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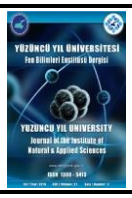

Araştırma Makalesi

DFT Investigations on Structural, Electronic and Vibrational Properties of LuN under High Pressure

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Abstract: In this study, the structural, electronic and lattice dynamics properties of cubic lutetium nitride (LuN) compound in the rocksalt structure have been investigated based on the Density Functional Theory with the Generalized Gradient Approximation. The structural properties, such as lattice constants, bulk modulus and bulk modulus derivative are in good agreement with literature. The phonon dispersion curves along high symmetry directions under various pressures were performed according to the Linear Response Approach of Density Functional Theory. Obtained positive phonon dispersion curves suggest that all studied materilas are stable. Moreover, the optical phonon band gap was found to be enhanced with increasing pressure. Accordingly, LuN is predicted to be a promising material for optoelectronic applications. This research is expected to shed light on many future works.

LuN'nin Yüksek Basınç Altında Yapısal, Elektronik ve Titreşimsel Özelliklerinin DFT ile İncelenmesi

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Öz: Bu çalışmada, kaya tuzu yapısındaki kübik Lütesyum Nitrit (LuN) bileşiğinin yapısal, elektronik ve örgü dinamiği özellikleri, Genelleştirilmiş Gradyan Yaklaşımı ile Yoğunluk Fonksiyoneli Teorisine dayalı olarak incelenmiştir. Örgü sabitleri, yığın modülü ve yığın modülü türevi gibi yapısal özellikler literatürle iyi bir uyum içindedir. Yüksek simetri doğrultuları boyunca, farklı basınçlar altındaki fonon dağılım eğrileri Yoğunluk Fonksiyoneli Teorisi'nin Doğrusal Tepki Yaklaşımı'na uygun olarak elde edilmiştir. Elde edilen pozitif fonon dağılım eğrileri, incelenen tüm materyallerin kararlı olduğunu göstermektedir. Ayrıca, optik fonon bant aralığının artan basınçla arttığı bulundu. Buna göre, LuN'nin optoelektronik uygulamalar için gelecek vaat eden bir malzeme olması öngörülmektedir. Bu araştırmanın gelecekteki birçok çalışmaya ışık tutması bekleniyor.

1. Introduction

The rare-earth (RE) monopnictides have interesting electronic and magnetic properties and have so much importance in the condensed matter physics (Duan et al., 2007; Pagare et. al., 2005). These materials show different characters from metallic to semimetallic or semiconducting, and there have been a lot of theoretical and experimental studies of binary rare earth semiconducting compounds (Re=La, Ce, Pr, Nd, Sm, Gd, Tb, Lu, …; ReN) (Granville, et al., 2006; Lambrecht, 2000; Kocak et al., 2010; Ciftci et al., 2012). The reason of this importance is due to their unfilled and highly delocalized 4f subshells. (Jakobsen et al., 2002; Rukmangad, et al., 2009). These materials have FCC-NaCl structure with space group Fm-3m (225) and each RE and N atoms are coordinated by six-N and six-RE atoms, respectively. These compounds have strong affinity because of large difference in electronegativity between N and RE. It is reported that 4f electrons of lanthanide atoms in mononitrides undergo delocalization at high pressures as these electrons are localized at ambient pressures (Natali, et al., 2013). For example, it has been declared that LaN and PrN undergo a transition from B1 to a tetragonal phase (B10) at ~23 GPa and ~40 GPa, respectively (Mukherjee, et al., 2013; Schneider, et al., 2012; Cynn et al., 2010). It is considered that these phase transitions are related to 4f electrons of lanthanide atoms (Sahoo et al., 2016). Nevertheless, the transport properties of these mononitrides are not understand, exactly. The electronic structure of RE nitrides in the NaCl phase structure (Larson, et al., 2007) and mechanical properties of the lanthanide nitrides in the rock salt structure (Yang, et al., 2010) are investigated theoretically by using density functional theory (DFT).

Lu is a RE metal used as an element for engineering electronic devices, for instance in the treatment of cancer in medicine, LED, bulbs. In some early studies, the crystal structure of RE pnictides have been predicted in detail (Escudero et al., 2017) and observed under a high pressure X-ray diffraction technique (Errandonea et al., 2000; Hayashi et al., 2000; Shirotani et al., 2003). Lutetium mononitride (LuN) is the last and heaviest member of lanthanide series and have completely filled 4f subshells. Therefore, it is one of the most important compound of the lanthanide series and has attracted the attention of many researchers due to its unusual properties. LuN crystallize in NaCl (B1) structure as other lanthanide series and have interesting properties and important applications, so there are a lot of investigations (Hayashi et al., 2000; Larson & Lambrecht, 2007; Yang et al., 2010; Painteret al., 2008; Yang et al., 2013). Especially, high-pressure investigations of Lutetium-pnictides (Lu-X; X=N, As, P,Bi, S) are important because of the little information about them. Furthermore these compounds are least studied among the rare earth pnictides.

By using first principles, Yanget al. (Yang et al., 2010) investigated hardness and elastic properties of lanthanide nitrides as well as the structural stability of LuN. LuN has first-order phase transition from NaCl-type structure (B1) to CsCl-type structure (B2) structure at 220 GPa pressure (Yang et al., 2013; Singh et al., 2015). Yadav et al. obtained that the electronic, mechanical and thermal properties by using the modified dielectric theory of solids. The values of energy gaps such as homopolar gaps (E_h), heteropolar gaps (E_c) and average energy gaps (E_g in eV) were evaluated with face-centered cubic (FCC) NaCl-type structure. (Yadavet al., 2016). The electronic and structural properties of LuN are investigated with a standard parameterization of the local density approximation (LDA) within DFT (Winiarski et al., 2019).

Oualdine et al. also studied LuN rare-earth nitride in rock salt structure to analyze the electronic, structural and elastic properties by using DFT full-potential linear muffin-tin orbital (FP-LMTO) (Oualdine et al., 2018). They show that band structure of LuN have semiconductor behaviour. The main purpose of this study is to reveal these unusual properties and investigate the effect of high pressures on the electronic properties of LuN. In the literature, there are also theoretical investigations based on Density Functional Theory (DFT) that have verified experimental results successfully.

2. Materials and Methods

The structural, electronic and dynamic properties of the LuN crystal in the ground state was performed with the Quantum-Espresso package (Giannozzi et al., 2009) based on DFT within the Generalized Gradient Approximation (GGA) (Perdew & Zunger, 1981). Perdew Burke Ernzerhof (PBE) parameterization scheme was used for exchange-correlation effects. LuN crystallizes in the B1 phase with space group Fm-3m. The calculations were generated for k-point meshes of 12x12x12 using the Monkhorst-Pack special k-points approach (Monkhorst & Pack, 1976) in the Brillouin zone. Both the plane wave cut-off energy, set at 150 Ry in all our calculations, and k-points gride size were optimized to determine total energy convergence. The total energy of the system was converged up to 10^{-8} Ry applying the self-consistent calculation. This convergence was considered as a sign of high accuracy calculations. The bulk modulus and its pressure derivative were obtained with Vinet equation of state (Vinet et al., 1986) using energy volume variation. Additionally, the phonon dispersion curve was taken into account with Fourier transform using dynamical matrices. The phonon dispersions were performed along symmetry directions at ambient and as well as at high pressures.

3. Results

3.1. Structural properties

Firstly, in order to investigate the ground state properties of LuN in NaCl crystal structure, we performed the structural optimization under the minimum condition of the total energy. Obtained ground state lattice parameter (a), bulk modulus (B_0), its pressure derivative (B_0') are tabulated and compared with experimental as well as other reported values in literature in Table 1. As shown, the results are in good agreement with experimental findings and verify the given theoretical works in literature.

Table 1. Lattice constant (a), bulk modulus (B_0) and its pressure derivative (B_0') for LuN.

	a (Å)	B_0 (GPa)	B_0'
This Work	4.84	162	4.23
Theory	4.87 (Larson &Lambrecht, 2007) 4.83 (Yang et al., 2010) 4.77 (Gupta & Bhat, 2013) 4.76 (Painter et al., 2008)	183 (Yang et al., 2010) 170 (Larson & Lambrecht, 2007; Chouhan et al., 2011) 164 (Gupta & Bhat, 2013)	3.81 (Gupta & Bhat, 2013) 4.12 (Chouhan et al., 2011)
Exp.	4.76 (Duan et al.,2007) 4.74 (Niwa et al., 2009)		

3.2. Electronic properties

The electronic structure of NaCl crystal structure with the equilibrium lattice parameter computed using GGA approach is presented in Figure1. The Fermi energy *(13.73* eV) was subtracted from all band energies and set at 0 eV. Rocksalt-LuN has $\Gamma \rightarrow X$ indirect gap of -0.162 eV and $X \rightarrow X$ direct band gap of 0.609 eV. This indicates that RS-LuN crystal is a semi-metal material. Our results are in good agreement with the data reported by Singh and Verma obtained via GGA calculation method (Singh and Verma, 2015). On the other hand the obtained band gap values are smaller than the experimental results (Larson & Lambrecht, 2007). Since GGA approach usually underestimates the band gap of semiconductors, these results are as expected.

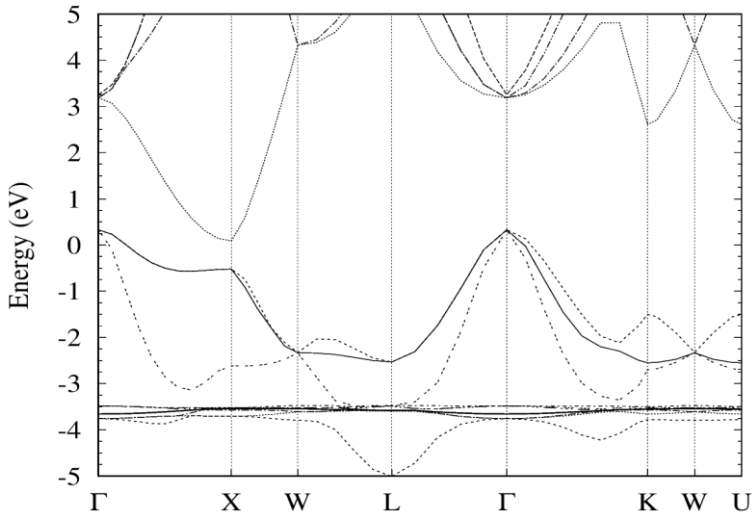

Figure 1. Energy band diagram of LuN crystal.

We also reported the effect of pressure on the band gap energy of LuN. The energy band gaps of LuN at different pressures are given in Table 2. The electronic band structures obtained for all pressures were similar with small changes. Therefore, only the band structure at zero pressure is presented. The variation of electronic band gap depending on the pressure is given in Figure 2. The direct band gap E^{X-X} as well as the indirect one $E^{\Gamma-X}$ are found to increase linearly with pressure. The band gap pressure coefficients are found as $\alpha = 22.76$meV /GPa and $\beta = 21.26$meV /GPa for indirect and direct band gap, respectively. To our knowledge there are not any experimental or calculated data for comparison of our results. It can easily be identified that the conduction band becomes closer to valence band with increasing pressure, thus the band gap narrows. Moreover, according to the band structure calculations, energy band gap disappears at around 10 GPa pressure values. It shows that LuN becomes semi-metalic at about 10 GPa.

Table 2. The energy band gaps of LuN at different pressures.

Presure (GPa)	E_{gap} (eV) $\Gamma \rightarrow X$	E_{gap} (eV) $X \rightarrow X$
-10	-0.0069	0.8288
-5	-0.1188	0.7166
0	-0.1621	0.6089
5	-0.0351	0.5045
7	-0.3948	0.4634
9	-0.4382	0.4228

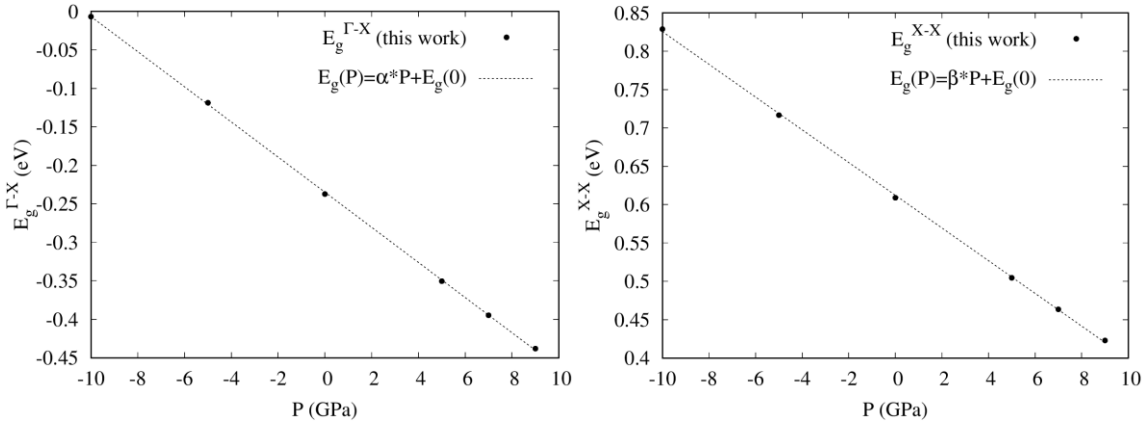

Figure 2. Pressure dependence of energy band gap of LuN. The dotted line gives the linear fit and the dots represent the calculated values.

3.3. Lattice dynamics properties

The phonon dispersion curve along the Brillouin zone and the phonon density of states of LuN are shown in Figure 3. The present compound contains two atoms in unit cell of NaCl type structure. Each atom has three degrees of freedom, thus this compound has six phonon branches, including three acoustic branches and three optical branches. The transverse acoustic (TA) and transverse optical (TO) phonon frequencies along the Γ- X and Γ- L high symmetries are double degenerated. Our results show that the degeneracy is partially resolved through the high-symmetry directions in crystal so that the phonon dispersion curves separates into transverse (TA and TO) and longitudinal (LA and LO) modes. The LO phonon branch at the Gamma point was obtained as 15.74THz. We also noticed an increase of that value in responce to increasing pressure.

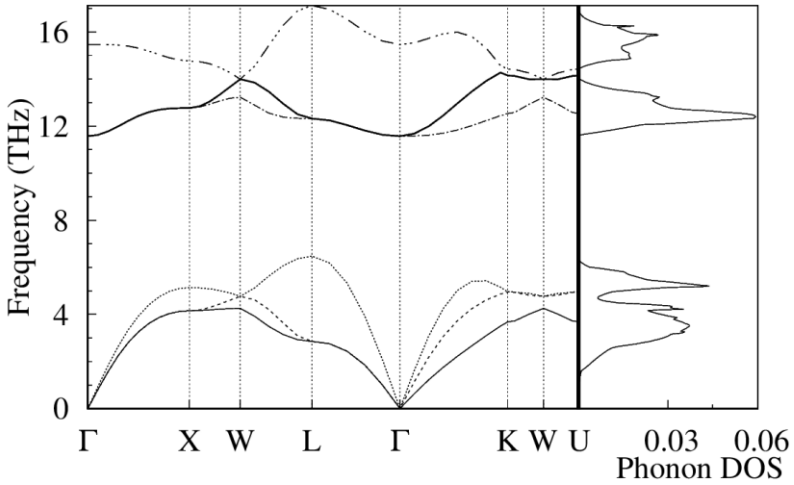

Figure 3. Calculated phonon dispersion curve and density of states (DOS) of LuN in rocksalt structure.

As shown in Figure 3, there is a wide gap (4.89THz) between the acoustic and optical modes owing to the high mass ratio of $m_{Lu}/m_N = 12.49$. The positive phonon frequencies of LuN in NaCl crystal structure have been found throughout the Brillouin zone, that clearly shows the dynamical stability of this compound.

In Table 3, we report the frequencies of TA, TO, LA and LO for Γ, X and L high symmetry points for LuN at zero and as well as various pressures. The acoustic phonons are compatible with the results reported by Mir et.al. (Mir et.al., 2016), while noticeable high optical phonons are obtained in this study. To best of our knowledge, there are no experimental data to compare our results. Since there are not enough theoretical studies especially on LuN's phonons under pressure, more comprehensive experimental and theoretical studies are needed.

Table 3: Transverse, longitudinal acoustic and optical frequencies at the high symmetry points (THz) under different pressures.

	Γ				X				X			
Pressure(GPa)	TO	LO	TA	LA	TO	LO	TA	LA	TO	LO	TA	LA
0	11.99	15.74	0.0	0.0	13.16	15.11	4.26	5.34	12.71	17.48	2.97	6.59
50	17.06	19.07	0.0	0.0	17.81	19.22	5.40	7.20	17.36	21.79	4.50	8.06
100	20.24	21.29	0.0	0.0	20.84	21.94	6.03	8.15	20.38	26.71	5.34	9.32
250	25.90	25.96	0.0	0.0	26.20	27.07	7.08	9.65	25.96	29.74	7.07	11.57
500	30.88	31.39	0.0	0.0	30.91	31.75	8.06	10.91	31.00	34.69	8.78	14.57

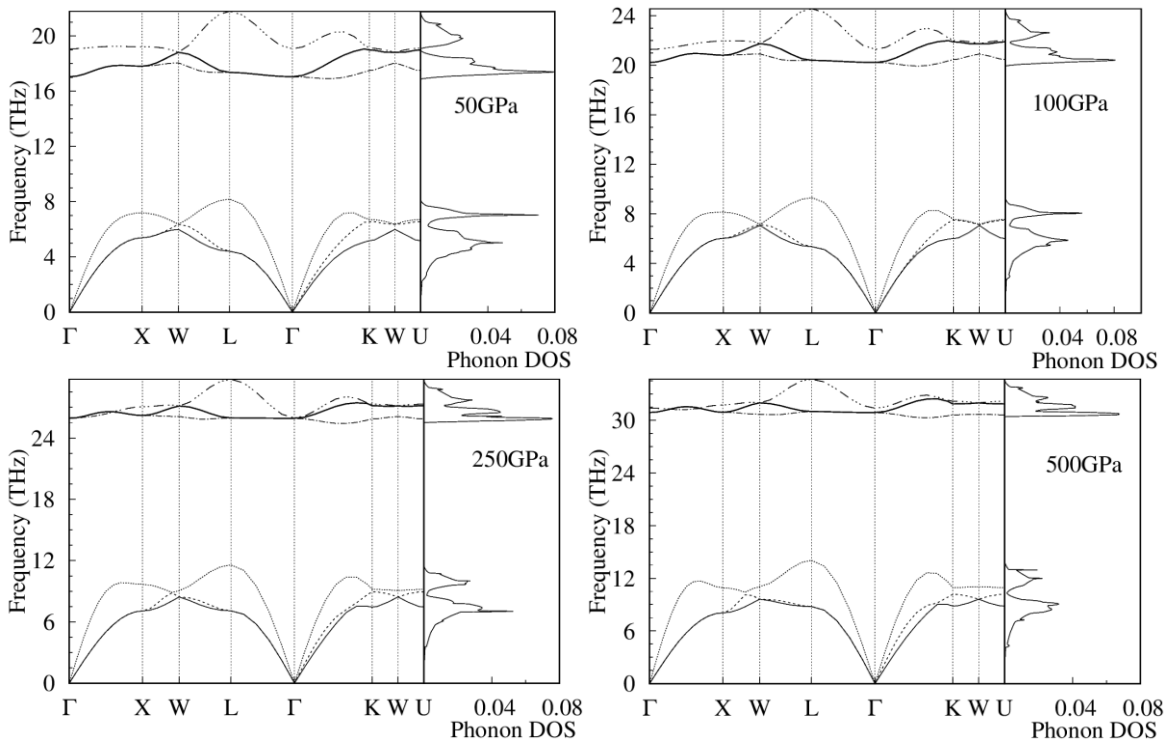

Figure 4. Calculated phonon dispersion curves and density of states of LuN in NaCl type structure under different pressures.

In Figure 4, phonon dispersion curves along several high symmetry directions and phonon density of states are illustrated for different pressure values. The frequencies in Brillouin Zone at high pressure values as well as at zero pressure value are positive. This results show that this crystal structure is dynamically stable. Moreover, the gap between the acoustic and optical branches increases with increasing pressure values.

4. Discussion and Conclusion

We reported the structural, electronic and dynamical properties of rocksalt LuN at ambient and high pressure using DFT within GGA. Band structure calculations under various pressures with optimized structural parameters indicate that energy band gap becomes narrower with increasing pressure. According to our results LuN compound in rocksalt structure becomes a metal at a pressure of around 10 GP. The phonon dispersion calculations of LuN performed up to a maximum pressure of 500 GPa show that this crystal structure is dynamically stable because of the positive values of frequencies throughout the Brillouin zone.

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