Advances in Physics Theories and Applications
ISSN 2224-719X (Paper) ISSN 2225-0638 (Online)
Vol.26, 2013
www.iiste.org

Half-metallicity in EuN: A First-Principles Calculation

Mona A. Huleil (Corresponding author)
Physics Department, Faculty of Science, Helwan University, Egypt
Tel:+2 01145380780 E-mail: soliman_offic@yahoo.com

Samy H. Aly
Physics Department, Faculty of Science, Damietta University, Egypt

Sherif Z. Yehia; M. Fadly
Physics Department, Faculty of Science, Helwan University, Egypt

Abstract

We report on the electronic and magnetic properties of the rock salt (RS) and cesium chloride (CsCl) phases of EuN. Our calculation was performed within the framework of the density functional theory (DFT), as implemented in the Wien2k package. We have used the generalized gradient approximation (GGA) for the exchange correlation potential and, in certain, cases the Local Spin Density (LSDA) approximation, with the Hubbard interaction taken into account. Our calculation demonstrates the presence of an energy gap in both of the RS and CsCl structures when only spin-polarized calculation is used. However, taking the Hubbard potential into consideration, via the LSDA+U scheme, led to the disappearance of the energy gap, and hence to the absence of the half-metallic behavior in this system.

Keywords: rare-earth nitrides; magnetic moment; DFT; DOS; half metallicity; spin density.

1. Introduction

Europium nitride is one of the rare earth nitride (RN) family. This class of materials displays a strong coupling between the electronic and magnetic properties of its member compounds. An accurate description of their electronic structure is a challenging problem because of their partially filled 4f shells, ranging from 0 to 14 through the series from La to Lu. RNs may form half-metallic ferromagnets as shown in the literature [1-2]. The half metallic (HM) behavior of these compounds is discussed by Duan et al [1-3]. The ambient structure of EuN is NaCl structure [4]. The electronic band structure has been calculated using the self- consistent TB-LMTO method [5-6] within the local density approximation (LDA) [7]. Von Barth and Hedin [8] parameterization scheme has been used for the exchange-correlation potential. The phase stability of its electronic structure and total energies were calculated at different cell volumes [9]. The pressure behavior of these compounds is important in understanding the systematic of the lanthanide and actinide mononitrides.The structural properties of this half metallic ferromagnet have been discussed at ambient and high pressure for NaCl and CsCl phases [9]. It has been found that the phase transition from NaCl to CsCl phase occurs at around 14.6 GPa. The two phases showed half metallicity with total magnetic moment of 6 μB. The band gap is 1.414 eV in the NaCl phase [9]. LSDA+U approach using a full potential Linearized muffin-tin orbital (FP-LMTO) program [10] with the exchange-correlation parametrization of Von Barth and Hedin [8] has been used in calculating the electronic structure and searching for half metallicity in the rock salt structure. In EuN a complicated hybridization occurs between an f level pinned at E_f and the nitrogen N 2p states, leading to a metallic band structure [11]. In this work, we present first-principles calculation of the magnetic and electronic properties of the NaCl and CsCl structures of EuN compound. In particular we report on calculation of the density of states (DOS), band structures, energy gap, charge and spin density maps and magnetic moment of the above mentioned structures. One important motive of this work is to investigate the interactions that may lead to the presence / absence of the half metallic property in this system.

2. Method of calculation

Our calculations are performed in the framework of the density functional theory using FLAPW [12] method and the tetrahedron Brillouin-Zone integration methods [13], as implemented in the Wien2k package [14]. The exchange and correlation effects are treated using the generalized gradient approximation (GGA) given by Perdew et al [15]. We consider in the present work both of the NaCl and CsCl structures of EuN. The NaCl

structure has the space group symmetry Fm3m (#225). The Eu atom is positioned at (0, 0, 0) and the nitrogen atom at (1/2, 1/2, 1/2). The space group of CsCl structure is Im3m (#221) and the atomic positions are (0, 0, 0) for Eu atom and (1/2, 1/2, 1/2) for N atom. The experimental lattice constant, of NaCl structure is 5 A0 [11] and that of CsCl, using energy minimization, is 2.99 A0 [9]. The self consistent band energy calculations are performed with 1000 k points in the irreducible part of the Brillouin-Zone. The potential cutoff extends up to Gmax=14. These systems with strongly correlated f states have been recently treated by several theoretical and experimental approaches [1]. In our work, all calculations are performed firstly within the bare spin polarized scheme. The spin orbit interaction and subsequently the LSDA+U approach were taken into account [1, 16, and 17]. The parameters U and J are equal to 0.58 and 0.07 Ry in the NaCl phase and 0.39 and 0.05 Ry in the CsCl structure respectively.

3. Results and Discussion

The minority-spin density of states, for CsCl structure, is shown in Fig.1. The schemes used in the calculation are the spin-polarized and the LSDA+U schemes (Fig.1a and 1b respectively). In contrast to the DOS structure of Fig. [1.a], the DOS of Fig. [1.b] shows non-vanishing counts at the Fermi level. This demonstrate that including the Hubbard interaction leads to introducing additional states at Ef, and consequently to the disappearance of the half-metallic property. We have performed the DOS calculation for the RS structure using the same schemes of Figs.1a and 1.b. These figures lead us to the same conclusion we have drawn for the CsCl structure, except that the LSDA+U approximation in this case does not eliminate the gap but shifts the Fermi energy to the lower energy side of the gap (Fig.2b). The energy gaps for these two structures are shown in table 1 together with the partial and total magnetic moments. Our calculation of the energy band structure was performed along a certain path in the Brillouin zone, using the spin-polarized scheme and the LSDA+U scheme (Figs.3.a and b respectively). The main features of Figs.3a and b are consistent with those of Figs. 2a and b and therefore support our conclusion concerning the metallic nature of the RS structure when the Hubbard interaction is considered. To understand the electronic structure more, the electron and spin density maps are constructed in the (110) plane in the RS phase. Figs. [4.a], [4.b] and Figs. [5.a], [5.b] show the charge and spin densities by using the pure spin polarized scheme (left panels of these figures) and by including the Hubbard potential into account (right panel). This plane contains six Eu atoms and three N atoms in the electron map. N atoms show no contribution to the spin density map. Only the Eu atoms are largely responsible for the total magnetic moment, in agreement with the calculated magnetic moment [table.1]. Including the Hubbard interaction in our calculation, led to an increase in the sphericity of both of the Eu and N atoms. In the CsCl structure, Figs. [6.a]: (left panel) and [6.b]: (right panel) show the electron density and spin density contours respectively for the (110) plane by using the spin polarized scheme. The electron map contains 4 Eu atoms and 1 N atom. The absence of the N contours in the spin density map indicates its small magnetic moment. The Hubbard potential seems to increases the sphericity of Eu atoms because of the spin-orbit interaction on these non-s state atoms (Figs.7a,b).

4. Conclusions

1- Half metallicity is predicted in both of the two structures, RS and CsCl only using the pure spin polarized calculation.

2- With taking LSDA+U into account, metallic behavior is predicted in both of two phases.

3- The very- near- to integer magnetic moments with the presence of a band gap confirm the half-metallic nature of these two structures, provided that only spin-polarized calculations are used.

4- LSDA+U including spin orbit interaction increases the sphericity of Eu atoms in the charge densities. Only the Eu atoms are largely responsible for the total magnetic moment. The absence of the N contours in the spin density map indicates its small magnetic moment.

References

[1] C. G. Duan, R.F. Sabirianov, W.N. Mei, P.A. Dowben, S. S. Jaswal and E. Y. Tsymbal, J. Phys. Condens. Matter 19, 315220 (2007).

[2] Reham M. Shabara, Sherif Z. Yehia and Samy H. Aly, Results in Physics, vol.1, iss.1, p. 30-35 (2011).

[3] Premlata Pandit, Vipul Srivastava, M. Rajagopalan, P. Sankar Sanyal, Physica B, vol. 403, p. 4333-4337 (2008).

[4] F. Hullinger, Hand book on the Physics and Chemistry of the Rare Earths Edited by K. A.Gschneidner and L. Eyring (North Holland, Amsterdam), Elsevier, vol. 4, p.153 (1979).

[5] O. K. Andersen, Phys. Rev. B 12, 3060 (1975).

[6] O. K. Andersen and O. Jepsen, Phys. Rev. Lett. 53, 2571 (1984).

[7] W. Kohn and L. Sham, J. Phys. Rev. A 140, 1133 (1965).

[8] U. Von Barth and L. Hedin, J. Phys. C 5, 1629 (1972).

[9] Gitanjali Pagare, Vipul Srivastava, Pooja Soni, Sankar p. Sanyal and Rajagopalan, Journal of Phys.: Conference Series 215, 012113 (2010).

[10] M. Methfessel, M. van Schilfgaarde, and R.A. Casali, in Electronic Structure and Physical Properties of Solids, The Uses of the LMTO Method, edited by Hughes Dreysse, Springer Lecture Notes, Workshop Mont Saint Odille, France, 1998 (Springer, Berlin), pp. 114-147 (2000).

[11] P. Larson , Walter R. L. Lambrecht and Athanasios Chantis and Mark van Schilfgaarde, Physical Review B 75, 045114 (2007).

[12] D.J. Singh, Planewaves, Pseudopotential and the LAPW Method. Kluwer Academic, Boston, 1994.

[13] O. Jepsen, O. K. Andersen, Solid State Commun. 9, 1763 (1971).

[14] P. Blaha, K. Schwarz and J. Luitz. (A Full Potential Linearized Augmented Plane Wave package for calculating crystal properties). Techn. University. At Wien, Austria, WIEN97 (1999).

[15] J. P. Perdew, K. Burke and M. Ernzerhof, Phys. Rev. Lett. 77, 3865 (1996).

[16] http:/www.wien2k.at.

[17] A. I. Liechtenstein, V.P. Antropov, and B. N. Harmon, Phys. Rev. B 49, 10770 (1994).

Table [1]. The calculated total and partial magnetic moments and energy gap for EuN in RS and CsCl structures.

Structure	Eu (μB)	N (μB)	Total (μB)Calc. Present work	Total (μB)Calc. TB-LMTO[9]	Energy Gap (eV)	Scheme Used	State*
RS	6.246 6.563	-0.396 -0.645	5.996 6.000	6.00	1.4	SP LSDA+U	HM M
CsCl	6.358 6.333	-0.485 -0.451	6.003 5.990	6.00	0.8	SP LSDA+U	H.M M

* HM = half metal and M = metal

Table 1 displays the partial and total magnetic moments together with the energy gap of the half-metallic states of the two structures. Our calculated total magnetic moments are in very good agreement with an earlier work [9]. The very- near- to integer magnetic moments together with the presence of a band gap confirm the half-metallic nature of these two structures, provided that only spin-polarized calculations are used.

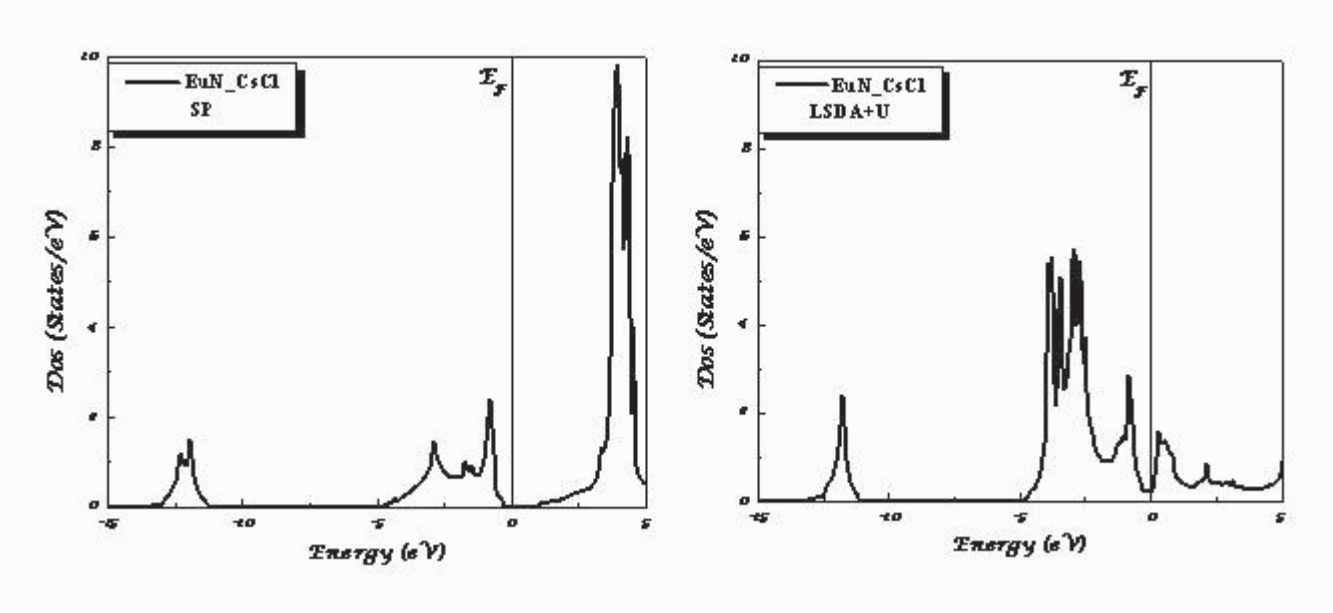


Fig. [1.a]: (left panel): The calculated spin-minority DOS in the CsCl structure (spin-polarized scheme). Fig [1.b]: using the LSDA+U scheme (right panel).

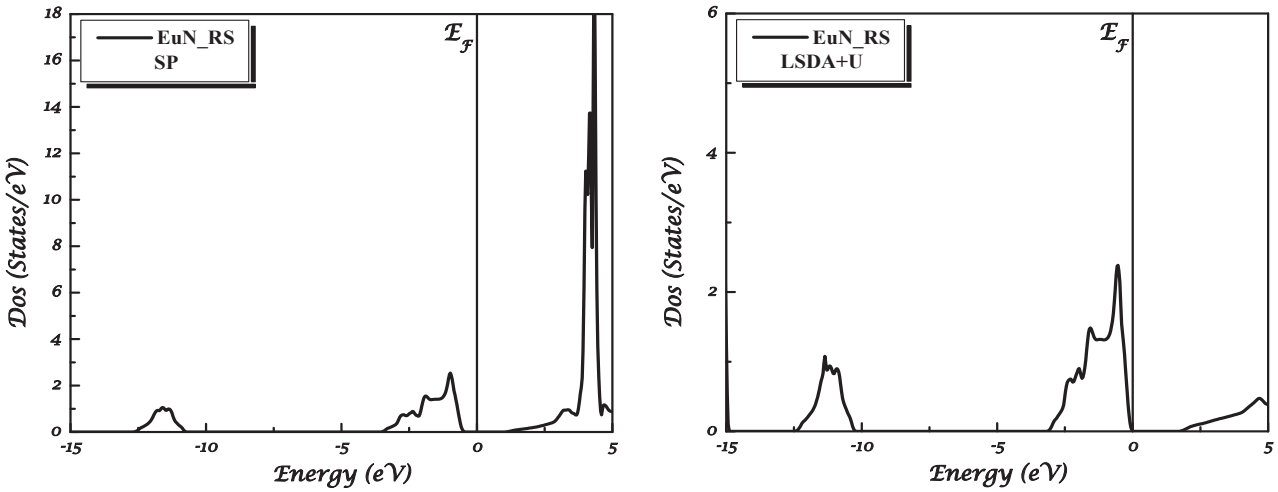


Fig. [2.a]: (left panel): The calculated spin-minority DOS in the RS structure (spin-polarized scheme). Fig [2.b]: using the LSDA+U scheme (right panel).

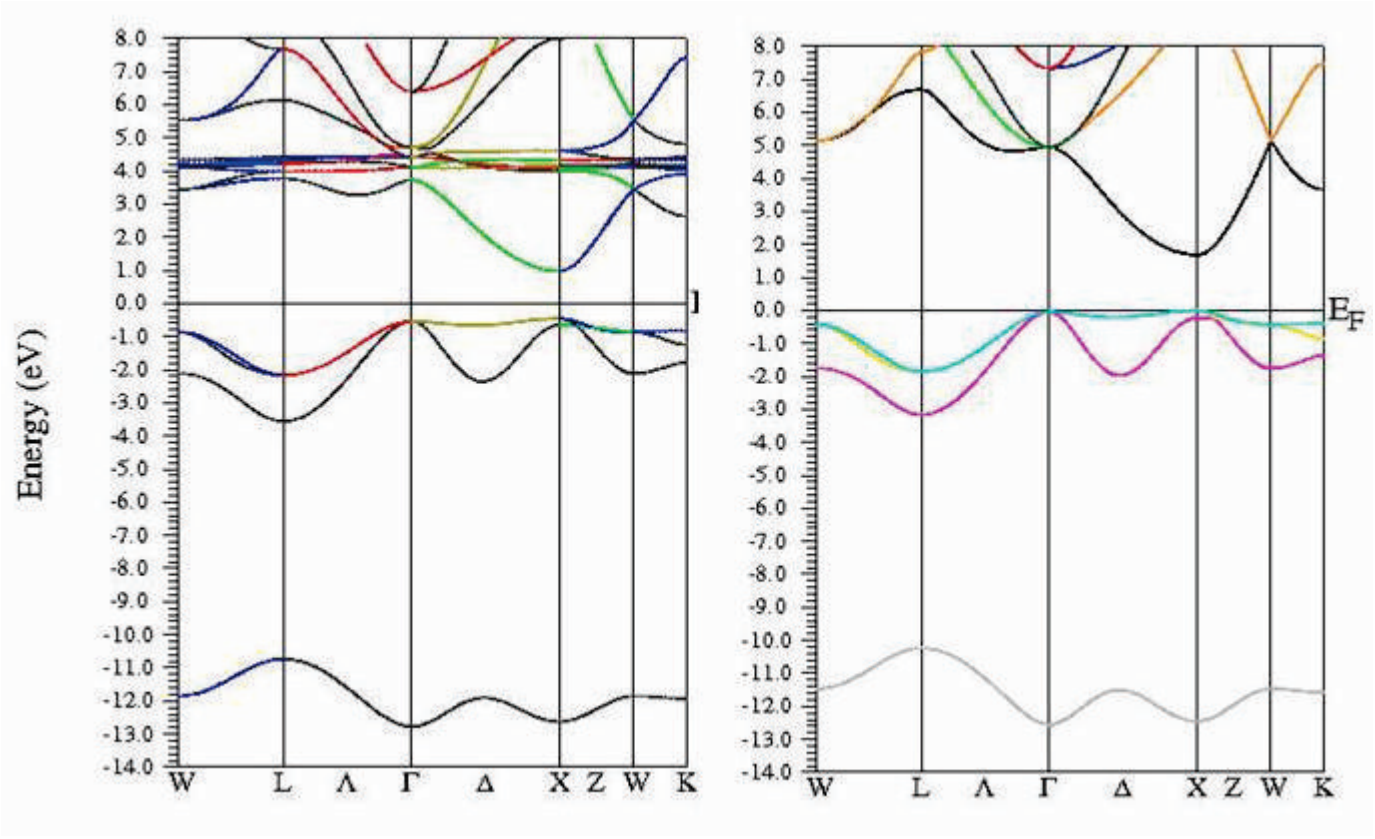
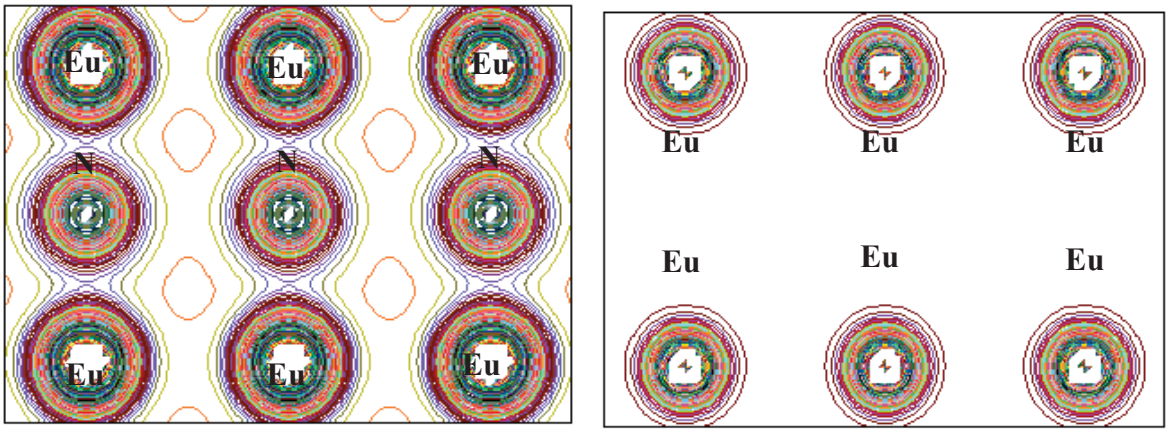
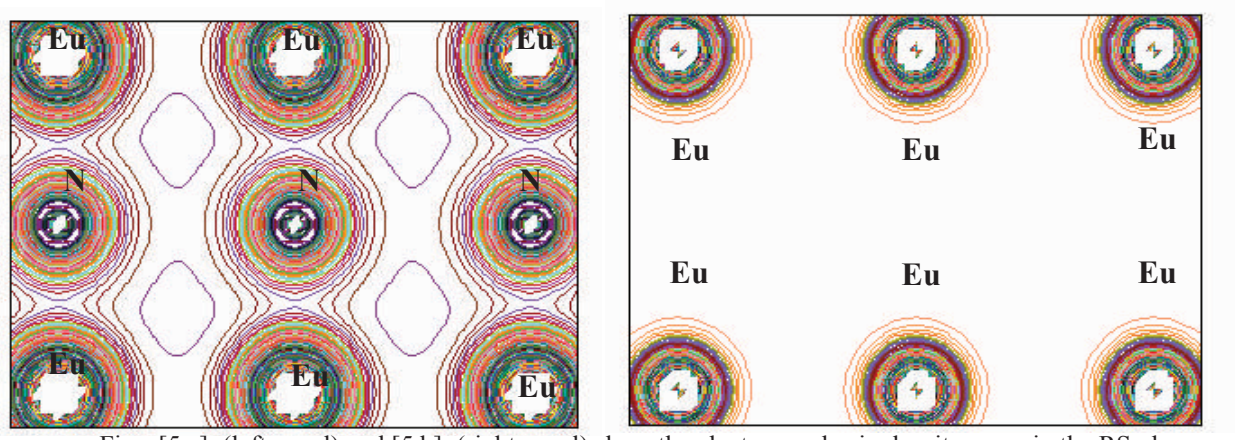


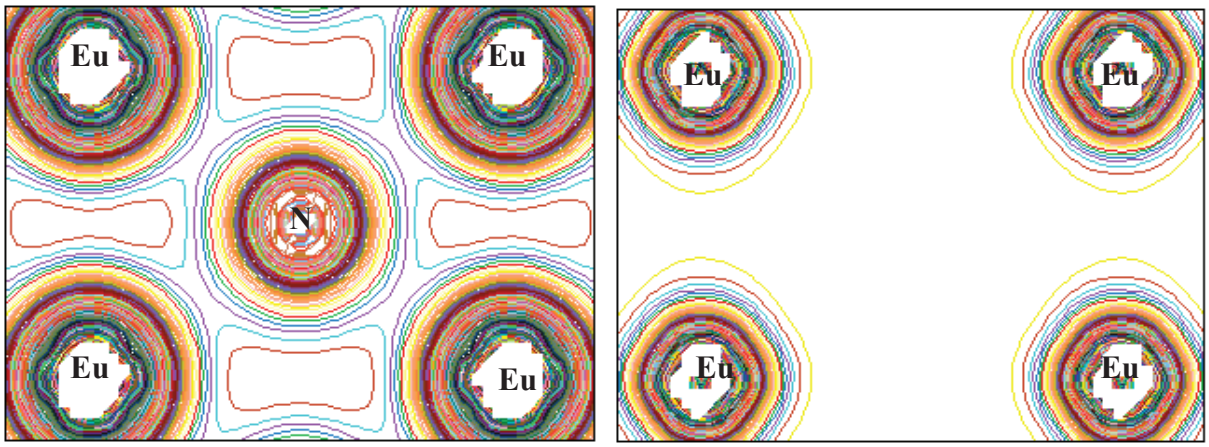
Fig. [3]: The minority band structure for the RS structure, without (a) and with LSDA+U (b)



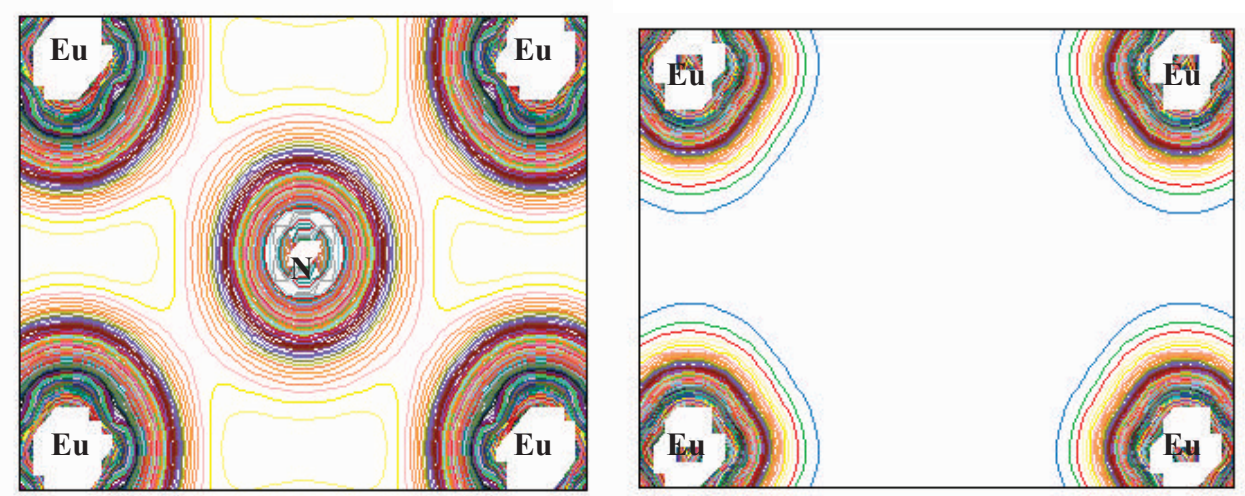
Figs. [4.a]: (left panel) and [4.b]: (right panel) show the electron and spin density maps in the RS structure respectively, using bare spin polarized calculation.



Figs. [5.a]: (left panel) and [5.b]: (right panel) show the electron and spin density maps in the RS phase respectively. The LSDA+U scheme is used.



Figs. [6.a]: (left panel) and [6.b]: (right panel) show the electron density and spin density contours in the CsCl phase respectively. Bare spin polarized calculation was used.



Figs. [7.a]: (left panel) and [7.b]: (right panel) show the electron density and spin density contours in the CsCl structure respectively. LSDA+U scheme has been used.