Magnetic Properties of CeAs: LDA+U Studies

Mohamed. M. A. Ismaeil[1] * K. Ayuel[2,] and Siddig T. Kafi[2]

[1]Master student, Physics Department, Faculty of Science, Neelain University, Sudan.
[2]Department of Physics, Al-Baha University, P.O. Box (1998), Saudi Arabia
[3] Physics Department, Faculty of Science, Neelain University, Sudan.
mutassimm@yahoo.com

Abstract: The present study applied the ab inito method implemented in Quantum Espresso to derive the densities of states (DOS), projected densities of states (PDOS) and magnetic moments of cerium monopnictides CeAs. The DOS and PDOS were displayed and studied. This study rivals that cerium monopnictides CeAs is a semimetal complicated antiferromagnetic material. These findings are in accord with the previous studies. The derived magnetic moments were compared with experimental results, this compression shows that our results are in good agreement with experimental ones.
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1. Introduction

For many decades cerium monopnictides CeX (X = N, P, As, Sb, Bi) shows a number of interesting unusual behaviors and they are subjects to many studies. The usual properties were first pointed out in the sixties where the magnetic susceptibilities versus temperature and magnetic moments versus applied fields of CeP, and CeAs and CeSb were measured [1] and since then several studies were done till now.

The member of the group CeAs is resembling features of these monnopnicdes. Anomaly related to temperature dependent of night shift was reported. Anomaly in the NMR shifts of CeAs and the evidence for a conduction-electron transition from pressure dependence of NMR in CeP and CeAs were also reported [2,3].

Low temperature measurements of the specific heat, the thermal expansion, the electric resistivity and the magnetization of CeAs and CeP were studied [4].

Neutron inelastic scattering experiments had been performed on cerium monopnictides CeX (X = N, P, As, Sb, Bi) [5]. The unusual magnetic properties of these compounds were reviewed [6].

High field magnetization of CeAs is investigated and successive multistep magnetization associated with Landu level crossing was found [7] also novel magnetic neutron diffraction under a magnetic field of CeAs was reported [8].

Pressure effects and mechanical properties on crystal electric excitations in CeAs and CeP, CeSb and CeBi had been performed [9]- [13].

The origin of the unusual properties was explored using neutrons, X-rays scattering, synchrotron X-rays, and polarized neutron scattering [14]-[19].

Electronic Structures in cerium monopnictides were performed using the linear muffin-tin orbital LMTO method [20], the self-interaction-corrected local-spin-density approximation an *initio* electronic structure calculation [21] and magnetic and structural phase transitions in CeAs under high pressure where studied [22].

Although the previous survey shows that electronic and magnetic structure calculations in cerium monopnictides had been studied experimentally and simulated theoretically using different methods, yet determination of some electronic structures and magnetic properties of these cerium using different simulation package are not yet exhausted. Nor there exist to our knowledge any detailed studies that invoves the electronic structure and magnetic properties of cerium monopnictides CeAs. The present study is an attempt to bridge this gap and aims at determination of electronic structure and magnetic properties of CeAs using quantum espresso computer package that employs ultra-soft pseudo-potential method and to get magnetic moments of these compound.

The layout of the rest of this paper will be as follows:

Methodology is presented in Section 2. Results and discussion will be given in Section 3. Section 4 will present conclusion and recommendations.

2. Material and Methods

The electronic configuration for neutral Ce and As, atomic mass, atomic number and are presented in Table 1. This compounds exhibit the NaCl crystal structure with space group $Fm3m$ (O_h^5) which is a faced-centered cube. This structure can be considered

as s two FCC sub-lattices Ce at atomic positions{ (0,0,0)} and As at one half of the body diagonal of the unit cell{ (1/2,1/2, 1/2)}. Figure 1 displays this structure. The lattice parameter of this compound is a=6.0809A^{o}.

Table 1: The electronic configuration for neutral rare-earth Ce, and As, atomic mass, atomic number and electronic configuration.

Atom	atomic mass	atomic number	electronic configuration
As	74.92	33	[Ar]3d^{10} 4s^{2} 4p^{3}
Ce	58	140.116	{Xe}4f^{1}5d^{1}

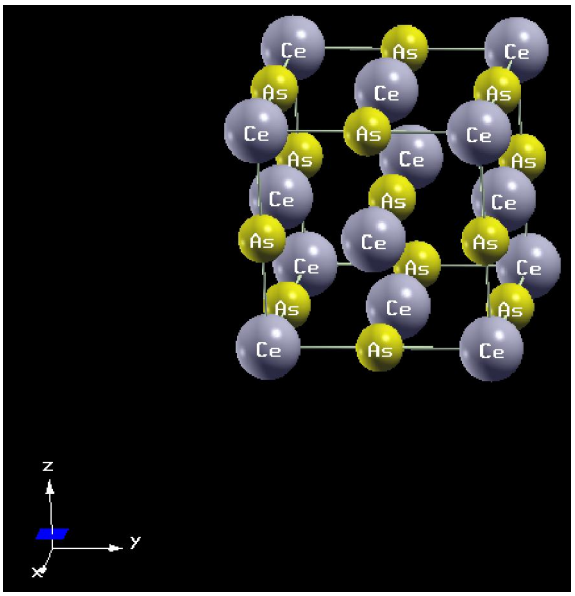


Figure 1: Crystal structure of CeAs

Quantum-Espresso computer package were used to simulate the electronic structure and magnetic properties of the monopnictide CeAs. Quantum Espresso [23] is a sophisticated collection of tools package implementing electronic structure calculation via density functional theory (DFT) using plane wave and pseudo potentials. Plane Wave Self Consistent Field (PWSCF) program uses both norm-conserving pseudo potentials (no-pp) and Ultra soft pseudo potentials (us-pp) within density functional theory (DFT). To get our results the following tasks have been performed: Self consistent field calculations were performed using *pw.x* code followed by a non-self-consistent field calculation using the same code. Then the density of states was calculated using *dos.x code* followed by the calculation of projected DOS using *projwfc.x code*. The obtained DOS and PDOS were plotted using GNUPLOT graphics package.

3. Results and Discussion

A NaCl unit cell that is depicted in Figure 1 for CeAs with the given lattice parameter were employed in a self -consistent calculation using pw.x program in Quantum Espresso package. The total energy, Fermi energy, Harris-Foulkes estimate energy and estimated self-consistent calculation (scf) accuracy for the compounds CeAs are listed in Table 2. It is evident from this table that the calculated energy converges within the estimated accuracy.

Table 2: Fermi, total energy, Harris Foukles estimate energy and estimated scf accuracy.

Compound	Fermi Energy eV	Total Energy Ry	Harris-Foukles Estimate Energy Ry	Estimated scf accuracy Ry
CeAs	9.4428	-481.83162016	-481.83160178	0.00000085

Magnetic moments calculated from the present work with their experimental values taken from references [24] are presented in Table 3. It is clear from this, which our results are in good agreement with experimental ones.

Table 3: Magnetic moments calculated from the present work (Present) with its experimental values (Exp).

Compound	**Magnetic moments Present in μ_B**	**Magnetic moments from experimental data in μ_B**	**Division from Exp. in μ_B**
CeAs	**0.86**	**0.85 (Ref 37)**	**0.01**

The derived density of state (DOS) of this compound (CeAs) is displayed in Figure 2. In this Figure the Fermi energy (=9.4428) is set to zero. The analysis and discussion related to this density of state is presented in the following paragraph.

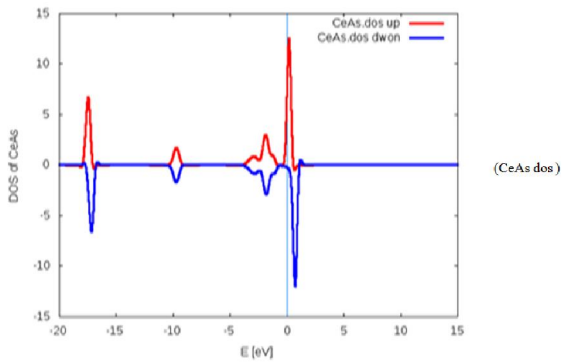


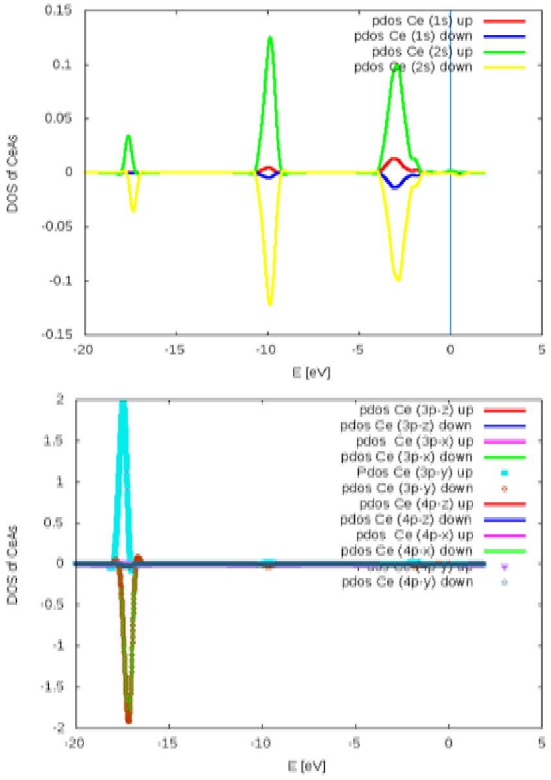
Figure 2: The density of states (DOS) of CeAs.

This figure shows that the DOS of CeAs is lying in four different zones. The first zone lays between $(-7.5472 \pm 0.1\ eV)$ $(-8.5672 \pm 0.1\ eV)$ and . The second zone is placed in the region $(-8.6572 \pm 0.1\ eV)$ $(-7.6772 \pm 0.1\ eV)$. and The third zone is situated in the range $(6.8739 \pm 0.1\ eV$ $(9.8139 \pm 0.1\ eV)$ and the $(10.3528 \pm 0.1\ eV$ fourth zone extended from to $(11.2428 \pm 0.1\ eV)$.

To analysis the contributions of the atomic states of the atoms/ions Ce, and As with orbital angular momentum $(l = 0, 1, 2, and\ 3)$ -those are usually denoted by the symbols s, p, d and f - to the DOS of Figure 2, the PDOS of the (1s, 2s), (3p,4p), 5d, 6d, and (7f, 8f) are displayed in Figures 3 (a)-(d) respectively. Also the PDOS of 1s, 3d and 4f of the As atom/ion are presented in Figures 3 (f)-(h). These figures rival that the contributions of 1s and 2s of atom Ce are only present in the first, second, and the third zones and it diminished in the fourth zone. The 3p and 4p states of Ce only contribute to the first zone. The 5d state of Ce atom contributes significantly in zones 2, 3 and 4. The 6d state of Ce is present in all zones but with minor contribution in the first zone. The Ce 7f and 8f (that are presented by Y_0-Y_6) are contributing only in fourth zone.

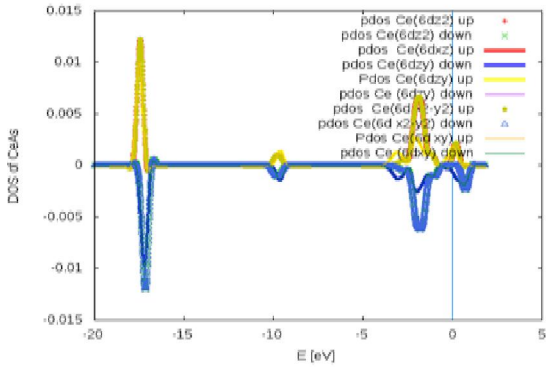
The accumulation of 1s state of As ion according to Figure 3 (f) is mainly in the second zone. The piling of 2p state of As ion is displayed in Figure 3 (g). The pilling is in……(h), the roundup of 3d state in As ion is dominated by the accumulations of it PDOS in the first zone, second, third zone, at Fermi level and in the conduction band. The concentration of 4f states in As ion are similar to those of 3d states as in Figure 3 (i). They are within the first, second zones, at Fermi level and in the conduction band. The conduction band is occupied by both spin up and down PDOS, but, the Fermi energy consists only of spin up.

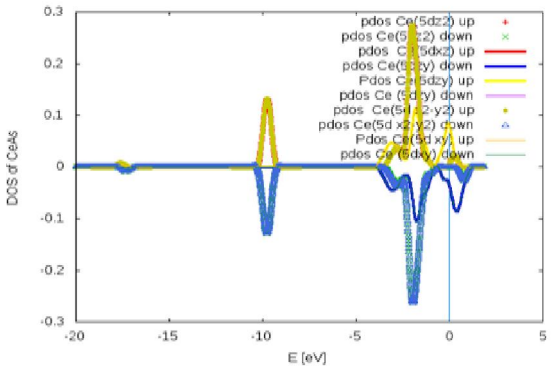
It is apparent from Figures 2 and 3 that the densities and projected densities of spin up of the conduction and the valance bands of this material are connected at the Fermi energy. So there is no gap between conduction and the valance bands of the spin up densities of these materials and they conduct electrons through the spin up channel. There is a relatively small gap between conduction and the valance bands of spin down densities, so the electrons are not conducting through the spin down channel. Since this gap is small. This spin channel forms a semi-conductor manner. Any material that behaves in this way is known as semimetals. So our studies characterized CeAs compound as semimetal. This funding is in full agreement with those of previous studies [25].

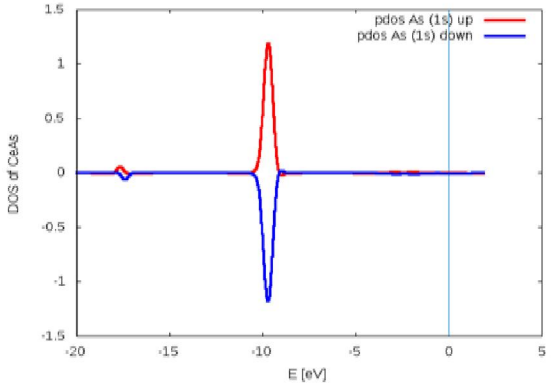


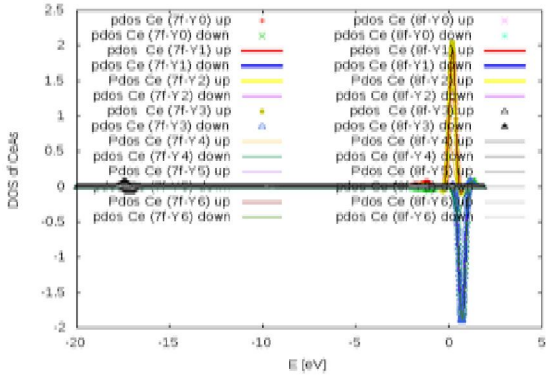
It was stipulated in previous studies [26] that the material CeAs is antiferromagnetic, but the behavior of the spin up and down in the DOS of Figure 2 is complicated as conformed by Figure 3 and it cannot be explain by simple antiferromagnetic model in which their patterns to be congruent. The spin up and down densities of this material is not congruent but shifted

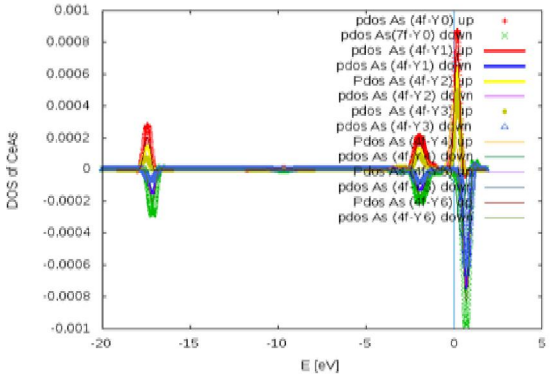
apart. So our result shows that CeAs is un-usual antiferromagnetic material that was shown in [19].

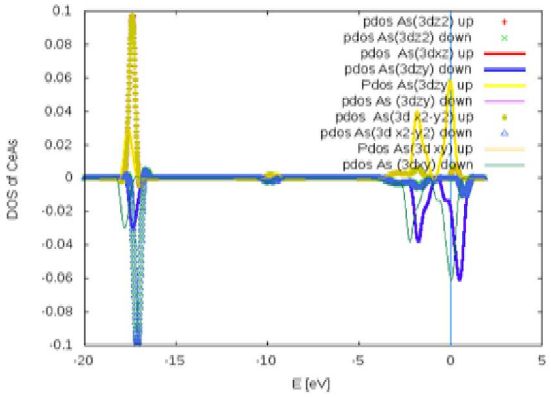












4. Conclusion and Recommendation

The electronic structure and magnetic properties of CeAs compound were studied using Quantum espresso ab initio package based on Density Functional Theory. Quantum espresso is capable of estimating the Densities and projected densities of states. It can also estimate the magnetic moment of materials.

Our study based on Quantum espresso enable the estimation of the magnetic moments of this material presented in Table 3. It is clear from this Table that our results are in good agreement with the experimental of [24] one. This study also, confirms that CeAs is a semimetal complicated antiferromagnetic material.

We recommend more investigations to be conducted in the further to clarify the nature of the behavior of spin up and down of CeAs.

Corresponding author
Mohamed A. Ismaeil
Physics Department, Faculty of Science, Al Neelain University, Sudan
mutassimm@yahoo.com

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