LSDA+U approximation-based analysis of the electronic structure of CeFeGe₃

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Abstract

We perform ab initio electronic structure calculations of the intermetallic compound CeFeGe₃ by means of the Tight Binding Linear Muffin-Tin orbitals-Atomic Sphere Approximation (TB-LMTO-ASA) within the Local Spin Density Approximation containing the so-called Hubbard correction term (LSDA+U[SIC]), using the Stuttgart’s TB (Tight Binding)-LMTO-ASA code in the framework of the Density Functional Theory (DFT).

KEYWORDS: Ab initio calculations, LSDA+U approximation, intermetallic compound.

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1 Introduction

The heavy electron compounds refer to those having a specific heat coefficient \( \gamma \) of the order of \( \text{Jmol}^{-1}\text{K}^{-2} \), which is much larger than that of simple metals (being typically in the range of \( \text{mJmol}^{-1}\text{K}^{-2} \)). In addition, this implies that such compounds—which have been given a great deal of attention for long time—possess a large effective mass \( m^* \), outweighing several hundreds of times the free electron mass \[1\]. They can be classified into two groups: the concentrated Kondo compounds CK and the intermediate valence compounds (IV) \[2,3\] depending on the position of the 4\( f \) or 5\( f \) level, relative to the Fermi level. The CK compounds have an integer valence at temperatures much higher \( (T \gg T_k) \) than the Kondo temperature \( T_k \), at which, there appears the Kondo effect (an effect observed in metals with a magnetic impurity). However, at comparatively low temperatures \( (T \ll T_k) \) they form a Fermi liquid state \[4\] with a reduction of its magnetic moment. On the other hand, the IV compounds do not possess an integer valence at room temperature as a result of the strong hybridization between the 4\( f \) electrons and the conduction electrons, due to the anomalous proximity between the 4\( f \) and the Fermi levels.

Remarkably, the CeFeGe\(_3\) compound here studied \[5\] apparently gives rise to two behaviors: A high \( T_k \) of the order of 100 K and an integer valence for Ce at room temperature. This study is motivated by the fact that such compound is known to present a strong electronic correlation character, which occurs when the Coulomb repulsion between electrons strongly inhibits their motion, thus becoming highly localized. Because of this, on compounds containing lanthanides the normally expected metal behavior—cerium ions with 4\( f \) electrons or uranium and neptunium ions with 5\( f \) electrons—is not observed. Some examples are: CeA\(_{13}\), CeCuSi\(_2\), CeCu\(_6\), UBe\(_{13}\), UCd\(_{11}\), U\(_2\)Zn\(_{17}\) and NpBe\(_{13}\), as well as transition metal oxides, organic metals and carbon compounds, i.e., carbon nanotubes, etc.

In the first stage of the present work \textit{ab initio} calculations were carried out to investigate the electronic structure of the intermetallic compound CeFeGe\(_3\) (tetragonal structure with spatial group 107) by using a DFT method \[7\] in the LMTO-ASA approximation \[8\], whereas in the second, an LSDA+U\text{SIC} approximation \[9\] was used, as implemented in the Stuttgart’s TB-LMTO-ASA code version 47 \[8\]. The density of states (DOS), total and partial, for cerium and iron, as well as the band structure (BS) are obtained from the compound geometrical conformation optimized by the CASTEP program (Cambridge Serial Total Energy Package) which makes use of the ultrasoft pseudopotentials theory \[10\]. The Coulomb and exchange parameters used in the calculations were \( U = 5.4 \text{ eV} \) \[11\] for cerium and \( U = 2.3 \text{ eV} \) \[12\] \((J = 0.9 \text{ eV})\) for iron, just obtained in the literature.
2 Computational approach.

2.1 LMTO-ASA and CASTEP Calculations.

The LMTO-ASA approximation employs the unitary cell splitting into overlapping Wigner-Seitz (WS) spheres with a maximum overlap of 15%, which is generally considered a reasonable approximation when having a spherically symmetric potential within the spheres. In addition, use is made of the ASA (Atomic Sphere Approximation) condition, i.e., a spherical approximation containing no zone of free electrons on the Muffin-Tin structure. For open structures, as the ones here considered, a set of empty spheres is introduced as a device for describing the repulsion potentials in the interstices (between an atomic and an interstitial sphere an overlap of 20% is allowed). The total volume of the WS spheres is equal to the unit cell volume, thus eliminating the interstitial region.

On the other hand, the Muffin-Tin (MT) orbital is energy dependent with the following linearized form:

\[
\phi_{\lambda}(\mathbf{r}) = i^l Y_{lm}(\mathbf{r}) \left\{ \begin{array}{ll}
\phi_{\lambda}(E, r) + p_{\lambda}(r/S_R)^l ; & r < S_R \\
(S/r)^{l+1} ; & r > S_R \end{array} \right. \tag{1}
\]

where \( \phi_{\lambda}(\mathbf{r}) \) is found by numerical solution of the radial Schrödinger equation, \( \lambda = RL \). \( R \) is the site index, whereas \( l \) and \( m \) are the orbital and magnetic quantum numbers of the angular momentum. The \( Y_{lm} \)'s refer to spherical harmonics and \( S_R \) is the MT radius. The numerical orbital \( \phi_{\lambda}(E, r) \) is augmented inside the sphere by a renormalized spherical Bessel function,

\[
J_{k\lambda}(r) = i^l Y_{lm}(2l+1)!! (S/S_R)^l j_l(kr), \tag{2}
\]

whereas outside the spheres, a renormalized spherical Hankel function is added:

\[
H_{k\lambda}(r) = i^l Y_{lm}(kS_R)^{l+1} (2l-1)!! h_l(kr). \tag{3}
\]

Here, \( h_l = j_l - in_l \) is a linear combination of spherical Bessel and Neumann functions. Thus, the tail of the MT orbitals at \( r > S_R \) is the solution of the Helmholtz equation with zero kinetic energy. The potential parameters \( p_{\lambda} \) are chosen so as to ensure that the wave function be continuous and differentiable at the sphere boundary.

In this approximation the potential \( V_{xc} \) is either von Barth-Hedin (vBH)[13] or Vosko-Ceperly-Alder [14] type at the Local Spin Density Approximation (LSDA) level, whereas at the Generalized Gradient Spin Approximation (GGS) level—which is a functional containing a density gradient correction—the potentials used the Langreth-Mehl-Hu [15] or Perdew-Wang type [16]. The exchange-correlation potential used in the present calculations corresponds to that containing the von Barth-Hedin parametrization, whose general form is

\[
ev_{xc}^\sigma = A(r_s) \left( \frac{2n_\sigma}{n} \right)^{\frac{3}{4}} + B(r_s), \tag{4}
\]
where $A(r_s)$ and $B(r_s)$ are analytical functions.

### 2.2 Geometry Optimization

The ternary system unit cell was optimized by means of ab initio methods, based on a DFT treatment within the Local Spin Density Approximation (LSDA) and with the Generalized Gradient Spin (GGS) approximation. In the CASTEP program [10] the wave function is expanded in planes waves for the valence electrons, whereas the core electrons (bound to the nucleus) are taken into account by means of their effective interaction on the valence electrons, in the form of pseudopotentials which are added to the corresponding Kohn-Sham Hamiltonian.

The pseudopotentials used in this work were generated by Vanderbilt [17] in the Kleinman-Bylander [18] representation. The parametrizations of polarized spin developed by Perdew-Zunger [19] and Perdew-Burke-Ernzerhof [20] for the exchange and correlation energy were used. The conjugated gradient method is employed to relax nuclear positions. The sampling of the Brillouin zone was of $7 \times 7 \times 8$ and $9 \times 9 \times 11$ for the LSDA and GGS approximations, respectively, using the scheme of Monkhorst-Pack [21]. The cutoff energy for the plane waves was of 400 eV approximately. Self-consistency in the calculations was attained whenever the total energy changes were $\leq 5$ meV, which corresponds to a criterion of reasonably good convergence.

To perform geometry optimization we let the lattice constants $a$, $b$ and $c$ vary as free parameters—though they are expected to undergo changes no larger than 5% relative to the experimental values. The crystal energy is minimized with respect to the degrees of freedom by taking into account the calculation of Hellmann-Feynman forces in the atoms and the components of the stress tensor [22]. Finally, the utilized optimization criteria were 0.00002 eV, 0.0010 Å and 0.050 eV/Å for energy change, quadratic mean displacement, and quadratic mean force per atom, respectively.

### 2.3 Mathematical Structure of the approximation LDA+$U^{SIC}$

In the LSDA+$U$ [9] method the electrons are separated into two subsystems (i and ii). For Ce, (i) delocalized $s, p$ and $d$ electrons, which are described by an orbital-independent one-electron potential (the LSDA potential), and (ii) localized $4f$ electrons, for which we take into account the orbital degeneracy and a Coulomb interaction of the form $\frac{1}{2}U \sum_{\sigma \neq \sigma'} n_{\sigma} n_{\sigma'}$, where $n_{\sigma}$ is the $f$-orbital (or $d$-orbital) occupancy. For Fe, (i) delocalized $s, p$ electrons, and (ii) localized $3d$ electrons.
The Hamiltonian for the spin orbitally degenerate systems is of the form

\[ \hat{H} = \sum_{i,j} \sum_{m,m'} \sum_{\sigma} t_{ij}^{mm'} \hat{c}_{im\sigma}^\dagger \hat{c}_{im'\sigma} + \frac{(U - J)}{2} \sum_i \sum_{m \neq m'} \sum_{\sigma} \hat{n}_{im\sigma} \hat{n}_{im'\sigma} + \frac{U}{2} \sum_{i,m,m'} \sum_{\sigma} \hat{n}_{im\sigma} \hat{n}_{im'\sigma} \quad (5) \]

where \( \hat{c}_{im'\sigma} \) is an electron annihilation operator with an orbital index \( m \) and spin \( \sigma (= \alpha, \beta) \). In the lattice site \( i \), \( t_{ij}^{mm'} \) are the hopping integrals and \( \hat{n}_{im'\sigma} \) is the number operator of the \( f \) (or \( d \)) electron at site \( i \), orbital \( m \) with spin \( \sigma \). The first term in Eq. (5) describes the hopping of electrons between lattice sites \( i \) and \( j \); the interactions between the localized electrons are described by the second and third terms, where \( U \) and \( J \) represent the on-site Coulomb and exchange interaction, respectively.

If we want to correct the LSDA functional for localized electrons we must first extract their LSDA treatment to avoid double count of the interaction. The spin density functional theory assumes a local exchange-correlation potential which is a function of the local charge and spin densities, so, fluctuations around the average occupations are neglected. In the mean field approximation (MFA) we can write

\[ \hat{n}_{m\sigma} \hat{n}_{m'\sigma'} = \hat{n}_m n_{m'\sigma'} + \hat{n}_{m'\sigma} n_{m\sigma} - n_m n_{m'\sigma'} \quad (6) \]

where \( n_{m\sigma} \) is the mean value of \( \hat{n}_m \sigma \) and \( n_{\sigma} = \sum_m n_{m\sigma} \). By introducing this approximation in Eq. (5), we obtain the expression for potential energy in the mean field approximation,

\[ E^{MF} = \frac{U - J}{2} \sum_i n_{i\sigma}(n_{i\sigma} - n_{i\sigma - 1}) + \frac{U}{2} \sum_i n_{i\sigma} n_{i-\sigma} \quad (7) \]

Solovyev et al. [23] propose to extract an energy function from the total number of electrons per spin \( n_{i\sigma} \) which would act as the LSDA potential. Such expression can be obtained from Eq. (5) in the atomic limit where occupation of the individual particle \( n_{i\sigma} \) is either 0 or 1:

\[ E^{LSDA}_{cor} = \frac{U - J}{2} \sum_{i\sigma} n_{i\sigma}(n_{i\sigma} - 1) + \frac{U}{2} \sum_{i\sigma} n_{i\sigma} n_{i-\sigma} \quad (8) \]

This energy is now subtracted from \( E^{MF} \) to obtain that associated with the total energy for localized states:

\[ \Delta E = E^{MF} - E^{LSDA}_{cor} = \frac{U - J}{2} \sum_{i\sigma} n_{i\sigma}(1 - n_{i\sigma}) = \frac{U - J}{2} \sum_{i\sigma} (n_{i\sigma} - n_{i\sigma}^2). \quad (9) \]
The fraction of the potential acting on the localized orbital \((m\sigma)\) is found by differentiating Eq. (9) with respect to the occupation number \(n_{im\sigma}\):

\[
\frac{d\Delta E}{dn_{im\sigma}} = \Delta V_{im\sigma} = (U - J) \left( \frac{1}{2} - n_{im\sigma} \right).
\]

An orbital dependent one-electron potential is thus obtained.

3 Results and discussion.

3.1 First Stage: LMTO-ASA calculations

Results obtained in the optimization of the intermetallic compound CeFeGe\(_3\) are shown in Table II. The LSD and GGS approximations yield values below the experimental parameters, which may be due to the fact that neither approximation removes the error introduced by the self-energy interaction term, arising from double count in the Hamiltonian. Furthermore, this material does not present a trend similar to that of semiconductors since otherwise, the LSDA and GGA results would give values remaining below and above the experimental parameters, respectively. A similar situation is found in the equilibrium properties of the plutonium (phase \(\delta\)-Pu)\([24]\), in which, results obtained with LDA and GGS give numbers that remain below the corresponding experimental values. We work with the CASTEP program at GGS level employing 446 K-points in the Brillouin zone. On the other hand, the density of states (total and partial) and band structure were obtained via the LMTO-ASA methodology within the DFT theory and the LSDA approximation, using the von Barth-Hedin parametrization at the optimized unit cell geometry. The corresponding results are compiled in Table I.

The total density of states (DOS) is given in Fig. 1, whereas the partial DOS associated with cerium \(f\)-states and iron \(d\)-states is illustrated in Figs. 2 and 3, respectively. They all indicate a metallic behavior for the material here analyzed, since we have the Fermi level slightly displaced from the central band. This is also supported by looking at the plot of band states (BS), as shown in Fig. 4, where a dense concentration of bands due to the cerium \(f\) states occurs around the Fermi level. Furthermore, the fact of having almost horizontal bands points to the characteristic behavior of a heavy fermion compound (in our case, \(\gamma = 150 \text{ mJ-molK}^2\)) \([1,5]\).

In the literature it is reported that the greater magnetic contribution stems from cerium (being the magnetic impurity responsible for the Kondo effect); a fact that is corroborated in the present theoretical calculations (see Table I). Once optimized the geometrical parameters, the material here analyzed turns out to be one of those classified as an intermediate valence compound. In our calculation, Ce has a magnetic moment of \(-0.00132 \mu_{\beta}\) whereas the compound’s total magnetic moment is \(-0.0010084 \mu_{\beta}\). Therefore, according to the criterion proposed by Vildosola and Llois \([25]\), i.e., by using calculations at the LSDA
level and the exchange-correlation potential of Perdew-Wang, they propose that the materials can be classified as follows:

\[
\begin{array}{|c|c|}
\hline
\text{Itinerant if } & \mu_{Ce} = 0, \\
\text{Intermediate valence if } & \mu_{Ce} < 0.5\mu_B, \\
\text{Magnetic if } & \mu_{Ce} > 0.5\mu_B. \\
\hline
\end{array}
\]

(11)

An intermediate valence system is usually defined in the literature as one having a noninteger average number of \( f \) electrons. Note that the charge on the Ce atom according with the LSDA calculation is of \(-2.4654\) a.u. with a magnetic moment of \(-0.00132\). This means that the normal atom configuration of \([Xe]4f^{1}5d^{1}6s^{2}\) is being added with almost 3 electrons whose alpha and beta spins pair off one another, which results in an overall moment of nearly zero magnitude.

3.2 Second Stage: LSDA+U calculations

As can be inferred from the analysis presented in the previous stage, the DFT theory—due to its intrinsic formulation—it cannot deal properly with strongly correlated systems, therefore, we have chosen to resort to the LSDA+U \(SIC\) approximation, developed by Anisimov \textit{et al.} [9], to calculate the electronic structure of the intermetallic compound \(CeFeGe_{3}\), as implemented in the Stuttgart’s TB-LMTO-ASA code version 47. For this calculation, we employed the parameters reported in the literature: \(U = 5.4\) eV [11] for cerium and \(U = 2.3\) eV (\(J = 0.9\) eV) [12] for iron.

The resulting density of states in this case is plotted in Fig. 5, whereas the partial DOS for cerium \(4f\)-states and iron \(3d\)-states are depicted in Figs. 6 and 7, respectively. By virtue of the approximation used in this stage, the latter include effects arising from strong correlation, not accounted for in those obtained by means of a conventional DFT calculation. The corresponding band structure is displayed in Fig. 8.

In the display of total DOS the greatest contribution comes from the cerium \(4f\)-states where an increased splitting within the energy bands—in addition to a relative overall shift around the Fermi level—can be seen in Fig. 5. This feature also shows up in the partial density of states, where a large band energy splitting arising from the cerium \(4f\)-states can be appreciated in Fig. 6 (being 5 eV wide, approximately), as compared with the corresponding energy band display (Fig. 2) obtained in the previous stage, in which, the presence of a nearly single peak dominates, located very close and above the Fermi level. The magnetic contributions to this material come partly from both cerium and iron, even prior to the introduction of the exchange parameter (previous stage), whereas the magnetic moment for germanium is almost null, as seen in Table I. Furthermore, the material presents metallic behavior. When carrying out calculations with an exchange parameter \(J\) equal to 0.90 eV for iron there occurs a reduction of the magnetic moment in a 42% rate, which probably follows from a slight localization effect of electrons on the iron \(3d\)-shell. On the other hand, the high
concentration of energy bands occurring around the Fermi level is consistent with a metallic behavior. In fact, a greater density of bands is observed in this stage (see Fig. 8) as compared to that observed without introducing the Coulomb parameter (see Fig. 4). Such feature—in this stage—points to a typical characteristic of heavy fermion materials.

According to the criterion mentioned in the first stage, proposed by Vildosola and Llois [25], and extended to handle the total magnetic moment per unit cell, one can notice that the magnetic moments for cerium, $-1.1407\mu_\beta$, iron, $(0.6147\mu_\beta)$, and $-0.00055\mu_\beta$ for the empty spheres, give altogether a total moment of $-0.552\mu_\beta$. This falls within the classification corresponding to a magnetic material. Also, the charge distribution shown in Table I (empty spheres introduced by the ASA condition), points to a possible covalent character among the atoms of cerium, iron and germanium, although this manifests itself very weakly, despite the fact of accounting for correlation effects in the theoretical calculation. Comparing the charge of the Ce atom in the LSDA(vBH) and LSDA(vBH)+U cases, it is seen to be similar for both: $-2.4654$ a.u. and $-2.3847$ a.u., respectively. However, the $U$ interaction gives rise to a complete change in the spin behavior: whereas in the absence of $U$ almost 3 electrons are added to the neutral atom—although the overall magnetic moment is nearly zero—now the salient effect in the presence of the $U$ interaction is to align the electrons, yielding an effective magnetic moment whose magnitude is $-1.1407\mu_\beta$.

Having no charge difference in the two cases, where the $U$ interaction acts only on the $f$ electrons, the filling of the $f$-shell proceeds via splitting of the $\alpha$ and $\beta$ levels by the energy $U$ and the occurrence of electron alignment on the $f$-shell only. The remaining charge distributes over the other shells: $s$, $p$ and $d$.

4 Conclusions

The calculations performed by means of the LMTO-ASA approximation, within the DFT theory, lead to results that are similar to those reported in the literature, in particular, the obtained magnetic contribution of the compound here analyzed, which practically corresponds to that of a nonmagnetic material. On the other hand, the partial DOS, together with the band structure, show a metallic behavior for the latter. Furthermore, results obtained with calculations carried out where the Coulomb parameters $U$ and $J$ (for iron) are introduced, also favor a metallic behavior and, in addition, a heavy fermion character for this material. The two-stage analysis performed in the present study also indicates a small charge covalent character. The pronounced magnetic moment reduction occurring in iron is here ascribed to an electronic cloud localization on the 3$d$-shell of this atom, which arises as a direct consequence of taking into account strong electronic correlation effects.
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**Table and figure captions**

**Table I:** Parameters utilized in the electronic structure calculations of the ternary compound CeFeGe$_3$ and theoretical data obtained by using the TB-LMTO-ASA approach.

**Table II:** Cell parameters optimized by means of the CASTEP program.

**Fig. 1:** Total density of states of CeFeGe$_3$ obtained by the LSDA-vBH approximation.

**Fig. 2:** Partial density of states (Ce 4$f$-states) obtained by the LSDA-vBH approximation.

**Fig. 3:** Partial density of states (Fe 3$d$-states) obtained by the LSDA-vBH approximation.

**Fig. 4:** Band structure obtained by the LSDA-vBH approximation.

**Fig. 5:** Total density of states obtained by the LSDA(vBH)+U approximation using the parameter U for cerium and parameters U and J (exchange) for iron.

**Fig. 6:** Partial density of states (Ce 4$f$-states) obtained by the LSDA(vBH)+U approximation.

**Fig. 7:** Partial density of states (Fe 3$d$-states) obtained by the LSDA(vBH)+U approximation.

**Fig. 8:** Band structure obtained by the LSDA(vBH)+U approximation using the parameter U for cerium and parameters U and J (exchange) for iron.
| Atoms in the Crystallographic MT sphere Positions radii (a.u.) | Charge\(^a\) (a.u.) | Magnetic\(^a\) (\(\mu_B\)) | Charge\(^b\) (a.u.) | Magnetic\(^b\) (\(\mu_B\)) |
|---|---|---|---|---|
| Ce (0.0, 0.0, 0.0) | 4.1077 | -2.4654 | -0.00132 | -2.3847 | -1.1407 |
| Fe (1.0,1.0,0.66) | 2.4566 | -0.3027 | 0.00033 | 0.3339 | 0.6147 |
| Ge\(_1\) (0.5,0.0,0.25) | 2.5320 | 1.1212 | -0.000005 | 1.1208 | 0.01274 |
| Ge\(_2\) (1.0,1.0,0.42) | 2.6284 | 1.064 | -0.000013 | 1.0499 | -0.02511 |
| E\(_1\)* (0.1224,0.1224,0.5684) | 1.1281 | -0.1396 | -0.000001 | -0.1432 | -0.00055 |
| E\(_2\)* (0.1224,-0.1224,0.5684) | 1.1281 | -0.1396 | -0.000001 | -0.1432 | -0.00055 |
| E\(_3\)* (-0.1224,0.1224,0.5684) | 1.1281 | -0.1396 | -0.000001 | -0.1432 | -0.00055 |
| E\(_4\)* (-0.1224,-0.1224,0.5684) | 1.1281 | -0.1396 | -0.000001 | -0.1432 | -0.00055 |

\(^a\)Positions of the empty spheres that fulfill the ASA condition within the LMTO-ASA approximation.

\(^b\)As obtained for the parameters optimized by means of the LSDA-vBH approximation.

\(^b\)As obtained via calculations performed with the LSDA(vBH)+U approximation.

Table II

| Experimental cell parameters (\(\text{Å}\)) | Optimized cell parameters (\(\text{Å}\)) LSDA | % of error Exp. vs LSDA | Optimized cell parameters (\(\text{Å}\)) GGS | % of error Exp. vs GGS |
|---|---|---|---|---|
| a=b=4.332 | a=b=4.1767 | 3.71 | a=b=4.234 | 2.314 |
| c=9.955 | c=9.5981 | 3.72 | c=9.73 | 2.312 |
This figure "DOS-CEf-CEFEGE3.gif" is available in "gif" format from:

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