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ELECTRONIC AND MAGNETIC PROPERTIES OF BERKELIUM MONONITRIDE BKN: A FIRST-PRINCIPLES STUDY

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ABSTRACT

Spin polarized ab-initio calculations have been carried out to study the electronic and magnetic properties of BkN compound in B_1 crystal structure. The calculations have been performed by using both generalized gradient approximation (GGA) and local spin density approximation (LSDA). The calculated values of lattice constant (a_0) with PBE-GGA is found to be 4.931 Å which in good agreement with the experimental data (4.950Å). The bulk Modulus (B), first order derivative of bulk Modulus (B') and magnetic moment (μ_B) are also presented. The band structure and density of states are plotted which reveal the metallic nature for BkN compound. The energy band structure and electron density of states are presented.

Keywords: Ab- initio Calculation, Electronic properties, Band structure, Magnetic moment, density of states, spin polarised.

I. INTRODUCTION

In recent years, the actinide mono-pnictides attracted a strong attention and they were the subject of many experimental and theoretical works due to their electronic, magnetic, mechanical and vibrational properties [1]. Most of the actinide mono-pnictides crystallize in NaCl-type (B_1) structure. Most of these unusual features, however, have been correlated with the existence of unfilled f-electron shells of the lanthanide ions which are delocalized [2] and therefore, interact strongly with the lattice. So far as the structural properties are concerned, several pnictides of actinide group which crystallize in NaCl (B_1) type crystal structure have been investigated by using high-pressure X-ray diffraction technique [3]. The Berkelium Nitride with the NaCl crystal structure has recently attracted particular interest as a proper reference material for the understanding of various anomalous physical properties of other actinide mono-pnictides. The temperature-dependent elastic and ultrasonic properties in the temperature range of 100–500 K of Berkelium Mono-pnictides were performed by Singh et. al.[4]. Although, there is no systematic study of structural, electronic and magnetic properties of BkN are found in the literature. For better understanding the physics of this compound, we have initiated a step to highlight the above properties in the present study.

II. METHOD OF CALCULATION

First-principles study of the BkN compound was performed by employing full potential linearized augmented plane wave (FP-LAPW) method [5] based on density functional theory within the generalized gradient

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approximation (GGA) and local spin density approximation (LSDA) incorporated in the WIEN2k code [6]. The density functional theory is derived from the N- particle Schrodinger equation and useful for system of many electrons. The exchange correlation potential is treated with LSDA[7] and generalized gradient approximations in the scheme of Perdew, Burke and Ernzhof (PBE-GGA) [8] to investigate the structural, electronic and magnetic properties of BkN compound. The basis function has been expanded up to Rmt* K_{max} = 7.0, where R_{MT} is the smallest atomic radius in the unit cell and K_{max} gives the magnitude of the largest k vector in the plane wave expansion. The maximum value for partial waves inside the atomic sphere is l_{max} = 10 while the charge density is Fourier expanded up to G_{max} = 12. The self-consistent calculations are converged when the total energy of the system is stable within 10^{-4} Ry. A dense mesh of 1000 k points and the tetrahedral method have been employed for the Brillouin zone integration. The total energies are fitted to Birch equation of state [9] to obtain the ground state properties. The energy band structure and corresponding density of states are prominent quantities that determine the electronic structure of a system. The spin polarized calculation has been performed using LSDA approximation to understand the electronic behavior of BkN compound in terms of electronic band structure (BS) and density of states (DOS).

III. RESULT AND DISCUSSION

3.1 Structural Properties

In order to calculate the structural properties of Berkelium Nitride, the total energy is calculated as a function of reduced volume in B_1-type (NaCl) structure using full potential linearized augmented plane wave (FP-LAPW) method. The total energies are calculated as a function of volume and fitted to Birch equation of state to obtain the ground state properties and to obtain the pressure volume relation. The results are listed in table 1. BkN compound is founded to be stable in B_1- phase at ambient pressure. As shown in table 1, the calculated lattice constant for the compound is compared with the available experimental data [3]. The ground state properties, such as equilibrium lattice constant (a_0), bulk modulus (B) and its first derivative (B') for BkN have been calculated in their B_1-phase by LSDA and PBE-GGA mentioned.

Table 1 The calculated structural properties and density of states at the Fermi level $N(E_f)$ for BkN

lid	Work	Approximation	a_0 (Å)	B (GPa)	B'	$N(E_f)$ *States/eV*	
						Spin Up	Spin Down
BkN	Present	LSDA	4.802	190.02	4.56	0.1	2.33
		PBE-GGA	4.931	148.56	4.87	-	-
	Experimetal	XRD	4.950[a]	-	-	-	-

[a]Ref[3]

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IV.SPIN POLARIZED ELECTRONIC AND MAGNETIC PROPERTIES

Electronic behavior of BkN has been shown in terms of energy bands and total, partial density of states. The calculated band structures along the high symmetry directions R→Λ→Γ→Δ→X→Z→M→Σ→Γ in the Brillouin zone for spin up and spin down channel are shown in Figs. 1(a) and 1(b). Zero value of energy gap in both spin up and spin down band structures indicates the metallic character. The Fermi level, E_F is considered at the origin. In both the cases (spin up and spin down channels), the bands are crossing the Fermi level (E_F) from valence to conduction region and overlapping significantly at the Fermi level (E_F) (i.e., zero energy gap), indicating typical metallic behavior. Figure 2 shows the total density of states (TDOS) and figure 3(a) and 3(b) present the partial density of states (PDOS) plots for BkN, respectively. It is observed that there are peaks in the majority spin channel below the Fermi level at around -1.8 to -5.0 eV which is due to 'd' and 'f' like states of Bk and 'p' like state of N. The peak at around -4.0 eV is due to mainly Bk-f states. For minority spin channel, the 'f' like state of Bk is observed near the Fermi level at 1.0 eV.

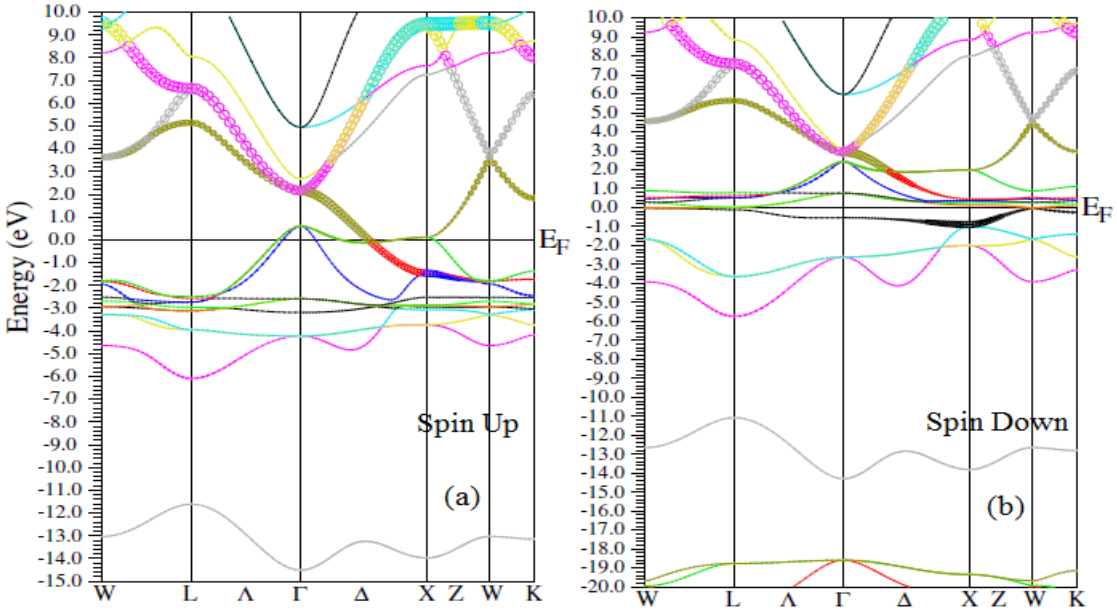

Figure 1 (a-b). Band structure of BkN in Spin Up and Spin Down Mode

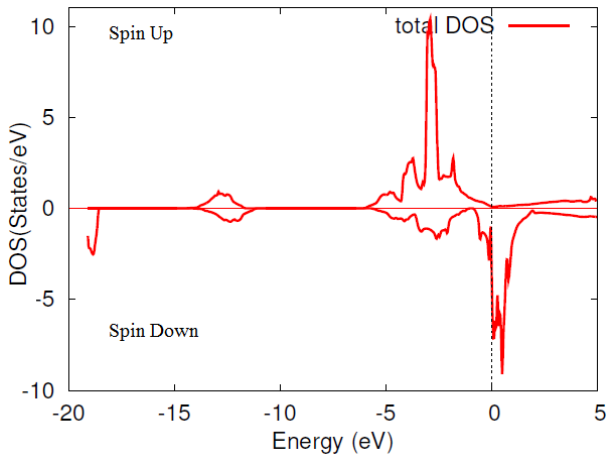

Figure. 2 Total Density of states of BkN in Spin up and Spin Down mode.

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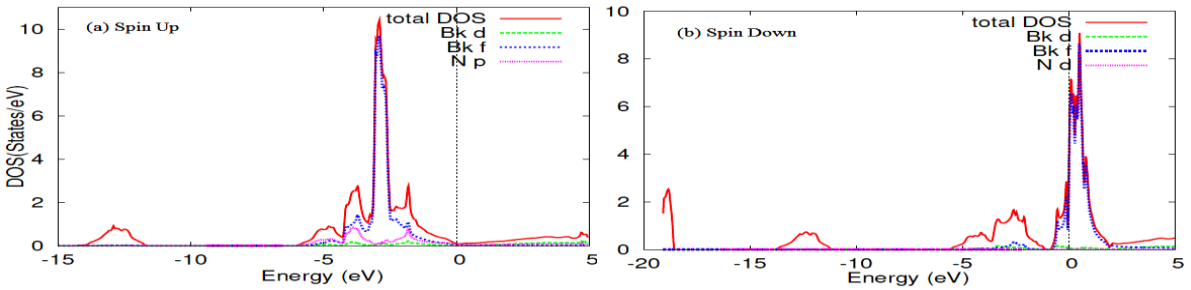

Figure. 3(a-b) Partial Density of states of BkN in Spin up and Spin Down mode.

In the present paper, we have studied spin polarized electronic band structure. Therefore, it is important to pay attention towards the magnetic behavior of Berkelium monopnicitide. Calculated magnetic moments on individual atoms and molecules are shown in Table 2. The total magnetic moment is found to be 5.9975 μ_B for BkN, which indicates that BkN is highly magnetic compound. The total magnetic moment is due to the contribution of the rare earth atom (Bk), Nitride (N) atoms and the interstitial region. Table2 shows that N atom and the interstitial region have negligible magnetic moments. Thus, it is concluded that total magnetic moment is dominated by the 4f-state electrons of the rare earth atom (Bk).

Table 2. The calculated Magnetic moment (μ_B) for BkN

Solid	Berkelium	Interstitial Region	Nitrogen	Total μ_B
BkN	5.80549	0.13267	0.05759	5.9975

V. CONCLUSION

An accurate method named full-potential linearized augmented plane-wave (FP-LAPW) using local spin density approximation and generalized gradient approximation (GGA) has been used to study the structural, spin polarized electronic and magnetic properties of Berkelium Nitride (BkN). The calculated lattice parameter for BkN is consistent with experimental/theoretical values. The spin polarized electronic calculation shows that studied compound is metallic in nature and shows the magnetic behavior which is mainly due to 4f-electrons of Bk.

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