Screened-exchange LDA-FLAPW investigations" J. Phys. Rev., B63(15) 5106-5109.

[5] Ghimire, M. P. and Thapa, R. K., 2008, "Calculation of dielectric functions and energy gaps in case of yttrium nitride" Proceedings of the First National Conference on emerging trends and recent advances in Electrical Engineering and Renewable Energy, Sikkim Manipal Institute of Technology, Sikkim, EIT004, pp. 26

[6] Blaha, P., Schwarz, K., Madsen, G. K. H., Kvasnicka, D., Luitz, J., 2008, "WIEN2k, An Augmented Plane Wave Plus Local Orbitals Program for Calculating Crystal Properties," (Vienna University of Technology, Vienna, Austria).

[7] Kohn, W. and Sham, L. J., 1965, "Self-Consistent Equations Including Exchange and Correlation Effects," Phys. Rev., A140, pp. 1133-1138.

[8] Perdew, J. P., Burke, S. and Ernzerhof, M., 1996,"Generalized Gradient Approximation Made Simple," Phys. Rev. Lett., 77, pp. 3865-3868.

[9] Kempter, P. Charles, Krikorian, N. H., and Joseph, C. McGuire, 1957, "The Crystal Structure of Yttrium Nitride," J. Phys. Chem., 61 (9), pp. 1237-1238.

[10] Murnaghan, F. D., 1944, "The compressibility of media under extreme pressures Proc. Natl. Acad. Sci.,USA, 30, pp. 244-247.