Theoretical Investigation of Properties of Semiconductors Materials Based Rare Earth

Asma KADRI
Department of engineering physics
University of Science and Technology of Oran -USTO- Mohamed Boudiaf
Oran, Algeria
asma.kadri@univ-usto.dz

Soumia BAHLOULI
Department of engineering physics
University of Science and Technology of Oran -USTO- Mohamed Boudiaf
Oran, Algeria
bsoumia56@yahoo.fr

Said HIADSI
Department of engineering physics
University of Science and Technology of Oran -USTO- Mohamed Boudiaf
Oran, Algeria

Mokhtar ELCHIKH
Department of engineering physics
University of Science and Technology of Oran -USTO- Mohamed Boudiaf
Oran, Algeria
m.elchikh@gmail.com

***Abstract*— In this work we present the structural, electronic, elastic and magnetic properties of semiconductors based rare earth nitrides ReN (Re=Sc, Y, Gd) in the three crystals cubic structures NaCl (B1), CsCl (B2), and ZB (B3), the properties have been determined by the first principle calculations based of the density function theory (DFT), using the WIEN2k simulation package. We have concluded that the rare earth nitrides ReN with (Re= Sc, Y, Gd) are semiconductors nature for the three compounds with direct bandgap 2.721eV for ScN, 3.044 eV for YN and 1.07eV for GdN compounds, at the normal conditions the rare earth nitrides are stable in the B1 structures, the results of magnetic properties showed that the two rare earth nitrides ScN and YN are nonmagnetic nature, in addition the GdN behave as ferromagnetic compound in rocksalt phase. The calculation of elastic constants proved that the compounds are mechanically stable. Our findings are in good agreement with the other experiments and theories results available.**

Keywords— The density function theory (DFT), WIEN2k, rare earth nitrides, ferromagnetic, semiconductors.

I. INTRODUCTION

Today, the world is broadly interested in studying the rare earth nitride materials because their important physical properties. The hardness of most rare earth nitrides are usually unstable at ambient conditions [1], therefore, we employed the theoretical calculation represented by the first principle technique for discover more properties about the rare earth nitrides. The goal of the present work is using the ab initio calculation to reveal more information and details of rare earth nitrides ReN with (Re=Sc, Y, Gd) properties.

II. THEORETICAL STUDY

These calculations have been performed using the full-potential (linearized) augmented plane wave (lapw+local orbital) [2,3] approach to the density functional theory [4] implemented in WIEN2k code [5], within the Generalized Gradient Approximation through Perdew-Burek-Eneerhof (GGA-PBE), which is used for treatment the electronic exchange-correlation energy function [6].

III. RESULTS AND DISCUSSIONS:

A. Structural properties:

The lattice constants, the bulk modulus B and its first derivative B' are calculated by minimizing the total energy of crystal at different values of the volume fitted to the Murnaghan equation state (EOS) [7], all these parameters are in the table 1.

The structural stability of the thre semiconductors compounds of rare earth nitride is analyzed among the three considered NaCl (B1), CsCl (B2), and ZB (B3) (figure 2.3.4) and it observed that B1 structure is the most stable for the three cubic structures at the ambient conditions.

Fig. 1. Unit cell of different cubic phases of rare earth nitrides ScN, YN and GdN compounds, the blue circle represent the Sc, Y or Gd atoms and red one represent the N atom.

At the ambient conditions it can be observed from the table and the figures that the rock salt phase is the most stable for the three semiconductors based rare earth nitrides as the total energy is minimum for B1 phase.

The lattice parameter a of ScN is computed as 4.5203 Å in B1 structure which is good agreement with the other theoretical and experimental results, 2.79 Å for the B2 structure which is 0.71% less than the theoretical result and 0.61 higher than the theoretical result in B3 structure with lattice parameter 4.91Å.

The present values of lattice parameter of YN compound in the B1 structure is about 0.71% higher than the experimental result, and 3.00Å, 5.8262Å for B2 and B3 respectively which are good agreement with other results.

The lattice parameter is calculated in rocksalt structure, Cesium chloride and Zinc Blend structures for the GdN compound and is in good accord with other results in the all cubic phases.

TABLE. 1. Calculated lattice parameter a (Å), equilibrium volume V (Å3), bulk modulus B (GPa), Shear modulus B'(GPa), total energy E (eV) of rare earth nitrides compounds Sc, YN and GdN.

		B1	B2	B3
ScN	***a* (Å)**	4.5203 4.50[8] (theo) 4.5018[9] (exp)	2.79 2.81[10] (theo)	4.91 4.88[10] (theo)
	***V* (Å^3)**	23.086	21.71	29.596
	***B* (Gpa)**	200.223	182.3277	148.467
	***B'* (Gpa)**	4.1232	3.9281	4.8297
	***E* (eV)**	-22289.1502	-22287.5170	-22288.9849
YN	***a* (Å)**	4.912 4.93[11] (theo) 4.877 [12] (exp)	3.00 3.01[11] (theo)	5.2862 5.28[11] (theo)
	***V* (Å^3)**	29.628	27	36.929
	***B* (Gpa)**	158.9976	147.0926	113.4592
	***B'* (Gpa)**	4.2336	4.4647	4.0139
	***E* (eV)**	-93623.3400	-93621.4560	-93622.8492
GdN	***a* (Å)**	4.99 4.98[13] (theo) 4.99[14] (exp)	3.0389 3.025[13] (theo)	5.3486 5.3[13] (theo)
	***V* (Å^3)**	31.062	28.063	38.252
	***B* (Gpa)**	148.703	141.0569	108.2775
	***B'* (Gpa)**	4.2372	6.6354	3.988
	***E* (eV)**	-308452.2825	-308450.6526	-308451.9328

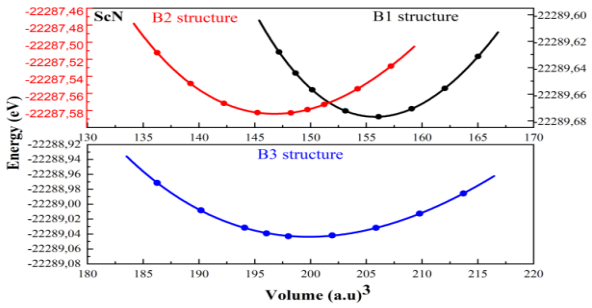


Fig. 2. Total energy (in eV) versus reduced volume for the three cubic phases of rare earth nitride ScN.

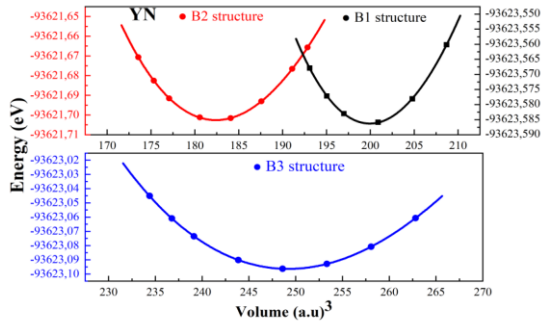


Fig. 3. Total energy (in eV) versus reduced volume for the three cubic phases of rare earth nitride YN.

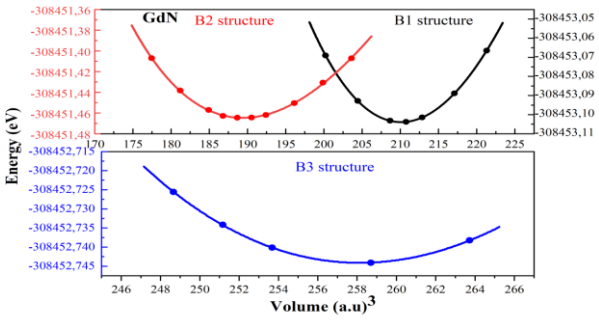


Fig. 4. Total energy (in eV) versus reduced volume for the three cubic phases of rare earth nitride GdN.

B. Magnetic properties:

The moment magnetic of the rare earth nitrides ReN (Re=Sc, Y and Gd) in the stable B1 structure is cheeked by studying the ferromagnetic (FM) and non-magnetic (NM) states by fitting the Munagan equation of state EOS of the total energy with relative volume.

The Figures 5 represent the total energy relative volume without and with spin polarization in B1 structure for rare earth nitrides compounds ReN (Re=Sc, Y, Gd). It observed that the compounds ScN, YN and GdN are stable in the nonmagnetic (NM) state at normal pressure, and for GdN, it can be seen that is more stable at the ferromagnetic (FM) state.

The table 2 represents the total and partial magnetic moment in Bohr magneton μ_B for the rare earth nitride GdN, the present work is good agreement with the other experimental and theatrical results.

TABLE. 1. Moment magnetic of rare earth nitride GdN in NaCl structure.

GdN		
μ_B (tot)	**μ_B (Gd)**	**μ_B (N)**
7.00	6.953	-0.0939

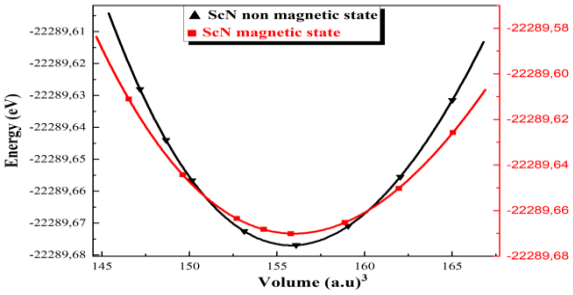


Fig. 5. Total energy versus relative volume in ferromagnetic (FM) and non-magnetic (NM)states of rare earth ScN.

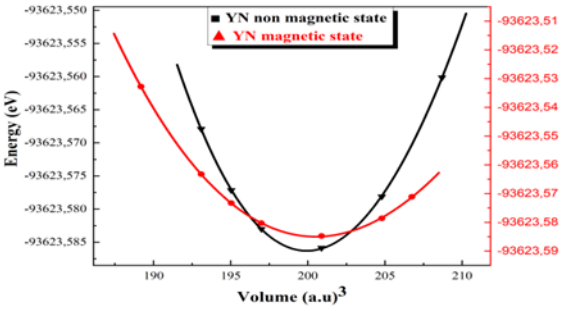


Fig. 6. Total energy versus relative volume in ferromagnetic (FM) and non-magnetic (NM)states of rare earth YN.

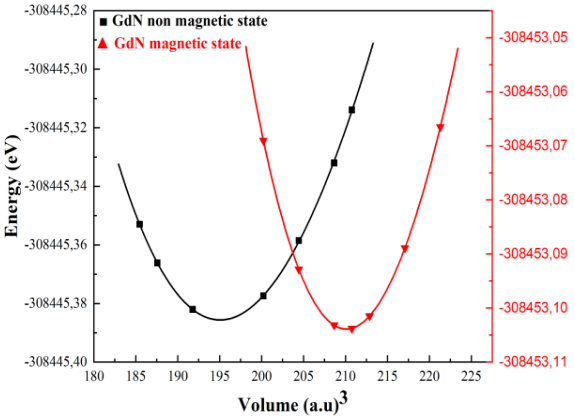


Fig. 7. Total energy versus relative volume in ferromagnetic (FM) and non-magnetic (NM)states of rare earth GdN.

C. *Electronic properties*

The electronic band structure of the rare earth nitride ReN (Re=Sc,Y, Gd) in NaCl structure are given in the figure 8,9,10 the Fermi level is located at zero energy.

It can be seen from the figure 5 (ScN compound) that band gap exists for the structures B1, there two bandgab direct 2.721 eV and 1.2 eV at Γ and X respectively, also there is a smaller indirect Γ-X bandgap with the Fermi level, about the YN compound we can observed the are two direct band gab 3.044 eV at Γ and 0.78 eV at X, also there is indirect Γ-X bandgap 0.23 eV.

In the GdN compound we can see there is no bandgap in the spin-up state and there is direct bandgap at X with 1.07 eV at X and indirect bandgap 1.09 ev at Γ-X.

From our work we can concluded that all the rare earth nitrides ReN with Re=Sc, Y, Gd are semiconductors nature, our results are close in agreement with the other results.

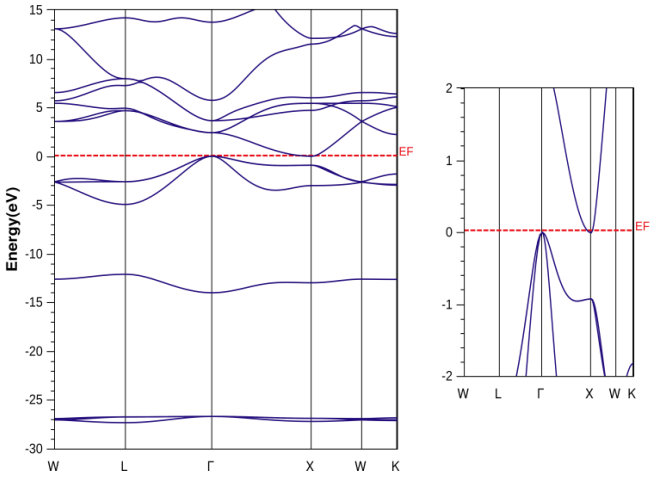


Fig. 8. Band structure of ScN in NaCl structure.

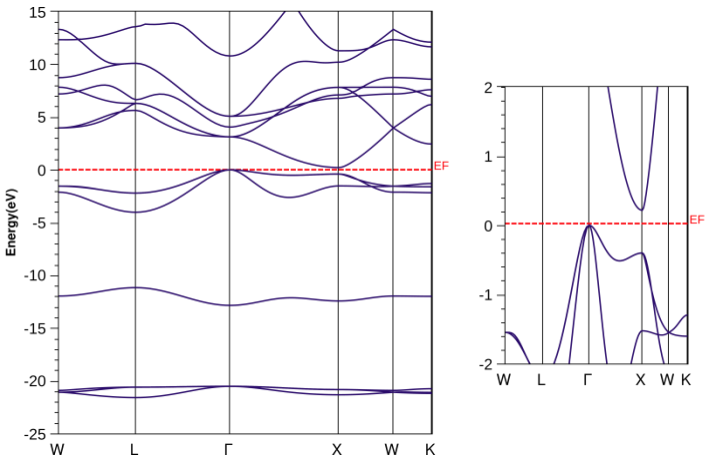
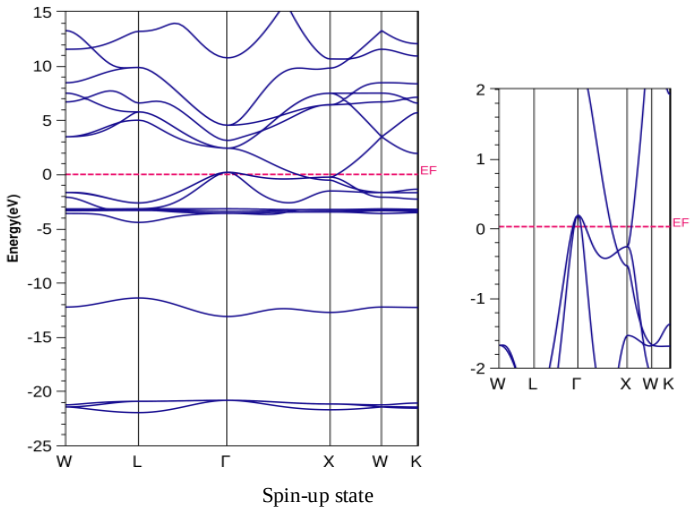
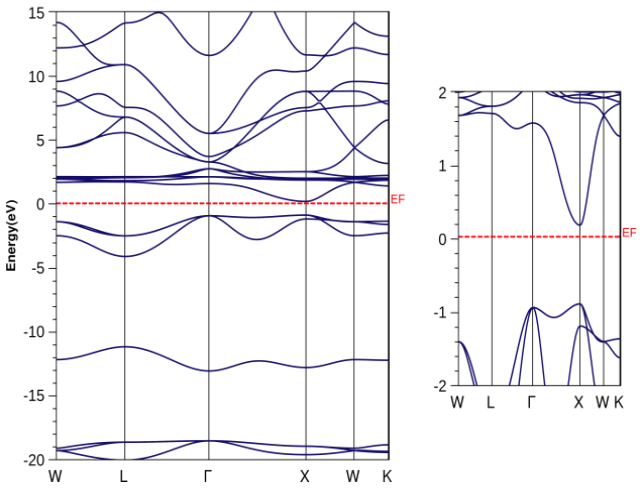


Fig. 9.Band structure of YN in NaCl structure.



Spin-up state



Spin-down state

Fig. 10. Band structure of GdN in NaCl structure for two states spin-up and spin-down.

D. Elastic properties:

The elastic constants of solids provide a link between the mechanical and dynamical behaviors of crystals, and give important information concerning the nature of the forces operating in solids. In particular, they provide information on the stability and stiffness of materials.

All cubic crystals have three independent elastic constants C_{11}, C_{12} and C_{44}, for the stability of cubic structure, the three elastic constants C_{11}, C_{12}, C_{44} should satisfy the Born-Huang [15] stability criteria:

$$C_{44} > 0, (C_{11}+2C_{11}) > 0, (C_{11}-C_{12}) > 0$$

The computed values of the elastic constants (C_{11}, C_{12}, C_{44}), bulk modulus B (GPa), Shear modulus B' (Gpa), Young's modulus E (GPa) and Poisson's ratio ν of the semiconductors based rare earth nitrides ReN (Re=Sc, Y, Gd) in the stable NaCl structure are listed in table 3.

It can be seen from the table 4 the elastic constants satisfy the Born-Huang criteria, we concluded that the rare earth nitrides ReN (Re=Sc, Y, Gd) are mechanically stable in normal pressure. The calculated elastic constants of rare earth nitrides ScN, YN and GdN are in close agreement with other theatrical and experimental results.

TABLE. 2. Calculated elastic constants C_{11}, C_{11}, C_{44} (GPa), bulk modulus B(GPa), Shear modulus B'(Gpa), Young's modulus E (GPa), Poisson's ratio ν, for rare earth nitrides ReN (Re=Sc, Y, Gd) in B1 structure

	ScN	**YN**	**GdN**
C_{11} (Gpa)	393.5978	327.0120	289.5688
C_{22} (Gpa)	104.0286	81.1886	78.5077
C_{44} (Gpa)	165.8863	125.0446	106.2940
B (Gpa)	200.551	163.129	148.861
B' (Gpa)	157.096	124.186	105.987
E (Gpa)	373.709	297.152	256.973
υ	0.189	0.196	0.212

.

E. Conclusion :

In conclusion, the structural, electronic, magnetic and elastic properties of rare earth nitride ReN (Re=Sc, Y, Gd) are analysed by the ab initio calculations using GGA-PBE approximation implemented in WIEN2K code with three cubic possible structures Rocksalt B1 , Caesium chlorides B2 and Zinc Blende B3.

ScN, YN and GdN compounds exhibit a semiconctor nature, the three rare earth nitrides ScN, YN and GdN are found that to be stable structurally and mechanically in NaCl (B1) phase at normal pressure. For the magnetic properties we was concluded the two compounds ScN and YN behave as non-magnetic compounds, on the contrary, the GdN compound is stable at ferromagnetic state.

The calculated results are in good agreement with the available results.

REFERENCES

[1] J. Yang, F. Gao, H. Wang, H. Gou, X., Z. Li, Materials Chemistry and Physics 119 499–504, 2010.

[2] E. Sjöstedt, L. Nordsrön, D. J. Singh, solid state communication 114, 15, 2000.

[3] G. K. H. Madsen, P. Blaha, K. Schwarz, E. Sjöstedt, L. Nordsrön, Phys. Rev B 64, 195134, 2001.

[4] W. Kohn, L. J. Sham, Phys. Rev. 140, A1133, 1965.

[5] P. Blaha, K. Schwarz, G. K.H. Madsen, D. Kvasnicka, and J. Luitz, "WIEN2k, an augmented plane wave ++ local orbitals program for calculating crystal properties," Karlheinz Schwarz, Techn. Universität Wien, Austria, ISBN 3-9501031-1-2, 2001.

[6] J. P. Perdew, K. Burke, M. Ernezerhof, Phys. Rev. Lett. 77, 3865, 1996.

[7] F.D. Murnaghan, Proc. Natl, Acad. Sci. USA 3 , 5390, 1994.

[8] C. Stampfl, W. Mannstadr, R. Asahi, A. J. Freeman, phys Rev B, volume 63, 155106, 2001.

[9] W. Lengauer, Journal of dolid state chemistry 76,4151,1988.

[10] N. Takeuchi, Phys Rev B, volume 65, 045204, 2002.

[11] L. Mancera, J. A. Rodriguez, N. Takeuchi, Journal phys : condens. Matter 15,3265-2633, 2003.

[12] P. Villars, L. D. Calvert, Pearson's Handbook pf cristallographie Data for Intermettalic phases American society for metals park, OF, 1985.

[13] R. M. Shabara, S. Z. Yahia, S. H. Aly, Results in phys 1, 30-35, 2011.

[14] W. Klemm, G. Z. Winkelmann, Among. Allg. Chem. 288-87, 1956.

[15] M. Born, K. Huang, Dynamical theory of crystal lattices, Clarendon, Oxford, 1956.