

First-principles investigation of electronic, structural, and magnetic properties of Si substituted cerium phosphide compounds $\text{CeSi}_x\text{P}_{1-x}$

A. Mahmood^{a,*}, W. A. Al Masary^a, S. M. Ramay^b

^a*Chemical Engineering Department, College of Engineering, King Saud University (KSU), Riyadh, 11421, Saudi Arabia*

^b*Department of Physics and Astronomy, College of Science, King Saud University (KSU), Riyadh, 11421, Saudi Arabia*

Cerium compounds have invited enough attention from scientists and researchers with respect to practical and fundamental implications having exotic physical, electronic, and magnetic properties like the kondo effect, anisotropic magnetic order, giant Hall effect and superconductivity. Hereby, we describe the mechanical stability and present the electronic, structural, and magnetic properties of new silicon-doped alloys of Cerium Phosphide with generic formula $\text{CeSi}_x\text{P}_{1-x}$ ($x=0, 0.25, 0.5, 0.75$ and 1.0) by using Wien2k code through DFT formalism. The simulation employs generalized gradient approximation through Perdew Bruke Ernzerhof with spin mode. The computed variables are lattice constants, volume, bulk modulus, pressure derivatives, and energy for structural studies. The partial and total densities of states and electronic energy band structures are calculated for electronic studies of these compounds. The magnetic properties of these compounds are described by computing spin magnetic moments. These doped alloys are predicated on being structurally stable, metallic, and non-magnetic materials.

(Received April 25, 2024; Accepted July 11, 2024)

Keywords: Cerium silicon phosphide, Generalized gradient approximation, Spin magnetic moment, Electronic energy bands, Density functional theory

1. Introduction

The rare-earth mono-pnictide compounds were described decades earlier, containing different elements with the pnictogen family (e.g. CeP, CeN, etc.). Mostly these RE compounds form crystals in simple rock salt (NaCl) with an fcc cubic crystal structure despite, the YbBi compound. On the other hand, they perform substantially different geometrical properties. All of these RE-alloys and compounds are reported anti-ferromagnetic at a small temperature [1-4], despite the lanthanum and yttrium being non-magnetic compounds and the praseodymium alloy and compounds being reported as para-magnetic of Van Vleck type [5]. The measurements of de Haas-van Alphen (dHvA) and Angular resolved photoemission spectroscopy (ARPES) about these alloys and compounds have been made [6-14] for investigation of their energy electronic band structure. The LDA+U and dynamical mean-field theory (DMFT) computations have proposed that the electrons of 4-f states are mostly completely localized in the compounds of $\text{Pn}=\text{Sb}/\text{Bi}$ [15-18], particularly regarding the bismuth alloys. In CePn, compounds the 4f -states of Ce element meagerly combine with the 5d sub-shells of Ce element (d-f combination) and p state orbitals of pn element (p-f combination) [6,19], and the prior go ahead to Kondo-type nature in this less density/minority carrier system, that mostly ceases for CeBi compound [16].

Under pressure, studies about the RE compounds with mono-pnictides have invited the attention of researchers due to their strange physical properties [20-22]. The said exotic properties of these RE-compounds should be normally described as the partially filled electron of f-states of atoms of rare earth alloys and compounds. These alloys show the B1 structural phase type at the ambient conditions of pressure and temperature, and experimental characterization through X-ray diffraction reports describe that large of these alloys shift their phase structurally either to B₂ phase

* Corresponding author: ahayat@ksu.edu.sa
<https://doi.org/10.15251/JOR.2024.204.467>

type or BCT type at large pressure [23,24]. The compounds of mono-pnictides with lanthanum elements have been investigated experimentally [25-32] as well as theoretically [33-42] because of their non-magnetic nature when compared with other elements of the rare earth family with mono-pnictides. Experimental studies of the compound CeBi have described a shift in phase structurally from B1 type to BCT type at about 13 GPa [43], and at 25 GPa pressure for CeP compound [44]. Haiyan Lu and Li Huang have studied the cerium mono-pnictides compounds about their unraveling with 4f-states of electronic structures [45]. Vedel et al. [46] studied electronic and crystallographic transition induced by pressure on CeP. Pagare and Sanyal [47] have studied the transition pressure at 12.7 GPa for B1 to BCT with 8.9% change in volume has also been observed about CeBi compound along with this phase transition, and similarly shift in phase about PrBi compound has been predicted at 13.5 GPa pressure along with 8.5% variation in volume, by using two body inter-ionic potential method.

With B1 phase (NaCl type) crystal structure, the mono-pnictides compounds of cerium CeX (X= P, N, Bi, Sb, As), described extraordinary magnetic properties [48] because of the existence of the 4th level near the Fermi energy level that is basically a normal behavior of anomalous rare earth compounds like the cerium. For the compounds of cerium mono-pnictides, Bear et al. [49] have experimentally studied by using XPS method, and it has described that the 4th level is near to or at the Fermi energy level for CeN compound, presenting it a combined valance orbital state, and large onwards to higher binding energy to CeBi from CeP compounds. The 4f state in the compound of CeP has been described below at 0.4 eV of Fermi level and at 10GPa [50] pressure, that pressure is much more suitable for predicting an electronic change as well as for a large volume minimization (~8%). Despite the same valance charge expectation from CeAs compound, Werner et al. [51] have described the CeAs compound that at pressure nearly 15Gpa, only structural phase change from B1 to B2-phase occurred. Due to the strong bonding of 4f electrons in CeSb and CeBi compounds, more strange magnetic properties are present there. The compounds of CeP and CeAs are naturally simple anti-ferromagnets, actually, but CeSb and CeBi compounds exhibit strange magnetic properties like much small crystal splitting field, a very high magnetic anisotropy, and a complex diagram of magnetic phase. The half-metallic nature is the basic cause for the existence of these properties of the aforesaid compounds. The computational investigation of electronic energy bands [52] reveals that the zone has fewer p-holes at its middle, and the 5d(t_{2g}) energy level electrons are concentrated at its boundary. The combined interaction with 4f electrons and the anion p-band is thus much higher than that has been described by the group of Kasuya [53], and hence the compounds CeSb and CeBi exhibit complex properties although the electrons of 4f level are far away from the Fermi energy level. Because of the combination of 5-f electrons with 5d conduction electrons, the mono-pnictides of cerium describe the anomalous transport properties up to some limit, similar to the compounds which present Kondo-like properties.

The Kondo interaction depending upon volume has been described in [54, 55] to show a minus involvement in the free energy and, thus, diminishing of the bulk modulus. The low pressure may thus produce variation in an electronic of first or second order lowering the temperature. A similar interaction has been reported in CeTe compound [56] to cause constant electronic change employed under pressure in the NaCl-type B1 phase structure. Basically, a much small decrease in bulk modulus because of combined interactions had been reported in CeSb compound [57]. However, the great f- p combining in CeBi described rise to a more effect and the P-V relation should then show an anomalous nature. Politecnico di Milano [58] has studied lattice dynamics as well as phonon anomalies in the compounds of cerium. Venn, H.Manked et al. [59] have described rare-earth bismuthides' phonon and thermo dynamical properties. Xu et al. [60] have investigated the topological and electronic tunable structural properties of LnPn (Ln= Pr, Ce, Gd, Sm, Ub, Pn= Bi, Sb).

J.Rossat-Mignod et al. [61] have conducted experimental studies about the magnetic ordering of the mono-pnictide compounds of uranium and cerium. The rare earth compounds of LaBi and CeBi have been studied for elastic and structural phase change at high pressure by V.Manked et al. [62]. At high-pressure changes occurred in the compound cerium phosphide have been observed by Jayaraman, et al. [63]. Hullinger, et al. [64] have studied magnetic phase variation properties of CeSb and CeBi compounds at less temperature. The elastic and structural

phase variations of XBi(X=Pr, Ce) compounds have been studied by Wenxia Feng et al. [65] Lenger et al [66] have experimentally studied lattice and magnetic properties of CeBi compound through X-ray diffraction technique. Azmat et al [67] have recently studied the computational analysis of the interplay between inter-magnetic and inter-metallic properties of lead-doped cerium-bismuthides CeP_xBi_{1-x} . The main cause of our interest developed about the study of these doped compounds because of their sensitive character of rare earth elements with pnicogen family over impurity addition, temperature and pressure variations. As per our knowledge, no study on doped compounds of CeP with Si has been reported up till now, and it is first time the researchers make an attempt for theoretical study about the electronic, structural, and magnetic properties of these doped alloys. This study is edited as follows. In portion 2, the detail of the computation is written briefly. Section 2 reports the results and discussions. In the end, the conclusion is described in part 4 with brief of the findings as a summary.

2. Computational detail

For the simulation of compounds, Silicon atoms are doped in CeP compound as per the generic formula $CeSi_xP_{(1-x)}$ (X= 0.0, 0.25, 0.5, 0.75, 1.0). The Si-doped alloys of CeP have been developed with NaCl(cubic) crystal type structure remaining in space group number 225(Fm-3m) to make an investigation employing the first-principles DFT computations. The compounds CeP have atomic positions in the form as Ce (0,0,0) and P(0.5,0.5,0.5), while the phosphide atoms are changed only with silicon atoms in doped alloys despite shifting the atomic positions. The ambient conditions of pressures and temperatures are maintained during the study of these doped alloys as well as B1 type crystal phase structure. The structural designs of the supercells of $CeSi_xP_{(1-x)}$ alloys compounds are developed employing the FP-LAPW technique by using the WIEN2K technique [68] through ab initio-principles DFT [69, 70] formalism. The exchange-correlation potential part of KSE by Perdew-Brucke-Ernzerhof (PBE), Generalized-Gradient-Approximation, has been used for total energy calculations [71] for the majority as well as minority spins polarization.

The k-points mesh of 100 for these doped compounds for optimized computations is taken, and 100 is chosen for these compounds about SCF calculations for summation through an irreducible Brillion Zone to converge the energy completely. The used $R_{MT} \times K_{max}=6$ in which K_{max} is the highest amount of wave vector for interstitial plane while R_{MT} is the smallest radii of the atomic sphere within the said expansion. The experimental lattice constants and data of CeP compound have been utilized for the optimization of the structure. The ratio of the doping concentration of Si element with P element in CeP compound has made as .00, 0.25, 0.50, 0.75 and 1 and the doped alloys of cerium phosphide have modeled such as they remained in the NaCl-type cubic crystals system. This happened by replacing 0,1,2,3 and 4 numbers of phosphide atoms with silicon atoms in order. Hence relating to 4 atoms of P exist in a supercell of alloys of $CeSi_xP_{(1-x)}$ (x=0.0,0.25,0.50,0.75,1.00), 8 atoms of CeP (P=4, Ce=4).

3. Results and discussions

3.1. Structural properties

The crystal structures have been developed to investigate the structural properties of doped alloys with a doping ratio of Si atoms in crystals as are 0,1,2,3,4, respectively, and are presented in Figure 1(a-e). The structural parameters computed about these doped alloys in optimized structure forms have been described in Table 1. It is evident from given in table1 that the calculated parameters of lattice constants of these doped alloys of $CeSi_xP_{1-x}$ are underestimated as compared to already obtained experimental values [44] as well as theoretical data [45] of CeP of various DFT formalism. There is a constant increase in lattice constants with an increased doping ratio of Si atoms, and it becomes overestimated when P is completely replaced with Si atoms. We have noted a regular enhancement in the volume and energy of doped crystal cells whereas the decrease in their bulk modulus is reported with enhancing the substitution concentration of Si/P. These

results are derived by using Murnaghan's equation of state [72] for simplicity and brevity, which is given as under.

$$E(V) = E_0 + \frac{9V_0 B_0}{16} \left[\left\{ \left(\frac{V_0}{V} \right)^{\frac{2}{3}} - 1 \right\}^2 B_0' + \left\{ \left(\frac{V_0}{V} \right)^{\frac{2}{3}} - 1 \right\} \left\{ 6 - 4 \left(\frac{V_0}{V} \right)^{\frac{2}{3}} \right\} \right] \quad (1)$$

In this equation, B_0 represents the Bulk modulus of the alloys crystal system, the value of the volume of stable alloys at the ground state is described by V_0 and $B_0' = dB_0/dP$, is the amount of the pressure derivative of Bulk modulus these alloys.

By considering the minimum energy of these selected doped alloys, the plots between volume and total energy (V - E) are described as shown in Figure 2.

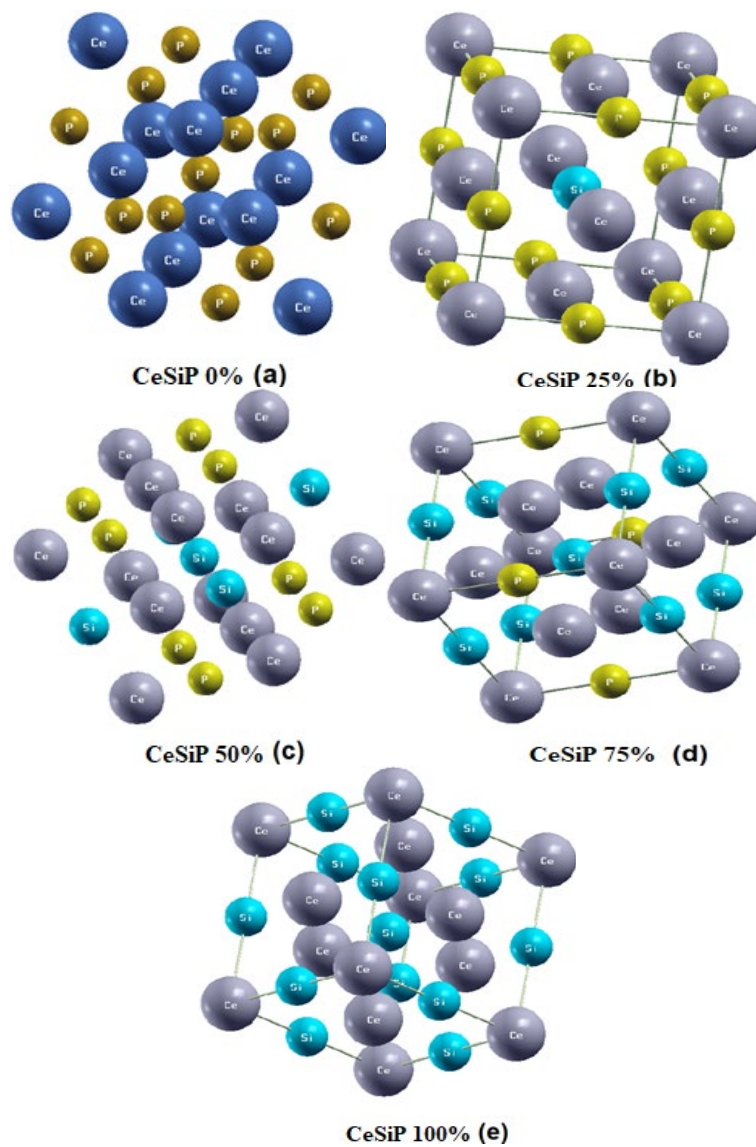


Fig. 1. Unit cell structures of silicon doped CeP compounds in $B_1(\text{NaCl})$ phase configuration (a) CeSiP 0% (b) CeSiP 25% (c) CeSiP 50% (d) CeSiP 75% (e) CeSiP 100%.

The total energy is kept in the MES and is theoretically calculated by the DFT technique through the FP-LAPW+lo scheme using PBE-GGA approximation. These doped alloys are observed as structurally stable through energy minima at various values of volumes of these doped alloys having their primitive unit cell. Bulk modulus of $\text{CeSi}_{0.75}\text{P}_{0.25}$ alloy calculated in our paper are agreed with already computed in Ref. [44,46]. We observe almost agreed values of lattice parameters of $\text{CeSi}_{0.0}\text{P}_{1.0}$ compound in this work with previous studies as presented in Ref. [44,45].

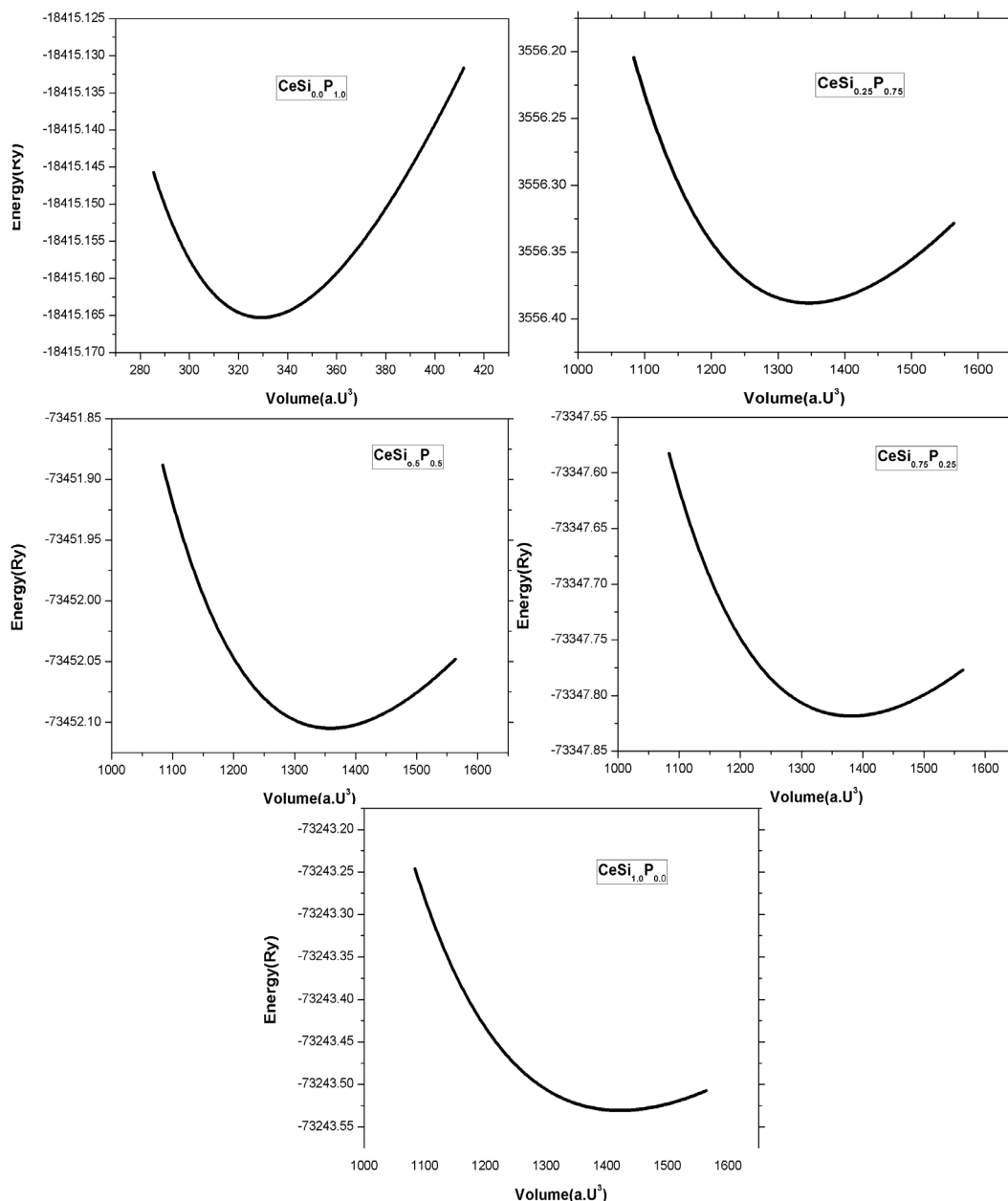


Fig. 2. Optimized Volume versus Energy graphs of doped compounds (a) $\text{CeSi}_{1.0}\text{P}_{0.0}$ (b) $\text{CeSi}_{0.25}\text{P}_{0.75}$ (c) $\text{CeSi}_{0.5}\text{P}_{0.5}$ (d) $\text{CeSi}_{0.75}\text{P}_{0.25}$ (e) $\text{CeSi}_{0.0}\text{P}_{1.0}$.

Table 1. Data of doped alloys of $CeSi_xP_{1-x}$ for their structural properties.

Sr. No.	Compound	Exp.Lattice constants(Å)	Computed Lattice constants(Å)	Volume(Å) ³	B(Gpa)	d/dpB(Gpa)	Energy(eV)
1	CeSi _{0.0} P _{1.0}	5.909[44]	5.8008 5.942[45]	329.3010	72.940 2 62 [44] 64 [46]	5.0000	-18415.9165250
2	CeSi _{0.25} P _{0.75}	Do	5.8431	1346.2267	66.669 9	5.0000	-73556.388066
3	CeSi _{0.5} P _{0.5}	Do	5.8611	1358.7058	70.868 4	5.0000	-73452.104776
4	CeSi _{0.75} P _{0.25}	Do	5.8936	1381.4667	64.401 3	5.0000	-73347.818327
5	CeSi _{1.0} P _{0.0}	Do	5.9506	1421.9042	58.10	5.0000	-73243.530598

3.2. Electronic properties

Interactions among electrons in solid materials play a central role in developing The overlapping of different atomic states from the electronic energy bands that total and partial densities of states can study. The approximation of PBE-GGA has been employed for minority as well as minority spins mode for the study of electronic properties against the said doped compounds. The Comparison of the structures of energy electronic bands is made in the form of plots of these five doped alloys of cerium silicon phosphide $Ce Si_xP_{1-x}$ ($x=0.0, 0.25, 0.5, 0.75, 1.0$) are given in Figure 3. It can be easily predicted that each doped alloy presents bands of electronic energy of similar nature against minority as well as majority spin polarization mode, despite the only change in graphs of electronic energy bands made by Si states through a change in the ratio of doping.

The first valence band (VB) at -10 eV develops mostly from P 2p states. For instance, in compound CeSi_{0.0}P_{1.0} a small VB was reported at -10 eV (Fig.3a) because of the filling of 2p states of the P atom. This could be verified by the density of state spectra of 2p orbital's of PDOS (Fig.4b) of same compound. The further thick atomic shape VB arises at -4 eV is developed through 4d states and in case of CeSi_{0.25}P_{0.75}doped compound, the next atomic-like VB exists at -7eV developed from 2s Pb orbital's that can also be confirmed from PDOS plot (Fig.4b) of the same doped compound. However, on enhancing the doping ratio of Si onwards from one to four atoms within supercells of $CeSi_xP_{1-x}$ compounds (see Figures 5-8), the atomic shape 2s Si states change slightly in the form of band-shape structure on going from 3a to 3e in plots. A larger VB at -2.5 eV from Fermi energy level at 0 eV is developed mainly through hybridizing 2p states of P and 4s states of Si with a small contribution of 6d orbitals of Ce atom.

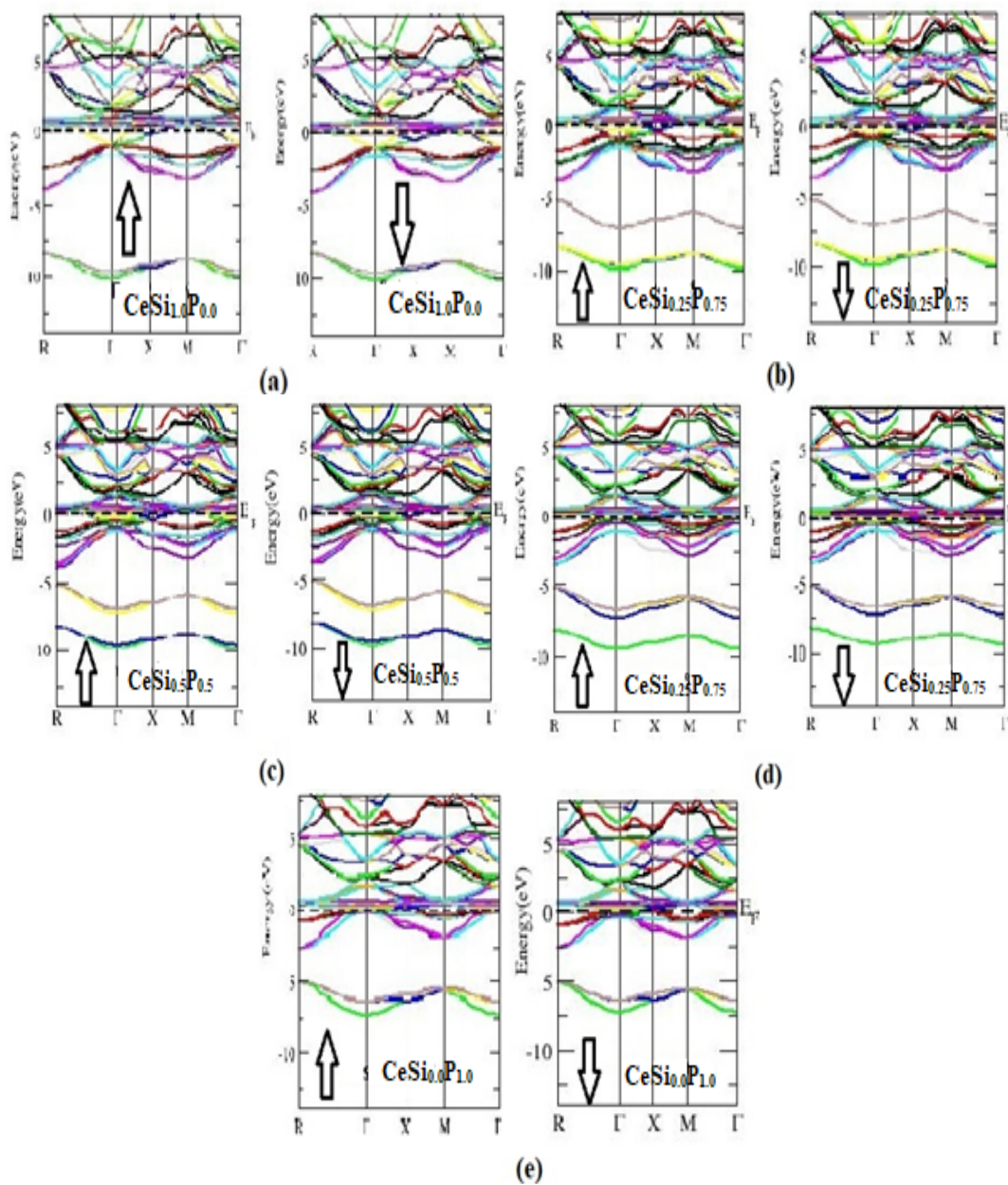


Fig. 3. A Comparison of electronic energy bands of cerium silicon phosphide with respect to substitution of silicon ratio for the minority and majority spin mode polarizations (a) $\text{CeSi}_{1.0}\text{P}_{0.0}$ (b) $\text{CeSi}_{0.25}\text{P}_{0.75}$ (c) $\text{CeSi}_{0.5}\text{P}_{0.5}$ (d) $\text{CeSi}_{0.25}\text{P}_{0.75}$ (e) $\text{CeSi}_{0.0}\text{P}_{1.0}$.

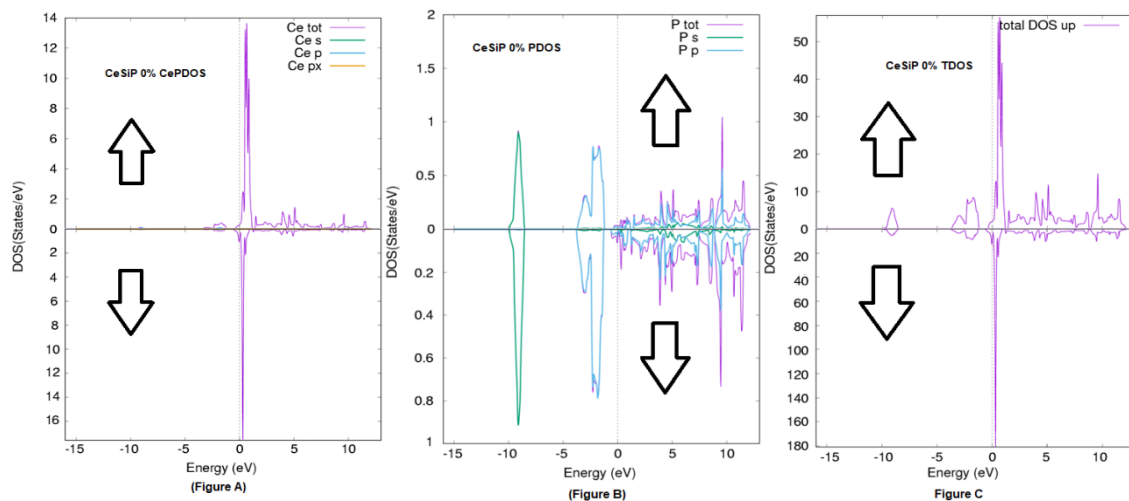


Fig. 4. Energy vs density of state graphs of partial and total densities of states for $CeSi_{0.0}P_{1.0}$ (a) PDOS of Ce (b) PDOS of P (c) TDOS of $CeSi_{0.0}P_{1.0}$.

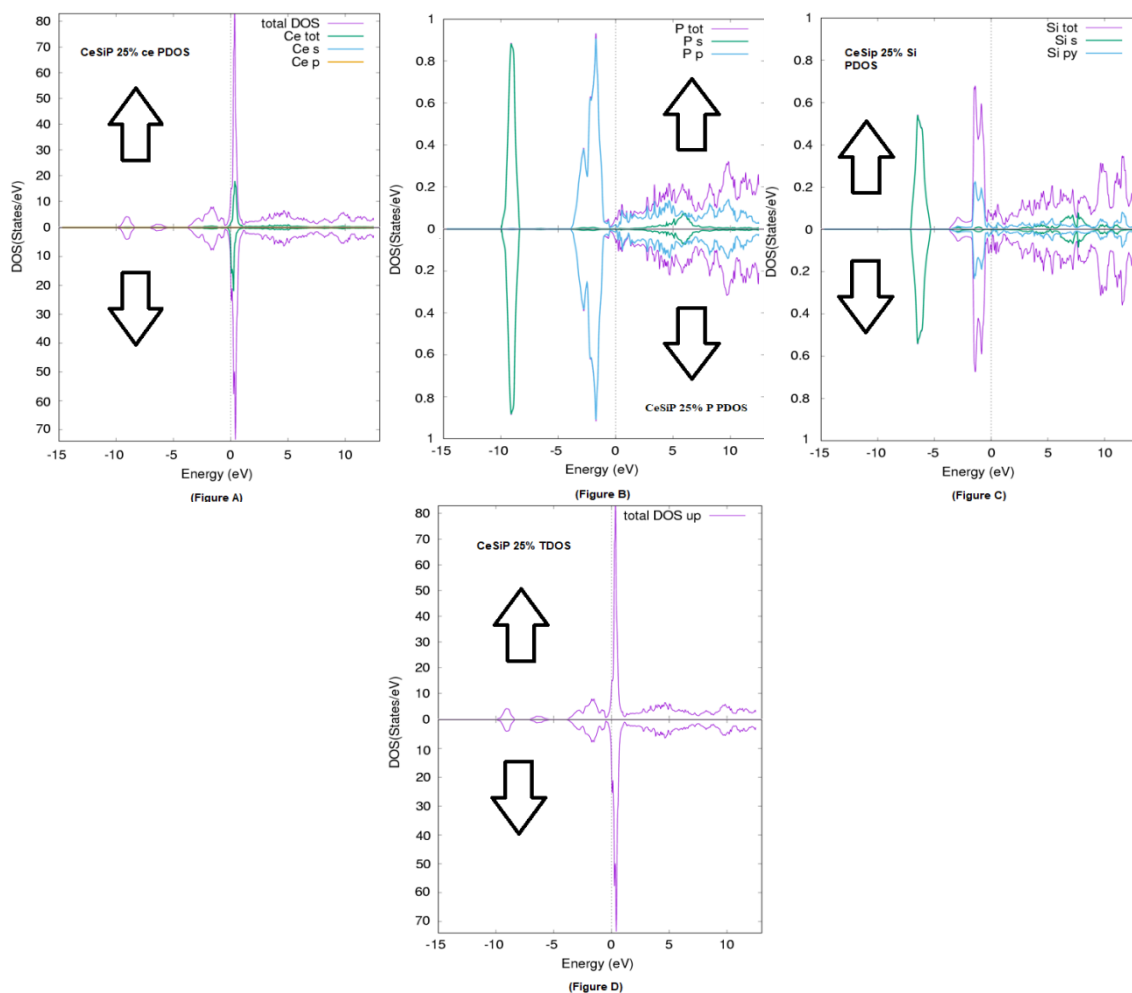


Fig. 5. Energy vs density of states graphs of partial and total densities of states for $CeSi_{0.25}P_{0.75}$ (a) PDOS of Ce (b) PDOS of Si (c) PDOS of P (d) TDOS of $CeSi_{0.25}P_{0.75}$.

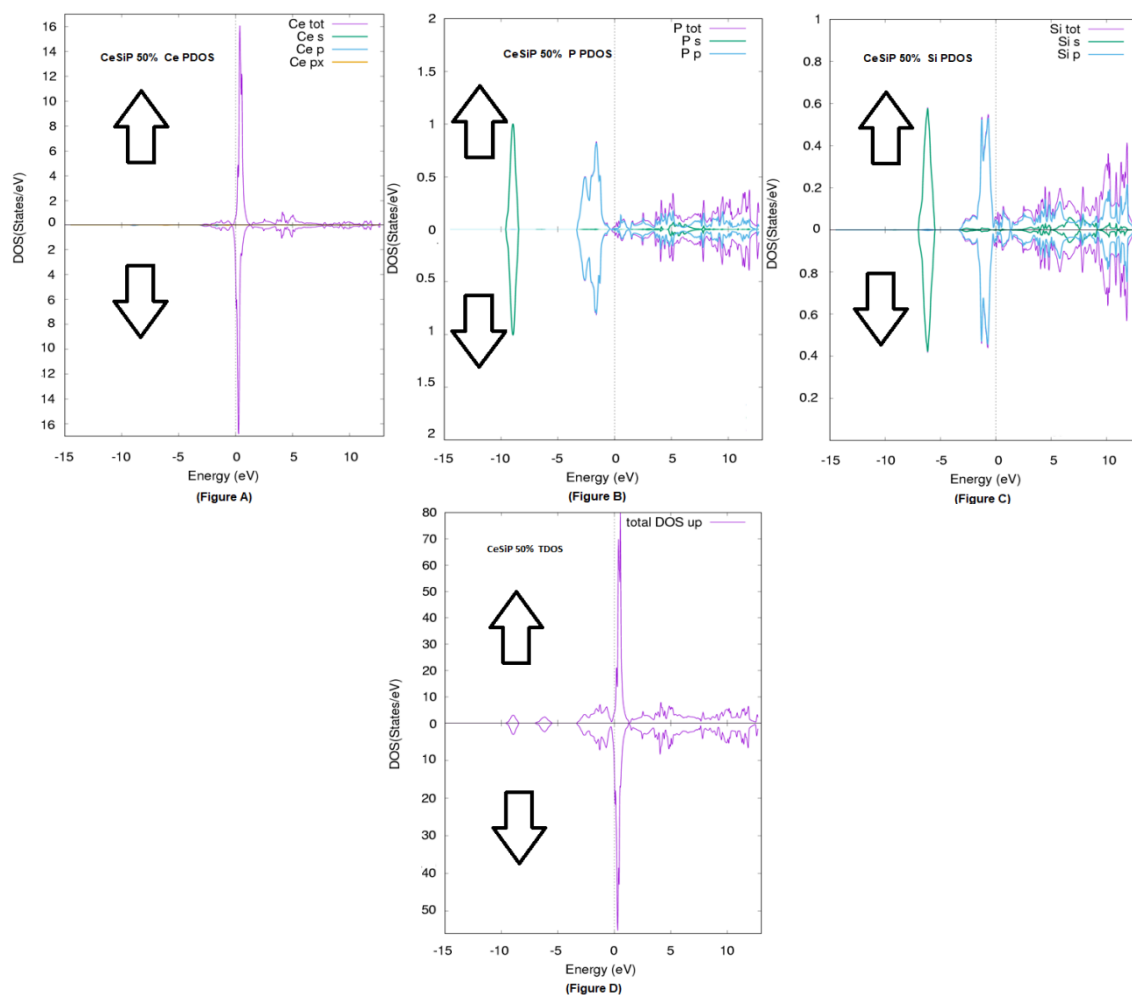


Fig. 6. Energy vs density of states graphs of partial and total densities of states for $\text{CeSi}_{0.5}\text{P}_{0.5}$ (a) PDOS of Ce (b) PDOS of Si (c) PDOS of P (d) TDOS of $\text{CeSi}_{0.5}\text{P}_{0.5}$.

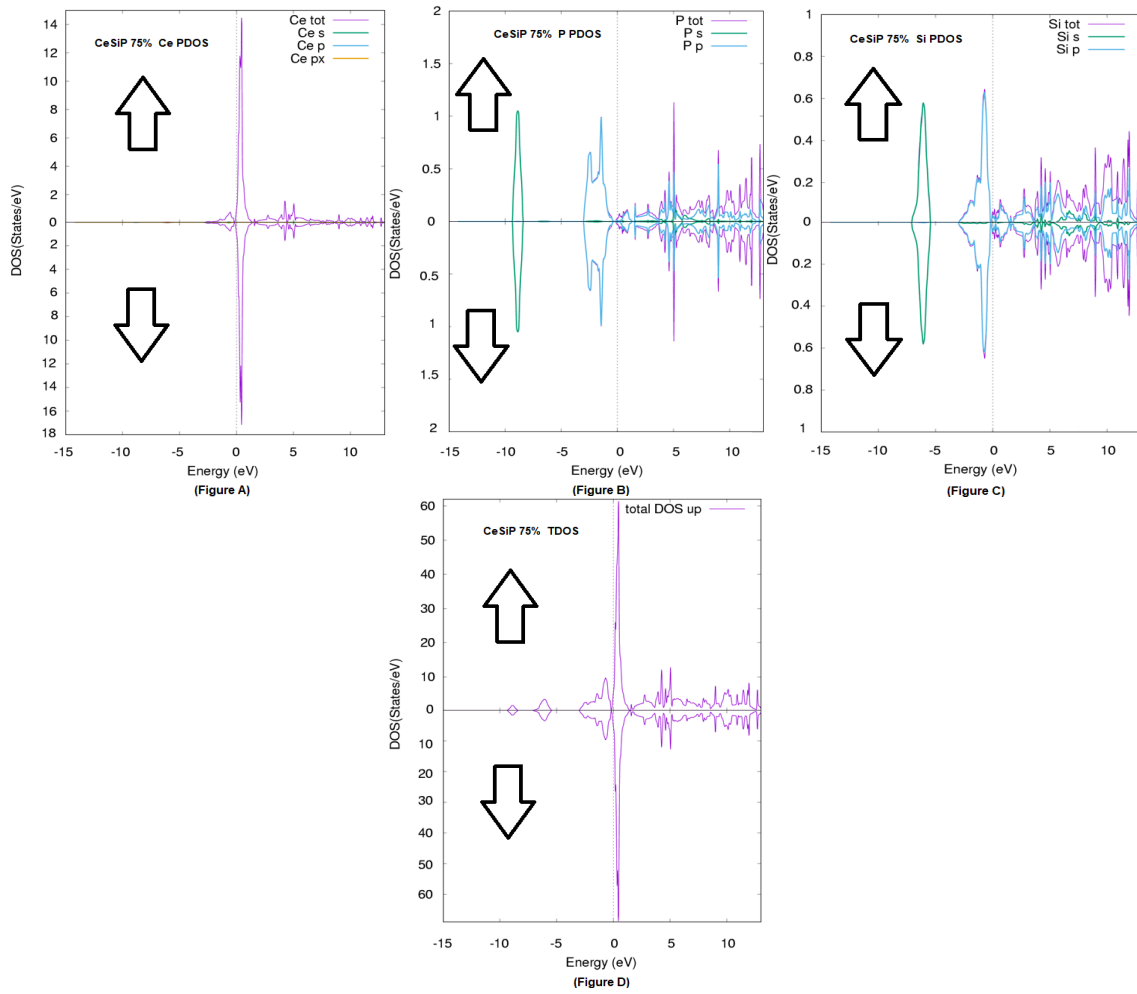


Fig. 7. Energy vs density of states graphs of partial and total densities of states for $CeSi_{0.75}P_{0.25}$
 (a) PDOS of Ce (b) PDOS of Si (c) PDOS of P (d) TDOS of $CeSi_{0.75}P_{0.25}$.

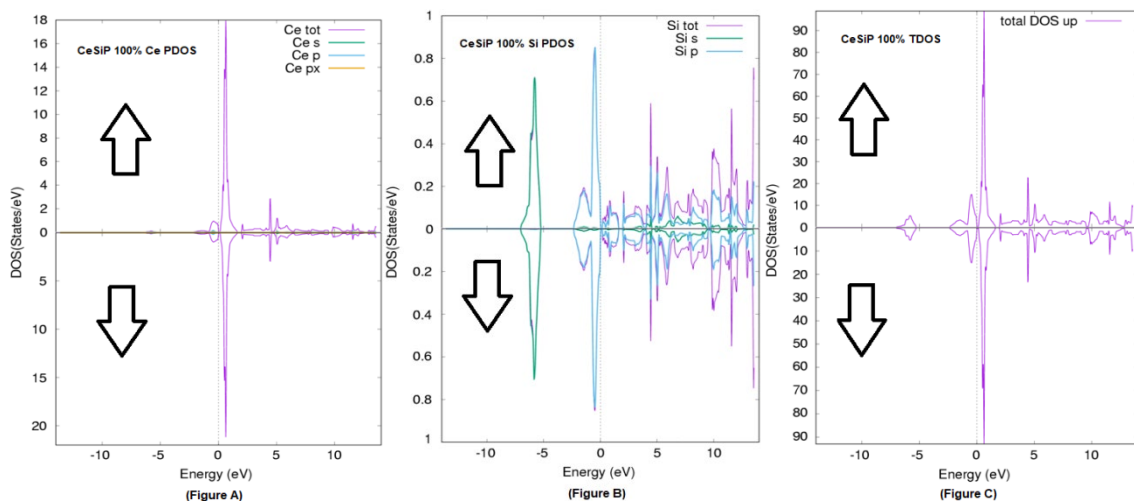


Fig. 8. Energy vs density of states graphs of partial and total densities of states for $CeSi_{0.250}P_{0.75}$ PDOS of Ce, PDOS of Bi, PDOS of Si and TDOS of $CeSi_{1.0}P_{0.0}$.

3.3. Magnetic properties

The magnetic properties of solid crystal materials can be described with spin magnetic moments and these magnetic moments occur in solid materials due to unpaired electrons. The net result of spin magnetic moments has zero value for diamagnetic materials due to the vanishing of different spins of electrons when they come in paired forms, but the non-zero net result of spin magnetic moments occurs in paramagnetic solid materials and the value of the moment is less developing though unpaired electrons. The net value of spin magnetic moments is high for ferromagnetic solid materials because of the presence of unpaired electrons in these materials. In the light of Hill theory [73], the value of overlapping of f-electrons wave function among attached f-electrons atoms determines solid materials' magnetic or superconducting nature. For example, solid materials with less f-electron atomic distance act as superconductors, and the situation in magnetic material differs. On the other hand, this standard does not cover in case of actinide compounds, while it is with agreement these material alloys.

According to the authors' study, the alloys had not been investigated before, despite the recent research about magnetic properties. It certainly will be a base and primary source for experimentalists for confirmation and further predictions. The computed spin magnetic moments about these doped alloys of $\text{CeSi}_x\text{P}_{1-x}$ along with silicon substitution ratio in percentages form are 0,25,50,75 and 100, respectively and are presented below in Table 2. As per computed data from the table, the largest amount of spin magnetic moment observed is $0.12771\mu_B$ for $\text{CeSi}_{0.25}\text{P}_{0.75}$ alloy and the value of spin magnetic moment diminishes with enhancing the substitution ratio of doping. The calculated values of spin magnetic moment are $-2.62322\mu_B$ and $-0.01496\mu_B$ for $\text{CeSi}_{0.0}\text{P}_{1.0}$ and $\text{CeSi}_{1.0}\text{P}_{0.0}$, respectively alloys and it predicts that on full substitution of phosphide atoms in place of silicon atoms, the thus developed alloy CeSi appears to be non-magnetic in nature presenting negative spin magnetic moment value. The remaining doped alloys are predicted to be magnetic in nature, the un-doped alloy $\text{CeSi}_{0.0}\text{P}_{1.0}$ observed as a non-magnetic material having less amount of $-2.62322\mu_B$ of spin magnetic moment, and others are observed as para-magnetic, containing slightly greater amount of spin magnetic moments.

Table 2. Data of computed spin magnetic moments of doped alloys of $\text{CeSi}_x\text{P}_{1-x}$.

Sr.No	Compounds	Spin Magnetic Moments(μ_B)
1	$\text{CeSi}_{0.0}\text{P}_{1.0}$	-2.62322
2	$\text{CeSi}_{0.25}\text{P}_{0.75}$	0.12771
3	$\text{CeSi}_{0.5}\text{P}_{0.5}$	-0.79591
4	$\text{CeSi}_{0.75}\text{P}_{0.25}$	0.00375
5	$\text{CeSi}_{1.0}\text{P}_{0.0}$	-0.01496

4. Conclusions

We have described the theoretical study of the electronic, magnetic and structural properties of alloys doped of cerium silicon phosphide through the generic formula $\text{CeSi}_x\text{P}_{1-x}$ ($X=0.0, 0.25, 0.5, 0.75, 1.0$) by employing the technique of first-principles of DFT formalism. In order to calculate the structural properties, a technique of full potential linearized augmented plane-wave+local orbital (FPLAPW)+lo is employed and the portion of exchange–correlation energy functional with Kohn-Sham equation is implemented through PBE-GGA approximation. The optimized lattice constants and other parameters of these crystals of cubic rock salt phase alloys of $\text{CeSi}_x\text{P}_{1-x}$ are computed and co-related, already reported in various studies. The structural stability is predicted from the said study. The partial and total densities of states and electronic energy bands graphs of doped alloys of $\text{CeSi}_x\text{P}_{1-x}$ predict that these doped alloys are naturally metallic, as overlapping in valance and conduction bands exists in energy band structures for both spin modes. The presence of mirror reflection in total and partial densities of states in both spin modes and zero energy band gap warrants that these doped compounds conductors are metals. The $0.12771\mu_B$ value of spin magnetic moments in $\text{CeSi}_{0.25}\text{P}_{0.75}$ doped compound reveals that the

compound is ferromagnetic and spin magnetic moment decreases on increasing the ratio of doping. The compound CeSi becomes diamagnetic with negative spin magnetic moment by changing all the phosphide atoms with silicon atoms. The compound CeP, which is un-doped, has a small amount of spin magnetic moment and is observed as paramagnetic. These fruitful and strange results warrant more investigation by scientists and researchers in order to describe the unique feature of these doped alloys. Especially, the structural, electronic, magnetic and thermoelectric properties of these doped alloys are still not studied experimentally to predict the potential candidacy of their technological as well as fundamental prospects.

Acknowledgements

Asif Mahmood would like to acknowledge the Researchers Supporting Project Number (RSP2024R43), King Saud University, Riyadh, Saudi Arabia.

References

- [1] Chattopadhyay, T. et al., Phys. Rev. B 49, 15096-15104(1994); <https://doi.org/10.1103/PhysRevB.49.15096>
- [2] Wakeham, N., Bauer, E. D., Neupane, M. Ronning, F. Phys. Rev. B 93,205152 (2016); <https://doi.org/10.1103/PhysRevB.93.205152>
- [3] Tsuchida, T., Wallace, W. E., J. Chem. Phys. 43, 2087-2092 (1965); <https://doi.org/10.1063/1.1697079>
- [4] Nereson, N. Arnold, G., J. Appl. Phys. 42, 1625-1627 (1971)
- [5] Tsuchida, T., Wallace, W. E., J. Chem. Phys. 43, 2885-2889(1965); <https://doi.org/10.1063/1.1660369>
- [6] Kasuya, T., Sakai, O., Tanaka, J., Kitazawa, H., Suzuki, T., J. Magn. Magn. Mater. 63-64, 9-14 (1987); [https://doi.org/10.1016/0304-8853\(87\)90507-5](https://doi.org/10.1016/0304-8853(87)90507-5)
- [7] Kumigashira, H. et al., Phys. Rev. B 56, 13654-13657 (1997); <https://doi.org/10.1103/PhysRevB.56.13654>
- [8] Kumigashira, H. et al., Phys. Rev. B 58, 7675-7680 (1998); <https://doi.org/10.1103/PhysRevB.58.7675>
- [9] Kumigashira, H. et al., Phys. Rev. B 54, 9341-9345 (1996); <https://doi.org/10.1103/PhysRevB.54.9341>
- [10] Norman, M. R., Koelling, D. D., Phys. Rev. B 33, 6730-6738 (1986); <https://doi.org/10.1103/PhysRevB.33.6730>
- [11] Morita, K. et al., Phys. B: Condens.Matter 230-232, 192-194 (1997); [https://doi.org/10.1016/S0921-4526\(96\)00587-X](https://doi.org/10.1016/S0921-4526(96)00587-X)
- [12] Ozeki, S. et al., Phys. B: Condens. Matter169, 499-500 (1991); [https://doi.org/10.1016/0921-4526\(91\)90295-P](https://doi.org/10.1016/0921-4526(91)90295-P)
- [13] Settai, R. et al., J. Phys. Soc. Jpn. 63,3026-3035 (1994); <https://doi.org/10.1143/JPSJ.63.3026>
- [14] Wu, F., Guo, C. Y., Smidman, M., Zhang, J. L. Yuan, H. Q., Phys. Rev. B 96, 125122(2017); <https://doi.org/10.1103/PhysRevB.96.125122>
- [15] Brooks, M. S. S., Eriksson, O., Wills, J. M., Johansson, B., Phys. Rev. Lett. 79, 2546-2549(1997); <https://doi.org/10.1103/PhysRevLett.79.2546>
- [16] Litsarev, M. S., Di Marco, I., Thunström, P. Eriksson, O., Phys. Rev. B 86, 115116 (2012); <https://doi.org/10.1103/PhysRevB.86.115116>
- [17] Larson, P., Lambrecht, W. R. L., Phys. Rev. B 74, 085108 (2006); <https://doi.org/10.1103/PhysRevB.74.085108>
- [18] Svane, A., Szotek, Z., Temmerman, W. M., gsgaard, J. L., Winter, H., J. Phys. Condens. Matter 10, 5309 (1998); <https://doi.org/10.1088/0953-8984/10/24/009>

- [19] Iwasa, K., Hannan, A., Kohgi, M., Suzuki, T., Phys. Rev. Lett. 88, 207201 (2002).
- [20] V. Srivastava, A.K. Bandyopadhyay, P.K. Jha, S.P. Sanyal, J. Phys. Chem. Sol. 64(2003) 907; <https://doi.org/10.1103/PhysRevLett.88.207201>
- [21] M. De, S. K. De, J. Phys. Chem. Sol. 60 (1999) 337; [https://doi.org/10.1016/S0022-3697\(98\)00286-8](https://doi.org/10.1016/S0022-3697(98)00286-8)
- [22] H. Takahasi, T. Kasuya, J. Phys. C 18 (1985) 2695; <https://doi.org/10.1088/0022-3719/18/13/019>
- [23] I. Shirotnani, K. Yamanashi, J. Hayashi, et al., J. Phys.: Condens. Matter 13 (2001)1939; <https://doi.org/10.1088/0953-8984/13/9/316>
- [24] I. Shirotnani, K. Yamanashi, J. Hayashi, et al., Phys. Rev. B 64 (2001) 132101; <https://doi.org/10.1103/PhysRevB.64.132101>
- [25] I. Shirotnani, K. Yamanashi, J. Hayashi, N. Ishimatsu, O. Shimomura, T.Kckegawa, Solid State Commun. 127 (2003) 570; [https://doi.org/10.1016/S0038-1098\(03\)00491-5](https://doi.org/10.1016/S0038-1098(03)00491-5)
- [26] T. Adachi, I. Shirotnani, J. Hayashi, O. Shimomura, Phys. Lett. A 250 (1998)389; [https://doi.org/10.1016/S0375-9601\(98\)00840-8](https://doi.org/10.1016/S0375-9601(98)00840-8)
- [27] J.M. Léger, D. Ravor, J. Rossat-Mignod, J. Phys. C: Solid State Phys. 17 (1984)4935; <https://doi.org/10.1088/0022-3719/17/28/010>
- [28] M. Yoshida, K. Koyama, T. Tomimsatsu, M. Shirakawa, A. Ochiai, M. Motokawa, J. Phys. Soc. Jpn. 70 (2001) 2078; <https://doi.org/10.1143/JPSJ.70.2078>
- [29] K. Koyama, M. Yoshida, T. Tomimatsu, T. Sakon, D. Li, M. Shirakawa, A. Ochiai, M. Motokawa, J. Phys. Chem. Solids 63 (2002) 1227; [https://doi.org/10.1016/S0022-3697\(02\)00053-7](https://doi.org/10.1016/S0022-3697(02)00053-7)
- [30] R. Settai, T. Goto, S. Sakatsume, Y. S. Kwon, T. Suzuki, T. Kasuya, Physica B 186(1993) 176; [https://doi.org/10.1016/0921-4526\(93\)90527-D](https://doi.org/10.1016/0921-4526(93)90527-D)
- [31] Y. S. Kwon, M. Tokeshige, T. Kasuya, Physica B 163 (1990) 328; [https://doi.org/10.1016/0921-4526\(90\)90202-6](https://doi.org/10.1016/0921-4526(90)90202-6)
- [32] H. Kumigashira, H.-D. Kim, T. Ito, A. Ashihara, T. Tokahashi, T. Suzuki, M.Nishimura, O. Sakai, Y. Kaneta, H. Harima, Phys. Rev. B 58 (1998) 7675; <https://doi.org/10.1103/PhysRevB.58.7675>
- [33] A. Hasegawa, J. Phys. C: Solid State Phys. 13 (1980) 6147; <https://doi.org/10.1088/0022-3719/13/33/012>
- [34] A. Hasegawa, J. Phys. Soc. Jpn. 54 (1985) 677; <https://doi.org/10.1143/JPSJ.54.677>
- [35] G. Vaitheeswaran, V. Kanchana, M. Rajagopalan, J. Alloys Compd. 336 (2002)46; [https://doi.org/10.1016/S0925-8388\(01\)01881-3](https://doi.org/10.1016/S0925-8388(01)01881-3)
- [36] G. Vaitheeswaran, V. Kanchana, M. Rajagopalan, Physica B 315 (2002) 64; [https://doi.org/10.1016/S0921-4526\(01\)01460-0](https://doi.org/10.1016/S0921-4526(01)01460-0)
- [37] G. Pagare, S. P. Samyal, P. K. Jha, J. Alloys Compd. 398 (2005) 16; <https://doi.org/10.1016/j.jallcom.2005.02.044>
- [38] E. Deligöz, K. Colakoglu, Y. O. Ciftci, H. Ozisik, J. Phys.: Condens. Matter 19(2007) 436204; <https://doi.org/10.1088/0953-8984/19/43/436204>
- [39] F. D. Khodja, A. Boudali, K. Amara, B. Amrani, A. Kadoun, B. Abbar, Physica B 403(2008) 4305; <https://doi.org/10.1016/j.physb.2008.09.030>
- [40] G. Gökoglu, A. Erkişi, Solid State Commun. 147 (2008) 221; <https://doi.org/10.1016/j.ssc.2008.05.013>
- [41] Z. Charifi, A. H. Reshak, H. Baaziz, Solid State Commun. 148 (2008) 139; <https://doi.org/10.1016/j.ssc.2008.07.038>
- [42] S. X. Cui, W. X. Feng, H. Q. Hu, Z. B. Feng, H. Liu, Solid State Commun. 149 (2009)996; <https://doi.org/10.1016/j.ssc.2009.04.012>
- [43] J. M. Leger, Physica B 190 (1993) 84; [https://doi.org/10.1016/0921-4526\(93\)90447-E](https://doi.org/10.1016/0921-4526(93)90447-E)
- [44] I. Shirotnani, J. Hayashi, K. Yamanashi, K. Hirano, T. Adachi, N. Ishimatsu, O. Shimomura, Physica B 334 (2003) 167; [https://doi.org/10.1016/S0921-4526\(03\)00042-5](https://doi.org/10.1016/S0921-4526(03)00042-5)

- [45] Haiyan Lu, Li Huang, 2020, J. Phys: Condens. Matter, 32485601.
- [46] I. Vedel et al, J. Phys. C 20 (1987)3439; <https://doi.org/10.1088/0022-3719/20/23/013>
- [47] G. Pagare, S. P. Sanyal, Phase Transitions 79 (2006) 935;
<https://doi.org/10.1080/01411590600979349>
- [48] Rossat-Mignod, J. Burlet, P., Quezel, S., Vogt, O., Physica 102B (1980) 237;
[https://doi.org/10.1016/0378-4363\(80\)90165-5](https://doi.org/10.1016/0378-4363(80)90165-5)
- [49] Baer, Y., Hauger, R., Zurcher, Ch., Campagna, M., Wertheim, G. K., Phys. Rev. B 18 (1978)4433; <https://doi.org/10.1103/PhysRevB.18.4433>
- [50] Jayaraman, A., Lowe, W., Longinotti, L. D., Phys. Rev. Lett. 36(1976) 366;
<https://doi.org/10.1103/PhysRevLett.36.366>
- [51] Werner, A., Hochheimer, H. D., Meng, R. L., Buchet, E., Phys. Lett. 97A (1983)207;
[https://doi.org/10.1016/0375-9601\(83\)90359-6](https://doi.org/10.1016/0375-9601(83)90359-6)
- [52] Hasega, Wa, A., J. Phys. C 13(1980) 6147; <https://doi.org/10.1088/0022-3719/13/33/012>
- [53] Takegahara, K., Takahashi, H., Yanase, A., Kasuya, T., Crystalline Electric Field Effects in f-electron Magnetism. Ed, R. P. Guertin, W. Suski, Z. Zol-mierek (Plenum Press) 1982, p.367;
https://doi.org/10.1007/978-1-4684-8646-9_42
- [54] Lavagna, M., Lacrolx, C., Cyrot, M., J. Phys. F13(1983)1007;
<https://doi.org/10.1088/0305-4608/13/5/014>
- [55] Allen, J. W., Martin, R. M., Phys. Rev. Lett. 49 (1982)1106;
<https://doi.org/10.1103/PhysRevLett.49.1106>
- [56] Leger, J. M., Epain, R., Loriers, J., Ravot, D., Rossat-Mignod, J. Phys. Rev. B 28, 12 (1983) 7125; <https://doi.org/10.1103/PhysRevB.28.7125>
- [57] Leger, J. M., Revat, D., Rasst-Mignod, J., J. Phys. C 17(1984) 4935;
<https://doi.org/10.1088/0022-3719/17/28/010>
- [58] Politecnica di Milano, Master Thesis in Engineering Physics, School of Industrial and Infracation Engineering, at ESRF (The European Synchrotron Radition Faculty, in Grenoble), 2016/2017.
- [59] Venn. H. Manked et al., Computational Material Science 65 (2012) 536-541;
<https://doi.org/10.1016/j.commatsci.2012.07.010>
- [60] Xu Duan, Fan Wu, Jia Chen, Perian Zhang, Yang Liu, Huiqiu Yuan and Chao Cao, Communications Physics (2018) 1:71;
<https://doi.org/10.1038/s42005-018-0074-8>
- [61] J. Rossat-Mignod, P. Burlet, S. Quezel, O. Vogt, Physik, 102B (1980) 237-248;
[https://doi.org/10.1016/0378-4363\(80\)90165-5](https://doi.org/10.1016/0378-4363(80)90165-5)
- [62] V. Mankad, S. K. Gupta, Z. Lukarevic, P. K. Jha, J. Phys. Conf. Ser. 377 012, 76 (2012);
<https://doi.org/10.1088/1742-6596/377/1/012076>
- [63] A. Jayaraman, Walter Lowc, L. D. Longinotti, E. Bucher, Physical Review Letters, Vol. 36, No. 7, (1976) page.366; <https://doi.org/10.1103/PhysRevLett.36.366>
- [64] F. Hulliger, M. Landolt, H. R. Ott, R. Schmcclzcer, Journal of Low Temperature Physics, Vol. 20, No. 3/4.(1975) page 269; <https://doi.org/10.1007/BF00117797>
- [65] Wenkia Fang, Heiquan Hu, Xiaoguang Xiao, Shouxin Cui, Zengtao Lv, Guiqing Zhang, Cheng Wu, Computational Materials Science 53 (2012) 75-78;
<https://doi.org/10.1016/j.commatsci.2011.09.019>
- [66] J. M. Leger, K. Oki, J. Russat-Mignot, O. Vegt, J. Physique 46 (1985) 889-894;
<https://doi.org/10.1051/jphys:01985004606088900>
- [67] A. Iqbal, Bashir, M. S, S. A, Amin-ur-Rahman, Computational Condensed Matter 31(2022) e00668; <https://doi.org/10.1016/j.cocom.2022.e00668>
- [68] P. Blaha, K. Schwarz, G. K. H. Madsen, D. Kvasnicka, J. Luitz, in: K. Schwarz (Ed). WEIN2K, an Augmented Plane Wave Plus Local Orbitals Programme for calculating crystal properties, Techn. University, Wein, Austria, 2001.
- [69] P. Hohenberg, W. Kohn, Phys. Rev. B 136(1964) 864;

<https://doi.org/10.1103/PhysRev.136.B864>

[70] W. Kohn, I. J. Sham. Phys. Rev. A 140(1965) 1133;

<https://doi.org/10.1103/PhysRev.140.A1133>

[71] J. P. Perdew, K. Bruke, M. Ernzerh, Phys. Rev. Lett. 77(1996) 3865;

<https://doi.org/10.1103/PhysRevLett.77.3865>

[72] F. D. Murnaghan, Proc. Natl. Acad. Sci., USA, 30 (1944) 244;

<https://doi.org/10.1073/pnas.30.9.244>

[73] H. H. Hill, in: W. N. Miner (Ed.), Plutonium 1970 and other Actinides, The metallurgical society of the AIMF, New York, 1970.