A first-principles theoretical study of structural, electronic, and magnetic properties of lead-doped alloys of praseodymium bismuth compounds PrPb$_x$Bi$_{1-x}$

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The magnetic, electronic, and structural properties of the cubic phase of lead-doped alloys of praseodymium bismuth compounds with the generic formula PrPb$_x$Bi$_{1-x}$ (x = 0, 0.25, 0.50, 0.75, and 1.0) have been reported in this paper by employing the formalism of density functional theory (DFT). For the analysis of physical properties, we have executed the full-potential linearized augmented plane wave plus local orbit (FPLAPW+lo) technique, while the exchange-correlation potentials in the Kohn-Sham equation (KSE) are implemented within the generalized gradient approximation (GGA) extended by the Perdew-Burke-Ernzerhof (PBE) correction. The structural parameters, lattice constants, volume, bulk modulus, pressure derivatives, and energy have been computed with the Wein2k code by fitting total energy through Murnaghan's equation of state. The structural stability of the compounds has been reported from the spin-polarized calculations. The electronic energy bands and total and partial densities of states of the compounds have been calculated in both majority and minority spins, depicting them as metallic. The similar spectrum intensities of the Pr(5d+4f) and (Pb +Bi)2p states account for the majority of the contribution to the density of states near the Fermi energy level. The spin magnetic moments computed for the supercell of the doped compounds have indicated that they are magnetic materials. From the comparison of spin magnetic moments in the PrBi compound, we noticed an improvement in the magnetic moments after doping lead into the PrBi compound.

1. Introduction

Even though various rare-earth (RE) chalcogenides and pnictides have a straightforward NaCl (rock-salt) structure, their magnetic and electronic characteristics greatly pique researchers' curiosity [1]. On the other hand, scientists' current focus has been on finding novel rare-earth materials for advanced spintronic devices [2–5]. The attention paid to the investigation of these solid materials has recently been enhanced greatly after the development of solid materials epitaxially from III-V semiconductors [6]. As a result, a method for creating electrical devices like metal-base transistors was discovered. Due to the potential uses of hyperfine increases in nuclear cooling and the investigation of mixed nuclear ordering and electron phenomena at far lower temperatures [7], praseodymium chalcogenide have attracted much interest. By categorizing the rare earths and related composites in terms of their valencies, a basic description of their physical properties can be made. Valency modification can be connected with variations in the lattice parameter of rare earths in particular [8]. The periodic table of the elements places praseodymium closer to cerium as several of cerium's distinctive characteristics, as well as those of its

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composites, are shared by praseodymium. As such, the investigation of lead-doped compounds of Pr mono-pnictides warrants to explore more varieties of the material's properties.

Earlier, the structural phase transition and electronic arrangement of lanthanum mono-pnictides [9, 10] and mono-chalcogenides [11] have been reported by employing the self-consistent tight-binding linear muffin-tin orbital (LMTO) technique under pressure. Their physical properties are influenced by the number of valence electrons [12, 13]. The optical and electronic characteristics of Pr pnictides [14] have been explored by using the LDA+U method. In another approach of local spin density (LSD), along with the LDA+U technique, the RE Sb compounds [15] and the Gd and Er pnictides [16] have been investigated. The theoretical study of Pr mono-chalcogenides and mono-pnictides was carried out using an ab initio electronic technique with self-interaction-corrected LSD correlation [17]. The electronic structures of trivalent and divalent rare-earth sulfides [18, 19] have already been studied using the SIC-LSD technique.

Electronic structure, structural phase transition, and under-pressure studies have been made about chalcogenides and pnictides of Ce [20, 21] by using SIC-LSD corrections. The phase change of PrP from B1 to B2, which occurs approximately at 2 GPa, has been reported experimentally [22]. Additionally, similar structural phase transitions from B1 to B2 at 27, 13, 14, and 9 GPa for PrAs [23], PrSb [24], PrBi [25], and PrTe [26], respectively, have been reported. Vaitheeswaran et al. [27] have theoretically studied the electronic structure of praseodymium mono-chalcogenides and mono-pnictides at high pressure by using LSD-SIC corrections.

The optical and electronic characteristics of praseodymium mono-pnictides have been investigated by De et al. [28] by employing the LMTO technique with LDA and atomic sphere approximation. Pagare et al. [29, 30] have reported the elastic constants and the structural phase transition in rare earth mono-antimonides and mono-bismuthides, along with the PrBi and PrSb compounds, at high pressure by employing the inter-ionic potential theory, where the body-centred (bc) tetragonal phase has been observed at large pressure. Soni et al. [31] have examined the elastic properties and high-pressure behavior of praseodymium mono-pnictides and mono-chalcogenides with a B1 (NaCl) type structure by employing interionic potential theory. In condensed matter physics, investigations on topological systems like topological insulators [32, 33], Dirac semimetals [34, 35], and Weyl [36, 37] report the relativistic Dirac-like low-energy excitations because of their strange bulk band topology like much large mobility, low carrier density, very large magnetoresistance, a Berry phase of π and chiral-anomaly driven negative magnetoresistance (MR).

Materials that show exotic properties both by mixing the electron correlation and topology with common 4f electron presence have been reported as examples in the pyrochlore iridates $R_2Ir_2O_7$ [36] and the Kondo insulator $SmB6$ [38]. Rare-earth materials which may provide possibilities of harbouring associated electrons with topological features are RY mono-pnictides (R = rare-earth, Y = Bi, Sb). A few rare-earth-dependent mono-pnictides have been investigated for similar unusual magneto-transport properties in topological semimetals [39–45]. Another study of rare materials like LaBi compound, shows that despite the presence of Dirac cones, the bands around the X point have a Dirac nodal line character [46, 47]. Many other composites like LaSb, LaAs, ScSb, PrSb, LuBi, YSb, and TmSb [39, 43, 48–52], in the rare-earth series, present transport properties similar to LaBi compound, although they are described trivially as topological. Due to the expected 4f-correlation electron effect on topological properties, the study of RY material's magnetic rare-earth would be strange and interesting [53]. Most magnetic RY materials exhibit large-range magnetic order at lower temperatures [54], making it difficult to investigate magnetotransport properties at lower temperatures. PrBi possesses partially full 4f states but exceptionally does not order at temperatures below 1.8 K; it is exceptional in this regard [55]. The PrBi compound is hence a unique semiconductor at which the existence of a strong correlated aspect of topological semimetals is increased by the existence of f electrons as well as the potential topological band framework that developed in ARPES. Belgin et al. [56] have worked on the elastic, structural, thermal, and lattice dynamics characteristics of PrZ (Z = Bi, Sb). Topological and adjustable electronic structural features of LnPn (Ln = Pr, Ce, Yb, Sm, Gd, Pn = Bi, Sb) have been reported by Xu et al. [57]. Recently, Amit et al. [58] have described the Fermi surface topology and substantial magneto resistance in the topological semi-metal applicant PrBi compound. The first-principles DFT study on the tunable Fermi surface topology and interplay

between magnetism and superconductivity of PrSb has been reported by Sn substitution [59]. Moreover, the interplay between intermetallic and intermagnetic of CePbxBi1-x RE bismuthides have been investigated with heavy-fermionic magnetic conduction [60].

As per our knowledge, no study about doped alloys of $PrPb_xBi_{1-x}$ on the target properties has been reported yet. Hence, the investigation of electronic and magnetic properties of such doped compounds may be notable, warranting attention, interest, and motivation. $PrPbxBi_{1-x}$ compounds are a part of the broader class of rare-earth pnictide compounds. The substitution of different elements by changing the composition (x) of Pb/Bi compounds can lead to tunable properties. By varying the composition of $PrPb_xBi_{1-x}$, researchers can investigate the effects of Pb/Bi ratio on various physical properties such as electrical conductivity, magnetism, thermal conductivity, or superconductivity. Rare-earth pnictide compounds, including $PrPbxBi_{1-x}$, have been of great interest in the search for high-temperature superconductivity. By doping or modifying the composition, researchers hope to discover or enhance superconducting behavior at higher temperatures. Understanding the relationship between composition, crystal structure, and superconductivity can provide insights into the underlying mechanisms of superconductivity and potentially lead to the discovery of new superconducting materials [59,60]. Rare-earth pnictide compounds exhibit a range of intriguing phenomena, such as quantum criticality, topological insulator behavior, superconductivity, and heavy fermion behavior. Taking this fact into account, we explore in this work novel electronic states that emerge as a result of doping or composition changes for $PrPb_xBi_{1-x}$, mainly focusing on clarifying the electronic, structural, and magnetic properties.

The field of rare-earth pnictide compounds, exemplified by $PrPb_xBi_{1-x}$, is currently at the forefront of emerging technologies, with promising applications spanning energy storage, spintronics, and quantum computing. In this project, we embark on an exploration of these compounds with the primary goal of unraveling novel functionalities and facilitating their practical application. Our research focuses on comprehending the intriguing structural, electronic and magnetic properties of these materials and deciphering the ramifications of doping or changes in composition on these properties. Through this endeavor, we aspire to contribute to the advancement of cutting-edge technologies and offer insights into the future possibilities these compounds hold. The structure of our work in this this paper is as follows: The second section delves into the preliminary aspects of our study, providing an overview of the research design and methodology. In the subsequent section, we present computational findings, engaging in in-depth discussions that elucidate the implications of our research. Lastly, we conclude with a summary of our study's key findings and offer a glimpse into the potential directions for future research in this fascinating and rapidly evolving field.

2. Computational details

The atoms of lead existing in the IV group of the periodic table of elements are substituted into PrBi compounds to obtain the objected compounds in the form of developed chemical relation $PrPb_xBi_{1-x}$ $(x = 1.0, 0.75, 0.5, 0.25,$ and $0)$. The substituted alloys of PrPbBi compounds in cubic crystal systems are modelled with space group Fm3m (225) for the first-principle DFT computations. The aforementioned compounds are examined in a NaCl-class arrangement with the B1 phase under no pressure or temperature conditions. The positions of the atoms in PrBi compounds exist at Bi (1/2, 1/2, 1/2) and Pr (0, 0, 0), and only bismuth atoms are changed with lead atoms in the doped compounds without any replacement of atomic positions. The supercell structures developed for $PrPb_xBi_{1-x}$ doped compounds are modelled through the FPLAPW+lo [61–64] technique employed by the WIEN2K code [65], implemented with the first-principles DFT [66,67] formalism. The total energy is calculated by the Perdew-Burke-Ernzerhof generalized gradient approximation (PBE-GGA) [68] by employing the Kohn-Sham equation in the exchange-correlation parts for both minority and majority spin polarizations. The effects of columbic interaction and orbital-dependent exchange among the electrons were taken into account in the DFT+U computations [69–72].

In an irreducible Brillouin zone with well-defined energy convergence, a mesh of about 100 k-points concerning the said doped compounds was computed. We utilized $R_{MT} x\ K_{max}= 6$, where R_{MT} is the smallest sphere of atomic radii and K_{max} is the largest value of the interstitial plane wave vector in the equation. The optimization of structures is made by using experimental data on the lattice parameters of the PrBi compound. The cubic crystals of the B1 phase (NaCl type) of the doped praseodymium bismuth alloys are constructed with lead impurity ratios of 0%, 25%, 50%, 75%, and 100%. This relates to the substitution of lead atoms with the numbers 0, 1, 2, 3, and 4 of bismuth. Relative to the 4 atoms of Bi that exist in the supercells of $PrPb_xBi_{1-x}$ (x = 1.0, 0.75, 0.5, 0.25, and 0.0), there are 8 atoms of PrBi (Pr = 4 and Bi = 4).

3. Results and discussions

3.1. Structural properties

The substituted impurity ratio of Pb atoms in every crystal structure is 0, 1, 2, 3, and 4, respectively. The structural parameters calculated regarding these substituted compounds are reported in Table 1 and present no large variations due to the impurity addition ratio. As given in Table 1, the computed lattice constants of $PrPb_xBi_{1-x}$ compounds are high as compared to the experimental value of PrBi [25] and theoretical data reported through different DFT formalisms [1, 28, 30, 58]. The lattice parameters calculated in our study are underestimated as compared to some already reported investigations, for instance, in Refs. [27, 57]. However, a small decrease in lattice parameters is observed on increasing the doping concentration, and similar results are reported regarding bulk modulus as well as the total energy of these doped compounds. The bulk modulus computed is underestimated when compared with already-made studies [27, 30, 57], and overestimation is observed in Ref. [25]. The said physical parameters are computed through Murnaghan's equation of state [73], which is given below.

$$E(V) = E_0 + \frac{9V_0B_0}{16}\left[\left\{\left(\frac{V_0}{V}\right)^{2/3} - 1\right\}^2 B'_0 + \left\{\left(\frac{V_0}{V}\right)^{2/3} - 1\right\}^2 \left\{6 - 4\left(\frac{V_0}{V}\right)^{2/3}\right\}\right]$$

where V_0, E_0, B_0, and B' are the volume, energy, bulk modulus, and pressure derivative of these doped compounds at ground states, respectively. The crystal structures modelled with doped compounds are shown in Fig. 1, and the optimized energy vs. volume plots computed are given in Fig. 2.

PrPbBi 0%
(a)

PrPbBi 25%
(b)

PrPbBi 50%
(c)

PrPbBi 75%
(d)

PrPbBi 100%
(e)
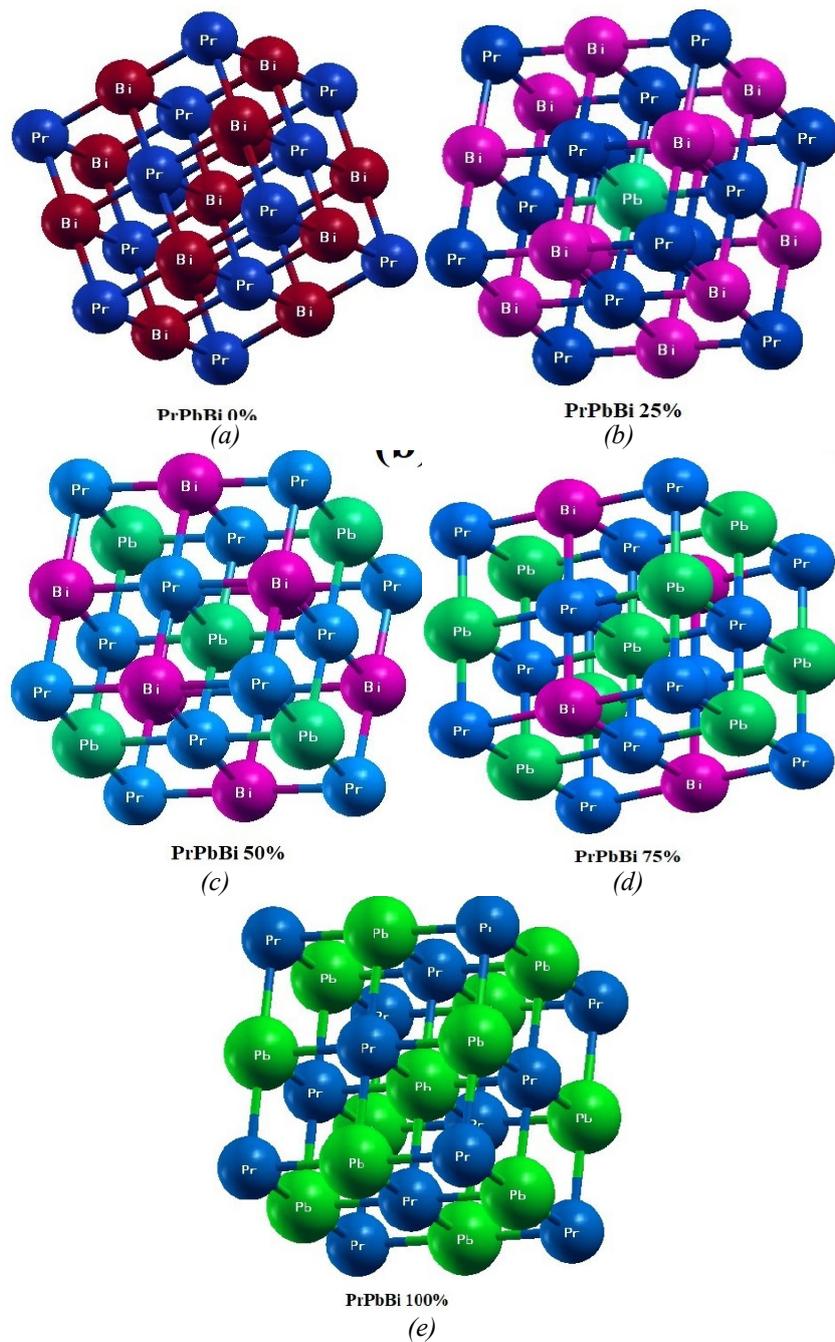
Fig. 1. Crystal structure of (a) $PrPb_{0.0}Bi_{1.0}$ (b) $PrPb_{0.25}Bi_{0.25}$ (c) $PrPb_{0.5}Bi_{0.5}$ (d) $PrPb_{0.75}Bi_{0.25}$ (e) $PrPb_{1.0}Bi_{0.0}$.
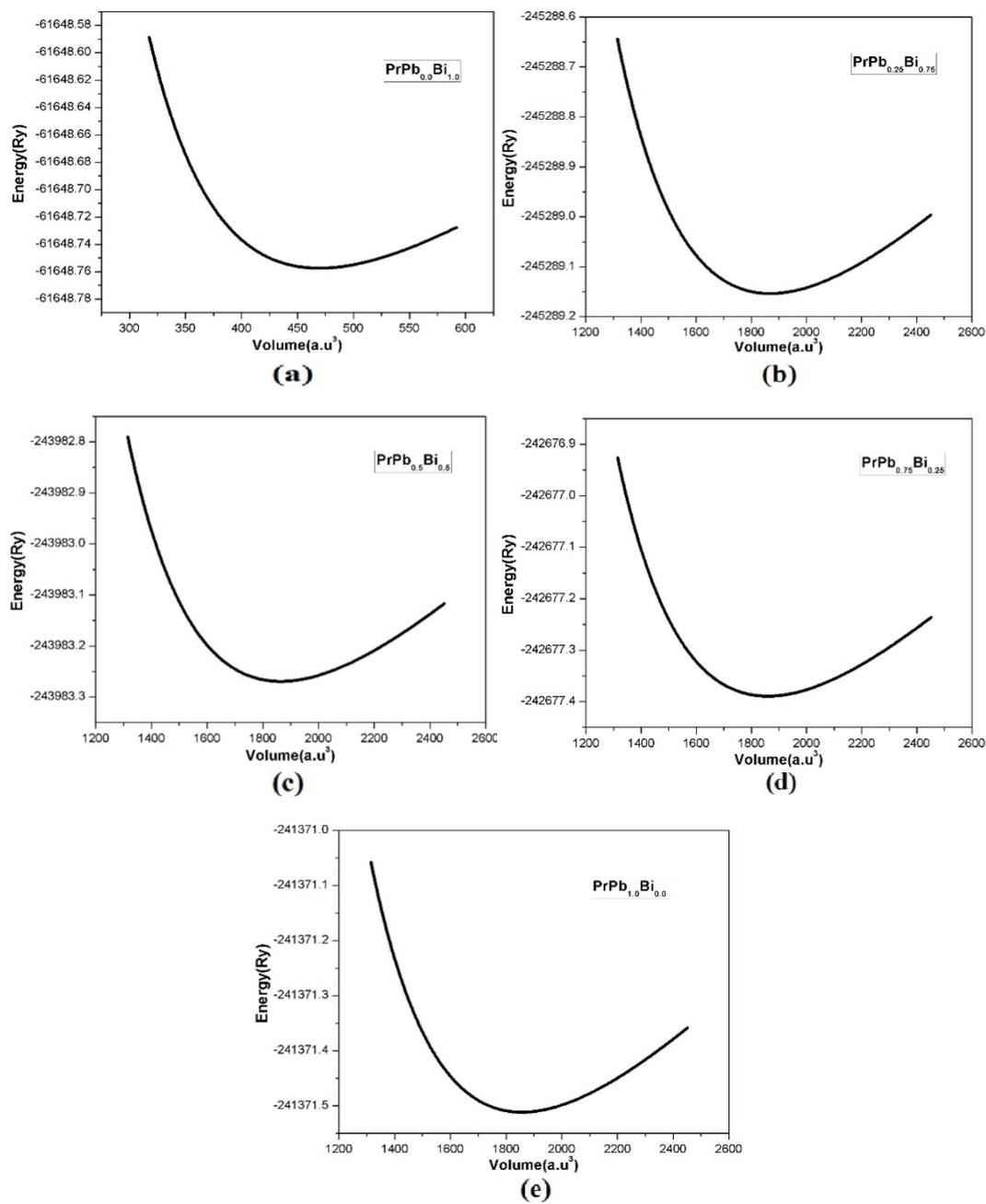
Fig. 2. The total optimized volume vs energy of (a) $PrPb_{0.0}Bi_{1.0}$ (b) $PrPb_{0.25}Bi_{0.25}$ (c) $PrPb_{0.5}Bi_{0.5}$ (d) $PrPb_{0.75}Bi_{0.25}$ (e) $PrPb_{1.0}Bi_{0.0}$.

Table 1. Data of structural parameters of substituted compounds of PrPb$_x$Bi$_{1-x}$.

Sr.No.	Compound	Approximation	Exp. Lattice Parameters (A^0)	Calculated Lattice Parameters (A^0)	Volume (A^0)^3	Bulk modulus B(Pa)	B'=dB/dp	Energy (Ryd)
1	PrPb$_{0.0}$Bi$_{1.0}$	PBE-GGA	6.455[25]	6.5295 12.210(a.u) [28] 6.566[56] 11.99(a.u)[27] 6.53[58] 3.2407[30]	469.6442	42.5040 48.940[28] 42.51[30] 51[27]	5.00000	-61648.757417
2	PrPb$_{0.25}$Bi$_{0.75}$	PBE-GGA	Do	6.5182	1868.8835	42.2722	5.0000	-245289.153524
3	PrPb$_{0.5}$Bi$_{0.5}$	PbE-GGA	Do	6.5138	1865.1126	40.4812	5.0000	-243983.269328
4	PrPb$_{0.75}$Bi$_{0.25}$	PBE-GGA	Do	6.5078	1859.9712	40.2980	5.0000	-242677.389234
5	PrPb$_{1.0}$Bi$_{0.0}$	PBE-GGA	Do	6.5044	1857.0401	39.7062	5.0000	-241371.511392

3.2. Electronic properties

Despite the different energies of the atoms in solids, electronic interactions are crucial in the creation of continuous electronic energy bands. The electronic energy band structure is described through the overlaps of different molecular shells that may be studied by utilizing the partial and total density of states (DOS). We have employed the PBE-GGA approach for both minority and majority spin polarizations in the study of the electronic characteristics of these substituated compounds. Comparable electronic band spectra of these five elements, PrPb$_x$Bi$_{1-x}$ (x = 0.0, 0.25, 0.50, 0.75, and 1.0), are given in Fig. 3. Similar energy bands have been reported for all compounds for minority and majority spin polarizations, except for variations in shape in the energy band developed through Pb shells with the change of doping ratio.

The first valence band (VB) in the range of -10.5 eV to -9.0 eV develops mostly from Bi 2s orbitals. For instance, in the case of PrPb$_{0.25}$Bi$_{0.75}$, a large VB from -10.5 to -9.0 eV (Fig. 3b) occurs mostly from the occupied Bi 2s shells. It may also be verified through the spectral intensity of Bi 2s orbitals from the partial density of states (Fig. 5c). The further small atomic-like VB at -8.0 to -7.0 eV is caused by Pb 2s states. However, by enhancing the concentration of Pb atoms from one to four in supercells of PrPb$_x$Bi$_{1-x}$, the atomic-like P 2s states change slowly into structure-like bands. When we go from Fig. 3a to Fig. 3e, the large VB is -2.0 eV at Fermi level E$_f$. E$_f$ is developed mostly by hybridization of Bi and Pb 2p orbitals, with less contribution from Pr 6d shells. The conduction band (CB) over the E$_f$ occurs mostly through the overlapping of Pr 4f shells with some involvement of Pr 5d orbitals and (Pb+Bi) 2p orbitals. It can also be verified from the total and partial DOS of about PrPb$_{0.25}$Bi$_{0.75}$ as given in Fig. 5. The significant overlap of CB and VB beyond and below the Fermi level demonstrates that praseodymium lead-bismuth is a good conductor of metallic nature. This agrees with earlier investigations on PrBi [19, 21]. It is interesting to note that by increasing the substitution of Pb, the topology of Fermi surface and energy bands spectra is modified considerably as observed earlier to explore the heavy fermionic nature and interplay between magnetic and superconductivity of RE compounds [59, 60].
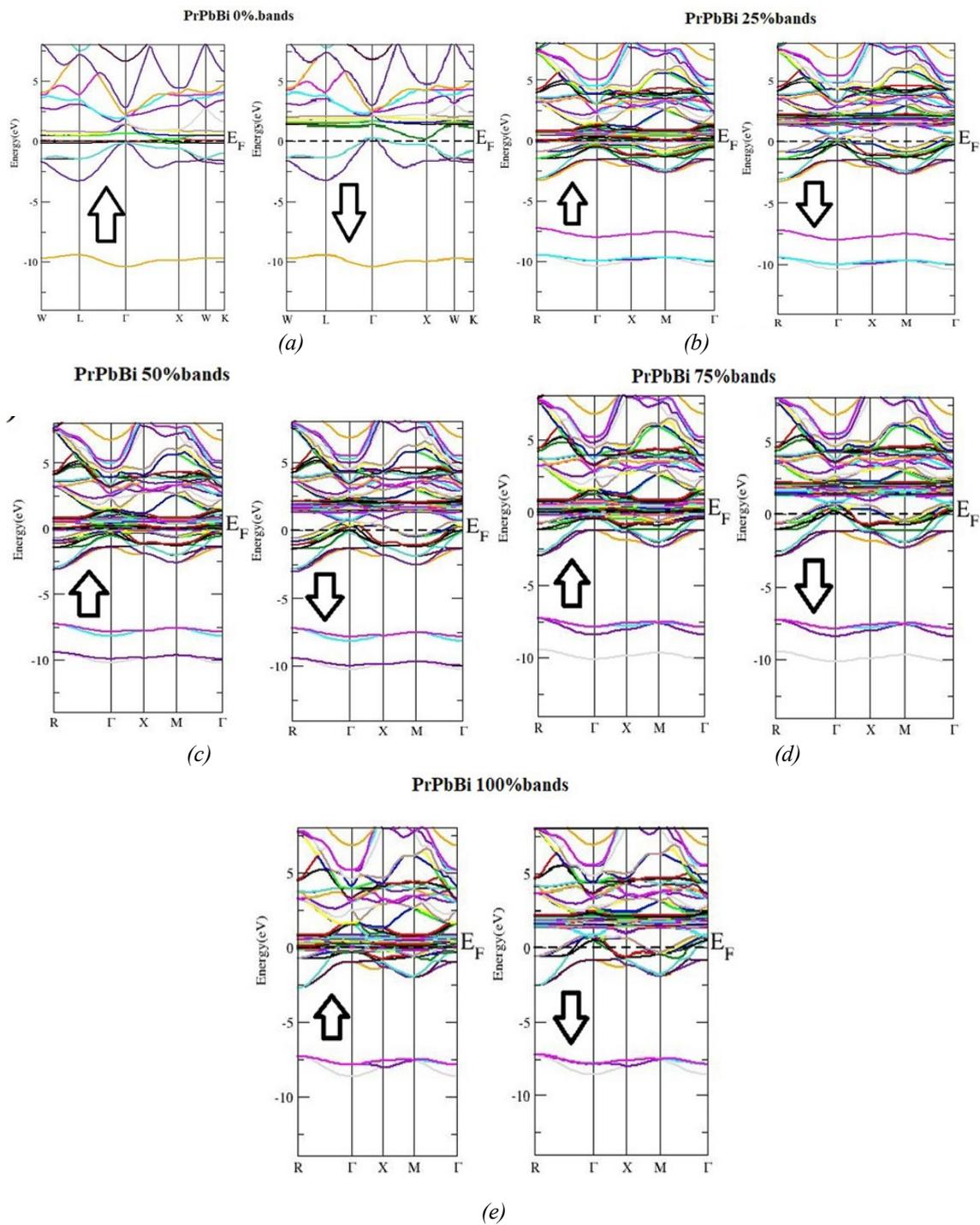
Fig. 3. Energy band spectra of (a) $PrPb_{0.0}Bi_{1.0}$ (b) $PrPb_{0.25}Bi_{0.25}$ (c) $PrPb_{0.5}Bi_{0.5}$ (d) $PrPb_{0.75}Bi_{0.25}$ (e) $PrPb_{1.0}Bi_{0.0}$.
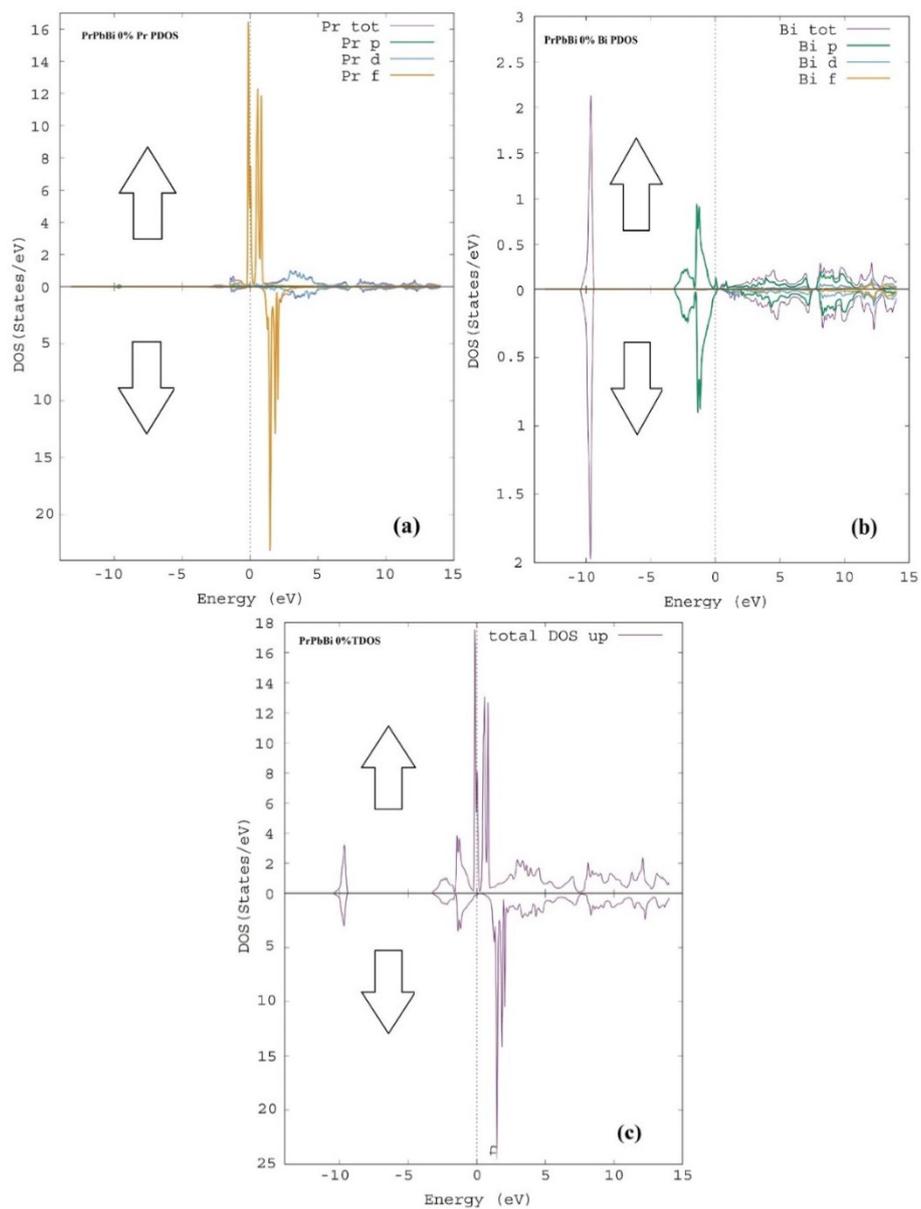
Fig. 4. Energy dependent plots of partial and total DOS for $PrPb_{0.0}B_{i\,1.0}$ (a) PDOS of Pr (b) PDOS of Bi (c) TDOS ofPrPb$_{0.0}$B$_{i\,1.0}$.
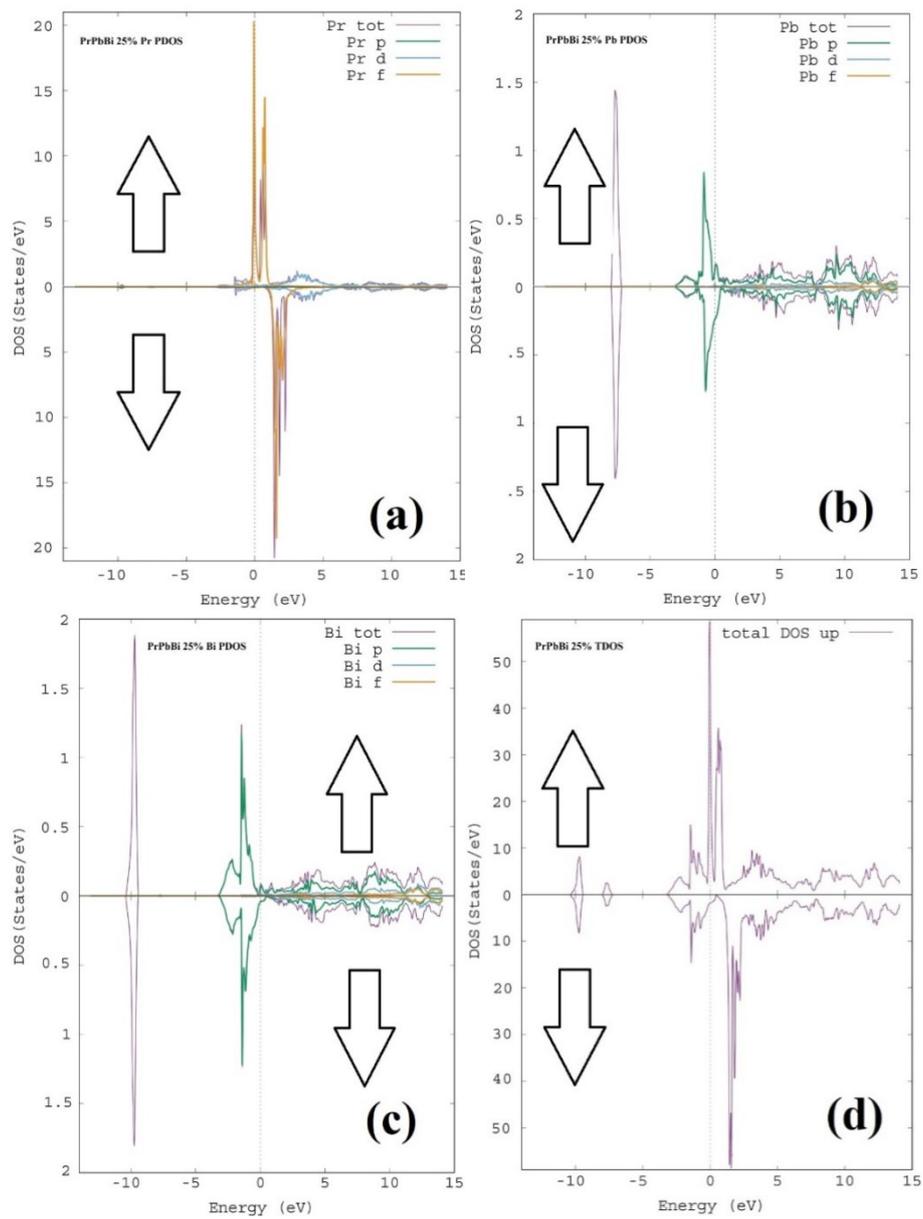
Fig. 5. Energy dependent plots of the partial and total DOS for $PrPb_{0.25}Bi_{0.25}$ (a) PDOS of Pr; (b) PDOS of Pb; (c) PDOS of Bi; (d) TDOS of $PrPb_{0.25}Bi_{0.75}$.
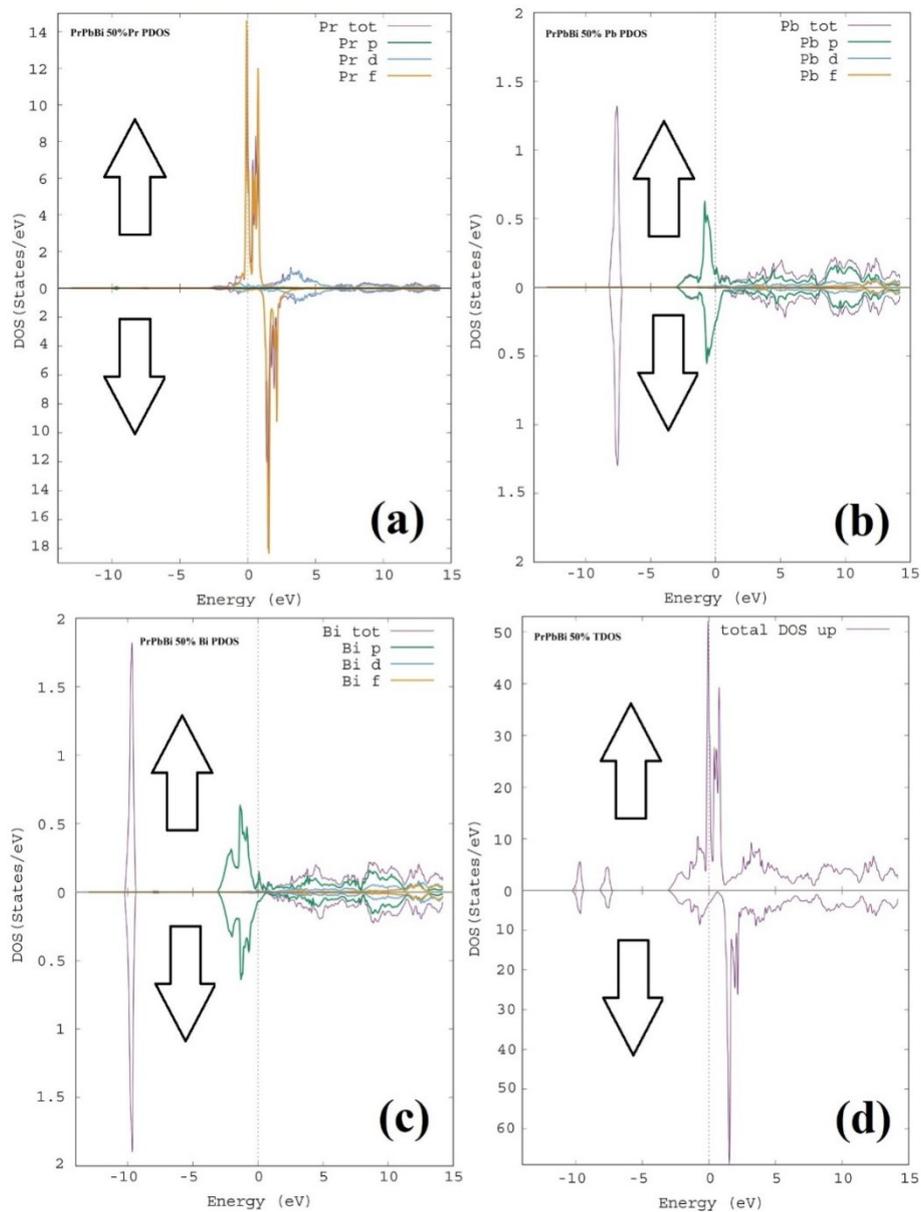
Fig. 6. Energy dependent plots of the partial and total DOS for PrPb$_{0.5}$B$_{i\,0.5}$ (a) PDOS of Pr (b) PDOS of Pb (c) PDOS of Bi (d) TDOS of PrPb$_{0.5}$Bi$_{0.5}$.
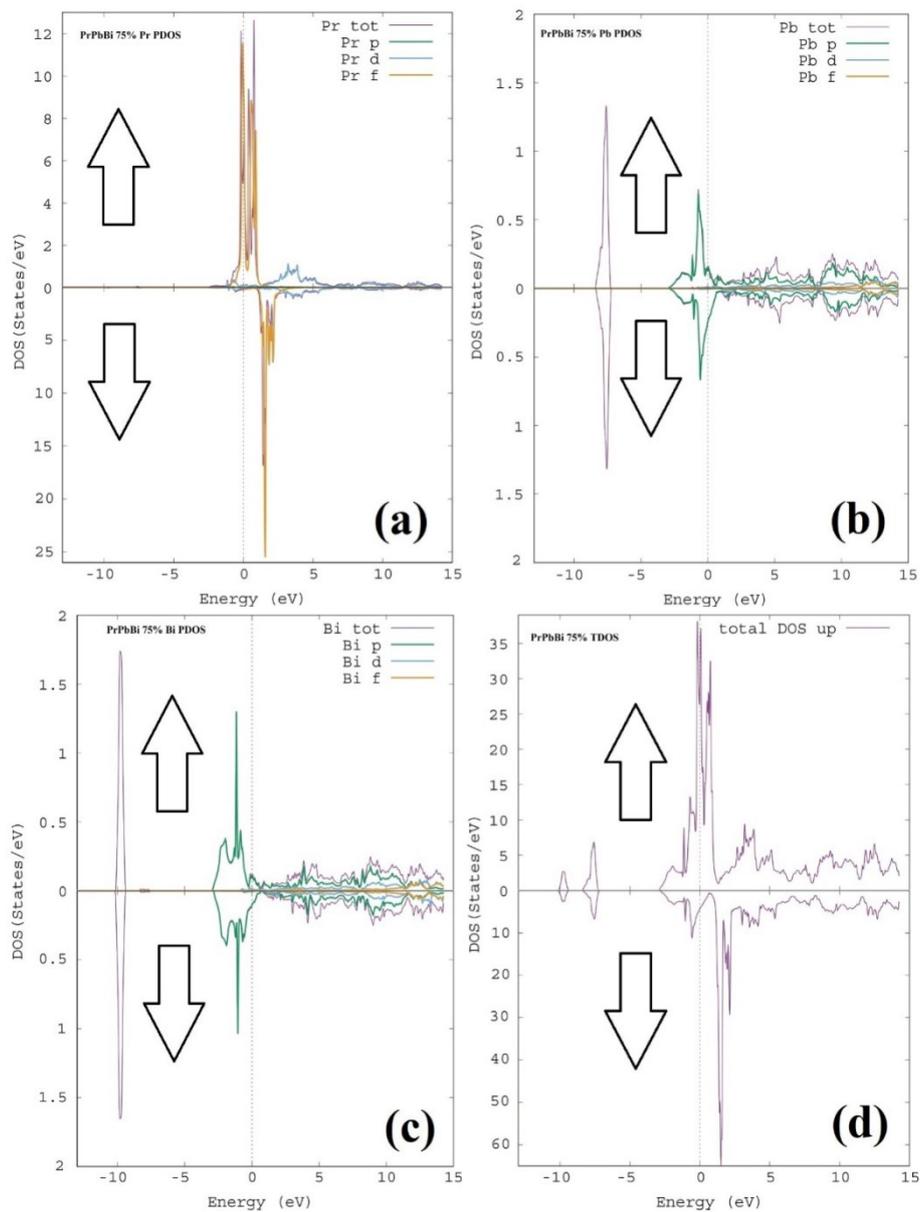
Fig. 7. Energy dependent plots of the partial and total DOS for $PrPb_{0.75}B_{i\,0.25}$ (a) PDOS of Pr (b) PDOS of Pb (c) PDOS of Bi (d) TDOS of $PrPb_{0.75}B_{i\,0.25}$.
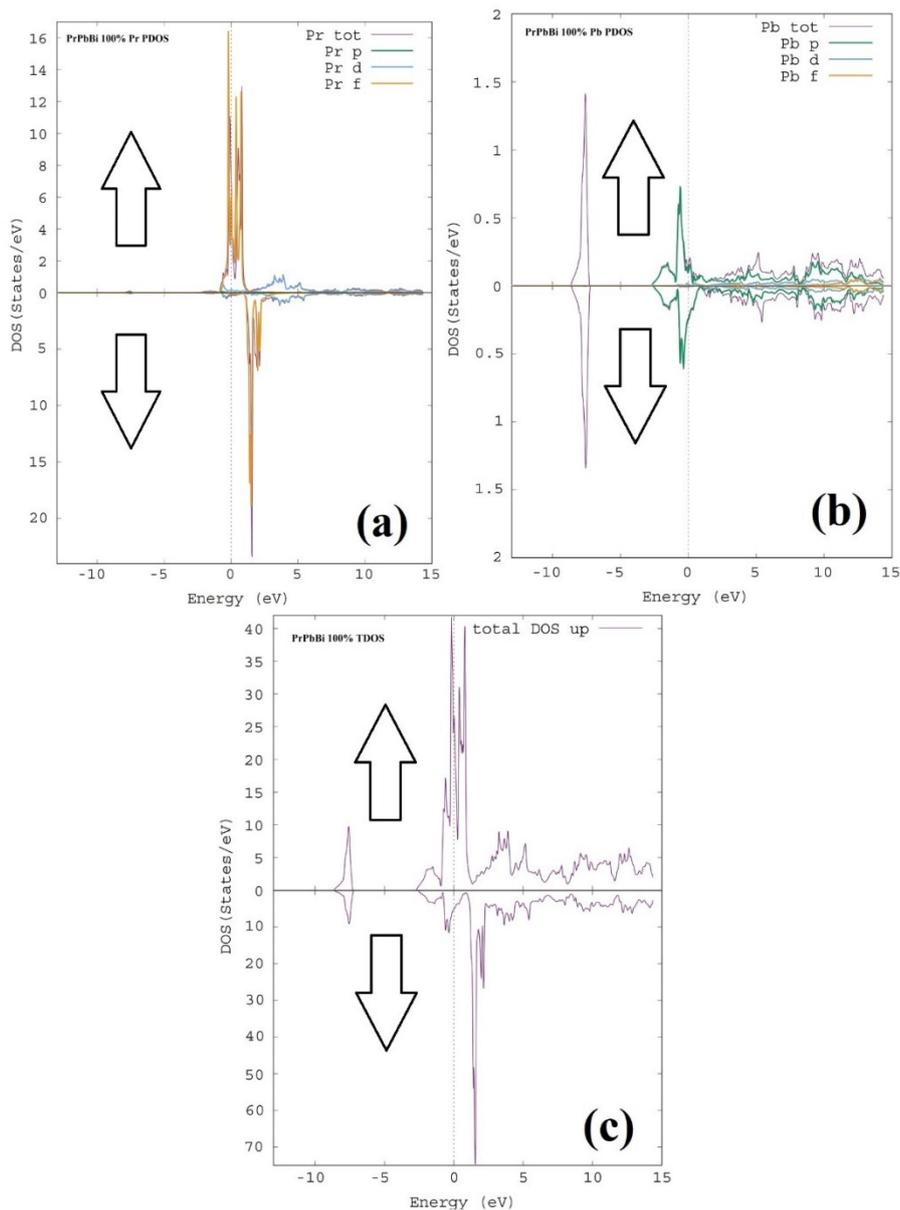
Fig. 8. Energy dependence plots of the partial and total DOS for $OrPb_{1.0}Bi_{0.0}$: (a) PDOS of Pr (b) PDOS of Pb (c) TDOS of $PrPb_{1.0}Bi_{0.0}$.

3.3. Magnetic properties

The contribution of constituents of unpaired electrons in materials determines their magnetic properties, like spin magnetic moments. In a magnetic material, the individual magnetic moments have a long-range magnetic order. Due to the absence of magnetic order (magnetic domains), diamagnetic materials have a zero cumulative spin magnetic moment, whereas paramagnets have a nonzero but smaller spin magnetic moment caused by smaller magnetic domains. Both materials are generally known as non-magnetic. Magnetic materials are divided into ferromagnetic and anti-ferromagnetic; in the former materials all the moments are aligned in one direction and in the later materials the moments are aligned in the opposite direction. The correlation between the magnetic nature and superconductivity [59] of the material may be determined by the value of the overlapping of wave functions having nonconducting f-electrons and conducing electrons. In contrast to band-like features of 5f-electrons and their overlapping in atoms of actinides [74], the 4f-electrons of lanthanides are localized considerably and hence contribute significantly to the magnetic properties of lanthanides compounds. As per our

knowledge, before this, no investigation had been reported on the Pb-doped PrBi compounds regarding their spin magnetic moments.

Table 2 displays the computed spin magnetic moments in the unit cell of PrBi and supercell of $PrPb_xBi_{(1-x)}$ compounds for lead substitution concentration of 0%, 25%, 50%, 75%, and 100%. The spin magnetic moment computed for or 0% Pb concentration with single Pr and Bi atoms in unit cell of PrBi is observed as 2.03210 μ_B. However, in supercell of the substituted compounds it is enhanced a little with doping of lead. There is a constant increase in spin magnetic moments due to increasing percentages of lead. When all lead atoms are replaced with bismuth atoms, the maximum value of the spin magnetic moment of the supercell with 4 Pr atoms is 8.70490 μ_B. Hence, all Pb-substituted compounds are magnetic materials. In the case of PrBi, the magnetic moment arises from the intrinsic magnetic properties of the praseodymium (Pr) atoms in the crystal lattice. Praseodymium is known to exhibit a magnetic moment due to its partially filled 4f electron shell. The magnetic moment of Pr depends on the valence state of Pr (2+, 3+ or 4+). The largest (theoretical) value obtained for Pr(3+) is 3.87, experimental value is normally less than this. In our case the calculated value of Pr(3+) in PrBi unit cell with single atom of each species is 2.06 μ_B, which is enhanced above 8 in the supercell as the number of Pr atoms increases from 1 to 4. For instance, the maximum calculated value in the supercell is 8.70490 μ_B in case of PrPb. Which is understandable by considering the average magnetic moment of Pr. The lowest value of magnetic moment of Pr owes to the fact that we did not apply spin-orbit coupling (SOC) in our calculations. The partially filled Pr atoms have large orbital angular momentum, and hence total angular momentum, so owing to large orbital magnetic moment Pr couples strongly with the lattice via SOC coupling. This in turn may lead to large magnetic moment of Pr and hence of the substituted compounds in supercell as compared to that for free Pr(+3) ion. Besides, the difference may also originate from the DFT methods employed and the fact that calculations were done at 0K.

Table 2. Data of computed spin magnetic moments of PrBi and $PrPb_xBi_{(1-x)}$ compounds.

Sr. No.	Compound	Spin Magnetic Moments, μ_B (Bohr Magnetron)
1	$PrPb_{0.0}Bi_{1.0}$	2.03210 (unit cell)
2	$PrPb_{0.25}Bi_{0.75}$	8.20995 (super cell)
3	$PrPb_{0.5}Bi_{0.5}$	8.40013 (super cell)
4	$PrPb_{0.75}Bi_{0.25}$	8.51802 (super cell)
5	$PrPb_{1.0}Bi_{0.0}$	8.70490 (super cell)

4. Conclusion

We have carried out a theoretical study about the structural, magnetic, and electronic properties of Pb-substituted alloys of praseodymium lead-bismuth systems along with a chemical generic formula $PrPb_xBi_{1-x}$ (x= 0.0, 0.25, 0.50, 0.75, 1.0) implemented with first-principles DFT formalism. We used the FPLAPW+lo technique to compute physical properties by incorporating exchange-correlation energy functional in the KSE with PBE-GGA correction. The cubic phase compounds of $PrPb_xBi_{1-x}$ are optimized, and their crystal structures are computed and compared with the earlies published data. The computed electronic energy bands and partial and total densities of states describe that the compounds $PrPb_xBi_{1-x}$ are magnetic metallic materials. The overlapping of (Pb+Bi) 2p shells and Pr (4f+5d) orbitals around the Fermi level necessitates a zero-energy band gap, implying that the doped compounds are metallic conductors. Spin magnetic moments increased as the Pb substitution concentration was enhanced, and a maximum spin magnetic moment of 8.70490 µB is observed for the Pb-substituted compound PrPb. The interesting outcome of our reported demands more research regarding the clarification of the noble features of the compounds under study. Especially, electronic and magnetic properties of theoretically investigated compounds are still to be computed experimentally to predict the

possible candidacy of the said compounds from basic as well as technological viewpoints. We are also interested in investigating thermoelectric as well as thermodynamic properties of the compounds in future to explore their potential in thermal management.

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Author contribution

M. I. Khan: Supervision; Writing - review & editing. Norah Alwadai: Conceptualization; Formal analysis; A. I. Bashir: Data curation; A.-Ur-Rehman: Formal analysis; M. Siddique: Investigation; Writing - original draft; S. Azam: Methodology; Software; Z. M. Elqahtani: Project administration; Resources; Funding acquisition; A. Nazneen: Visualization; Validation

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