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Theoretical Study of Structural and Electronic Properties of Rare Earth Transition Metal Gallides

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Abstract
The ternary compound Ho4XGa12, (X = Pd and Pt), displays unconventional physical properties such as heavy fermions behavior, notable magnetoresistance, and future applications in superconductivity. These applications occur because of the molecule's tight connection among its electrons. Ho_4XGa_{12} (X = Pd, Pt) crystallize in the cubic phase consisting of Im-3m space group. To exhibit the relevance character of Ho_4XGa_{12} (X = Pd, Pt), we have inquired about the electronic structure, magnetic and thermodynamic properties of Ho_4XGa_{12} (X = Pd, Pt) using density functional theory (DFT) with help of WIEN2K software. Electronic properties show that metallic behavior of both compounds.

Keywords
Gallium, Electronic properties, DFT, Magnetoresistance

INTRODUCTION

In the end of the nineteen centuries, it assumed that magnetic material does not reveal the superconducting phenomenon. Heavy-fermions superconductivity much attracted after the discovery of superconductivity in $CeCu_2Si_2$. This adventure opened a vast area for research to study new intermetallic compounds of gallides with rare earth and transition metal. A substance or a phenomenon in the field of condensed matter physics that displays characteristics such as heavy fermion behavior, magnetism, significant magnetoresistance, and superconductivity. Heavy fermion compounds are a type of material renowned for their ability to exhibit these features. Heavy fermion compounds are a kind of intermetallic compound characterized by the behavior of their conduction electrons, which exhibit an effective mass significantly greater than their intrinsic mass. The observed phenomenon can be attributed to the significant interplay between the conduction electrons and localized magnetic moments present in the material. The existence of localized magnetic moments in the combination can be ascribed to the inclusion of rare earth or actinide ions. The manifestation of heavy fermion behavior is commonly observed under conditions of low temperatures, and it is characterized by the presence of a substantial concentration of electronic states at the Fermi level. The phenomenon gives rise to a significant electronic specific heat, a distinctive characteristic shown by heavy fermion materials. The investigation of correlated electron systems is significantly enriched by the presence of heavy fermion behavior, as it engenders a diverse range of intriguing and technologically significant phenomena, such as magnetism, substantial magnetoresistance, and superconductivity, as previously indicated [1-4]. Hybridization of orbital electrons of rare earth and conduction electrons play an important role in magnetism, superconductivity and magneto resistance. Rare earth transition metal gallides exist in different phases with different structures [5-9]. At lower temperatures, these interactions have the potential to generate a diverse range of captivating and technologically significant phenomena. The comprehension and utilization of the characteristics exhibited

by strongly correlated electron systems possess the capacity to bring about transformative advancements in diverse domains of technology, encompassing energy, electronics, and quantum computing. Scholars persist in investigating these substances to gain basic insights into the field of condensed matter physics and to further the creation of novel technologies. In the present research article, the focus of our research is on RE_4XGa_{12} (RE = heavy rare earth elements X = Pd, Pt) type gallides. RE_4XGa_{12} compounds are condensed in the cubic phase consisting of Im-3m space group [10]. The metal flux growth method is widely utilized in the field of crystal development for the purpose of synthesizing a diverse range of materials, encompassing ternary layered intermetallic complexes. The present methodology involves subjecting a blend of metallic elements, frequently accompanied by a flux substance, to elevated temperatures, therefore facilitating the formation of the intended compound through the constituents' mutual reactions. Subsequently, the compound undergoes a gradual cooling process, facilitating its crystallization from the molten amalgamation. The selection of gallium is a strategic decision. The substance's relatively low melting point enables it to undergo easy liquefaction and serve as a flux. Conversely, its elevated boiling point allows it to remain in the liquid state across a broad spectrum of temperatures, rendering it well-suited for promoting the formation of specific compounds. The synthesis of ternary layered intermetallic compounds by this approach frequently results in the emergence of distinctive electronic, magnetic, or other physical characteristics. These qualities hold significant potential for many applications in fields such as electronics, superconductivity, and magnetism. The properties and applications of the compound will be contingent upon the precise amalgamation of rare earth elements, transition metals, and gallium employed [11] and studied the magnetic properties. Magnetic study of Ho_4PdGa_{12} and Er_4PdGa_{12} indicates that these compounds are anti-ferromagnetic at transition temperatures. Study of electrical resistivity of these compounds confirms that these materials exhibit metallic nature [12]. Based on literature survey, we can say that a few studies on structural and magnetic properties have been presented by several authors [1-12] but no detailed studies have been made on temperature and pressure dependent electronic behavior and electronic structure for RE_4XGa_{12} (RE = heavy rare earth elements X = Pd, Pt) type rare earth transition metal gallides. The aim of present research work express and yield an interpretation of more strong properties of rare earth transition gallides on band structure (BS) curves, density of states (DOS) determine the electronic.

COMPUTATIONAL METHOD

In the present research article, the Density function Theory (DFT) calculations were carried out to explore the electronic structure using an accurate full potential linearized augmented plane-wave plus local orbital (FP-LAPW + lo) method with GGA exchange correlation as inserted in WIEN2k software [13-17]. Optimization has been made with the charge accuracy of 0.0001 ec. The cutoff energy for optimization has been taken out -6.0 Ry. The calculated values of Fermi energies for Ho_4PdGa_{12} and Er_4PtGa_{12} are shown in table 1.

RESULT AND DISCUSSION

Structural and electronic properties

In this paper, we have calculated structural properties of Ho_4XGa_{12} (X = Pd, Pt) compounds in terms of Crystal structure of unit cell and Volume Vs Energy curve. The unit cell structure of Ho_4XGa_{12} (X = Pd, Pt) is illustrated in Figure 1(a-b) with help of XCrySDen software. In this figure, the lattice parameters $a_0 = b_0 = c_0 = 8.549$Å for Ho_4PdGa_{12} and $a_0 = b_0 = c_0 = 8.540$Å for Ho_4PtGa_{12} [12]. This exhibit the material Ho_4XGa_{12} (X = Pd, Pt) have cubic structure with space group Im-3m. In figure 2(a-b) indicates that Volume Vs energy curves plots with help of Birch–Murnaghan equation of state [BM-EOS]. In this curves, we have analysis some structure parameters such as equilibrium volume (V_0), Bulk modulus (B_0), derivate of Bulk modulus (B_0'), and equilibrium energy (E_0) shown in table -1 for Ho_4XGa_{12} (X = Pd, Pt) compounds[18-20].

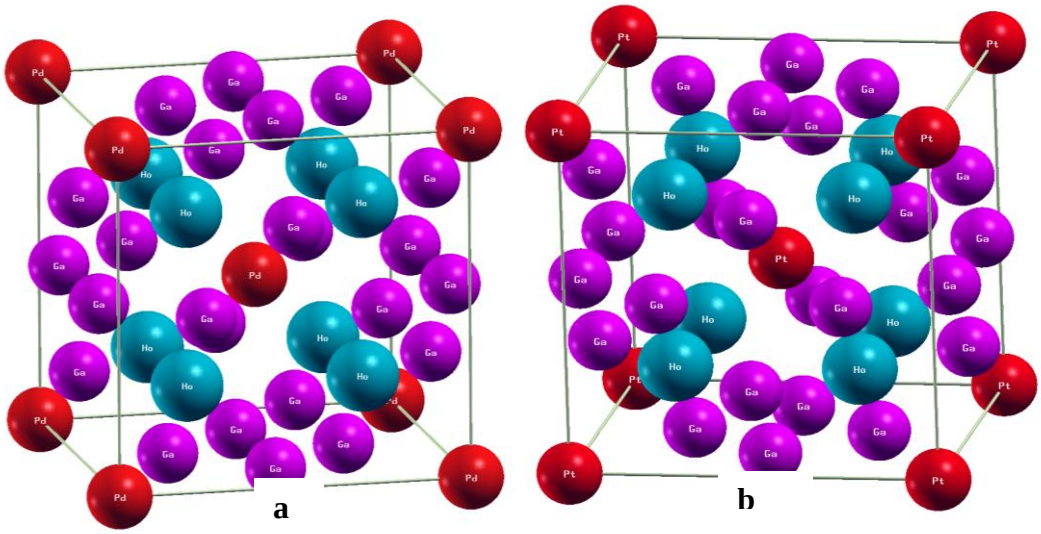

Fig. 1 Unit cell structure of (a) Ho_4PdGa_{12} and (b) Ho_4PtGa_{12}

Table 1

S. No.	Parameters	Ho_4PdGa_{12}	Er_4PdGa_{12}
1.	Lattice constant $a_0 = b_0 = c_0$ (Å)	8.2516	8.2215
2.	Equilibrium volume (V_0) $a.u^3$	1895.7251	1875.2381
3.	Bulk modulus (B_0) GPa	40.5370	42.4482
4.	Derivate of Bulk modulus (B_0') GPa	3.8971	3.9657
5.	Equilibrium energy (E_0) Rayd	-134452.040348	-161251.380180
6.	Fermi energy (E_f) eV	0.29918	0.30771

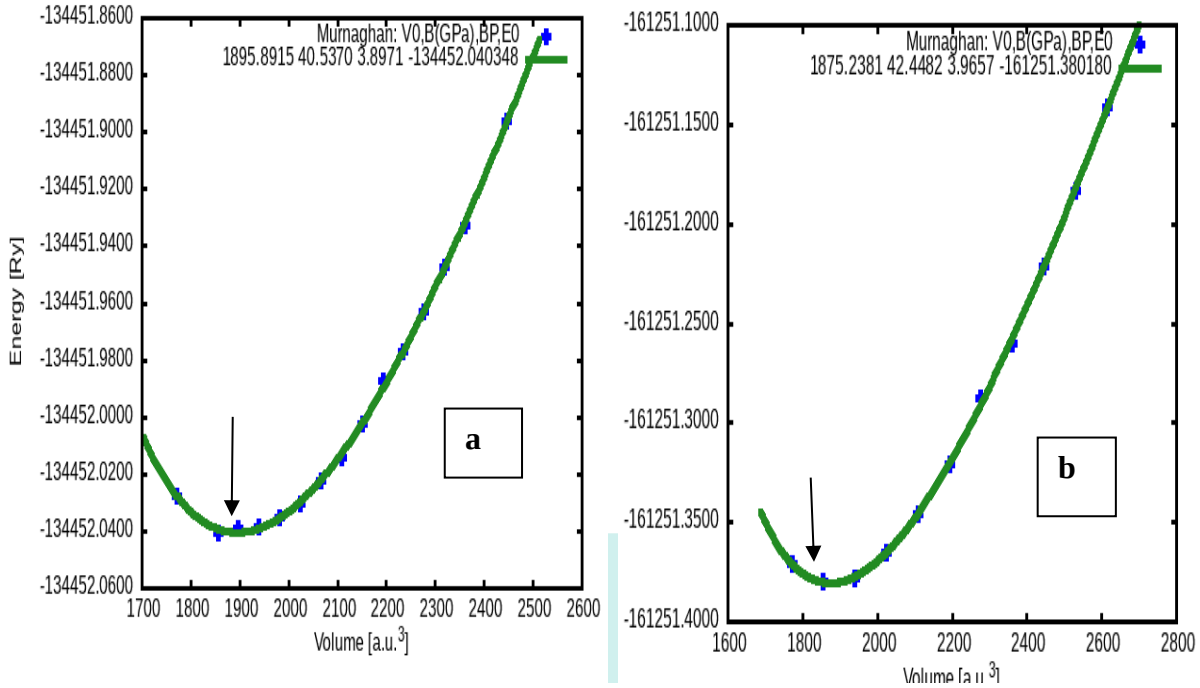

Fig. 2 Energy Vs Volume curves with help of Brich-murnaghan equation of (a) Ho_4PdGa_{12} and (b)

In this phase the electronic properties of the selected material is determined by band structure (BS) curves (behavior of valence electron near the Fermi level) in figure 3(a-d) and density of states (total number of allowed electronic state per unit volume) in figure 4(a-h) for Ho_4PdGa_{12} and figure 5 (a-h) for Ho_4PtGa_{12} compound. The BS for both states for Ho_4PdGa_{12} and Ho_4PtGa_{12} compound shown in Figures 3(a, b) and 3(c, d) respectively. In Figures 3(a, b) and 3(c, d), different colors correspond to different energy range along different symmetry directions. These figures stipulate that valence bands and Conduction band overlap to each other, and fermi level located at origin. In figure 3(a-d) shows that BS of Ho_4PdGa_{12} and Ho_4PtGa_{12} compound is metallic nature. This metallic character of Ho_4PdGa_{12} and Ho_4PtGa_{12} is due to existence of Ho-f bands at the Fermi level with small contribution of Pd-p bands. Now it's confirmed both compounds are show that metallic nature. Furthermore, TDOS and PDOS for both Ho_4PdGa_{12} and Ho_4PtGa_{12} have been shown in Figures 4(a-h) and 5(a-h) respectively. In Figure 4(a), it can be noticed that three distinct peaks were detected in both the spin up and spin down channels. The first peak is located at -3.0 eV, followed by a second peak at -2.0 eV, and finally a third peak at -1.75 eV. The steep peaks observed at around -3.0 eV and -2.0 eV in the Ho4PdGa12 compound are primarily attributed to the Ho-f states, as depicted in Figures 4(a, b). On the other hand, the peak observed at roughly -1.75 eV is mainly a result of the Pd-d states and the significant hybridization between Pd-s and Ga-p, as illustrated in Figure 4(a). Three distinct peaks were seen in the minor spin down channel at around -1.5 eV, 0.0 eV, and +1.2 eV, as shown from the observations. The density of states (DOS) at an energy level of around -1.5 eV is mostly attributed to the Pd-d states. Conversely, the energy levels around 0.0 eV and +1.2 eV are predominantly influenced by the Ho-f states and the significant hybridization of Pd-p and Ga-p states. The presence of a density of states (DOS) at about 0.0 eV can be attributed mostly to the Ho-f spin down states, which play a crucial role in conferring metallic properties to these materials. The intense peaks at around 0.0 eV and +1.2 eV above the Fermi level are also contributed mainly Ho-f spin down states which are empty states and available for conduction. Once more, it is evident from figure 4 (a) and 4 (e) that Ho-f orbital states have large difference between spin up and spin down states near the Fermi level. Thus, Ho-f states are also responsible for providing the magnetic moment and hence magnetic character. Almost similar, features of TDOS and PDOS for Ho_4PtGa_{12} have been obtained which can be explained in similar manner.

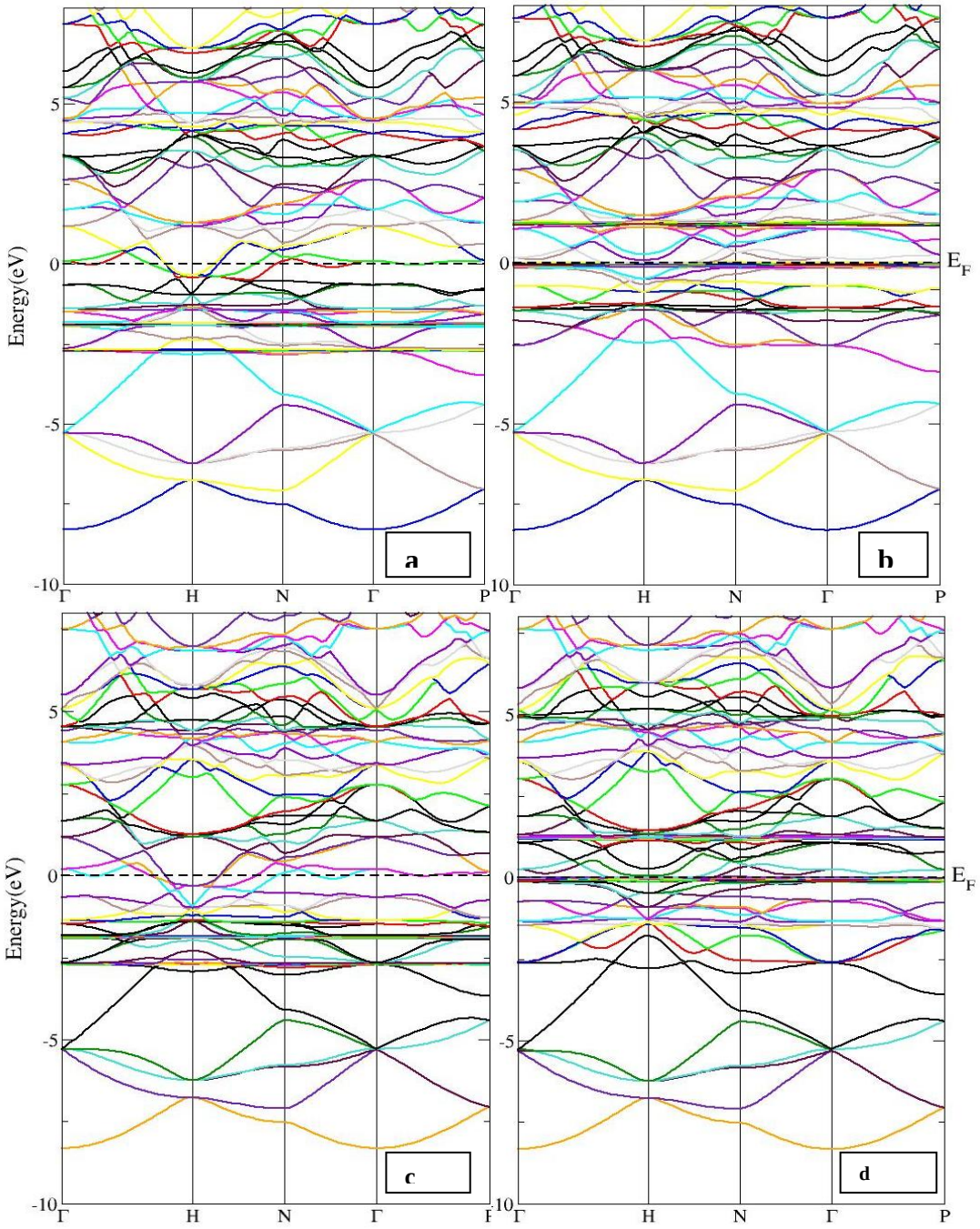

Fig. 3 Band Structure of (a) Ho_4PdGa_{12} spin up, (b) Ho_4PdGa_{12} spin down, (c) Ho_4PtGa_{12} spin up, and (d) Ho_4PtGa_{12} spin down

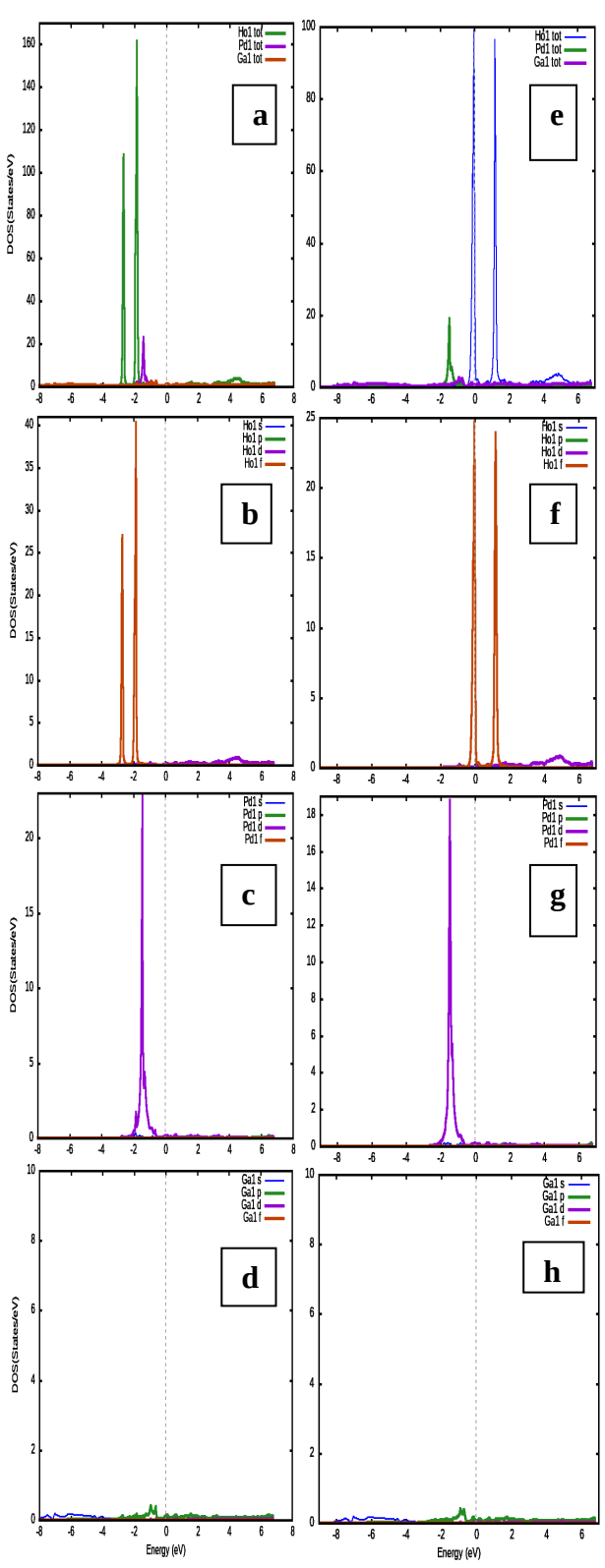

Fig. 4 TDOS and PDOS of (a) TDOS of Ho_4PdGa_{12} spin up, (b) PDOS of Ho spin up, (c) PDOS of Pd spin up, (d) PDOS of Ga spin up, (e) TDOS of Ho_4PdGa_{12} spin down , (f) PDOS of Ho spin down, (g) PDOS of Pd spin down, (h) PDOS of Ga spin down

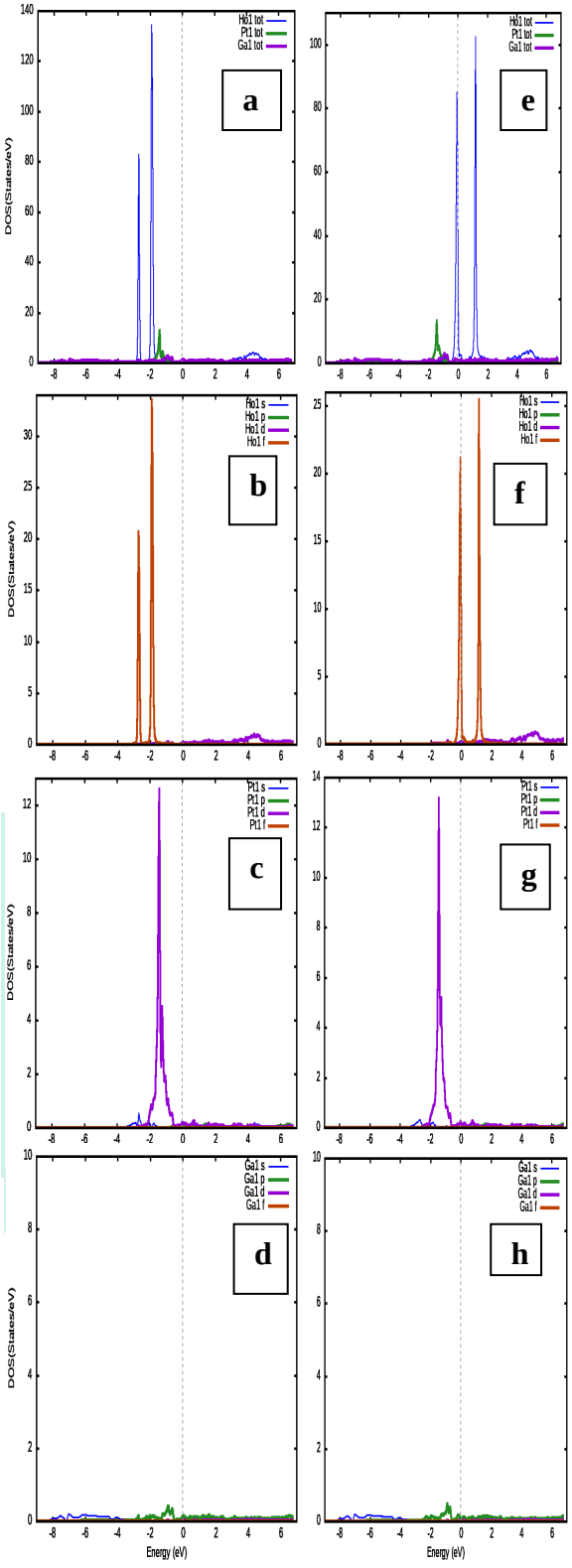

Fig. 5 TDOS and PDOS of (a) TDOS of Ho_4PtGa_{12} spin up, (b) PDOS of Ho spin up, (c) PDOS of Pt spin up, (d) PDOS of Ga spin up, (e) TDOS of Ho_4PtGa_{12} spin down , (f) PDOS of Ho spin down, (g) PDOS of Pt spin down, (h) PDOS of Ga spin down

CONCLUSIONS

The spin polarized structure and electronic properties, properties have been estimated using DFT for rare earth transition metal gallides (Ho_4PdGa_{12} and Ho_4PtGa_{12}). The calculated structural parameters were found in good agreement with literature values. The studied rare earth transition metal gallides show the conducting nature due to Ho-f conduction electrons. Ho-f orbital electrons have dominant character at the Fermi level in conduction and these Ho-f orbital electrons in TDOS and PDOS are accountable for magnetic nature. The total magnetic moment and magnetization of Ho_4PdGa_{12} and Ho_4PtGa_{12}compounds was found to be lesser than experimental/theoretical values. Total magnetic moment/magnetization is mainly contributed by Ho^{3+} ions in which Ho-f orbital electrons are dominant over other orbital electrons.

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