Journal of Natural Sciences and Mathematics
Qassim University, Vol. 8, No. 1, PP 63-75 (January 2015/Rabi I 1436H.)

LMTO-ASA electronic and magnetic structures calculations of the (3d–5d) mixed double perovskite oxides $Ba_2BB'O_6$ (BB'=V-Hf, Cr-Ta, Mn-W)

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Abstract. The electronic and magnetic structures of series of double perovskite oxides $Ba_2BB'O_6$, have been calculated by using the ab-initio linear muffin-tin orbital method with the atomic-sphere approximation (LMTO-ASA). The calculations were performed using the local spin density approximation with the coulomb interaction method (LSDA+*U*) in the framework of density functional theory (DFT). The results show that Ba_2VHfO_6 is half-metallic and Ba_2CrTaO_6 is conductor. The conduction bands in two compounds form mainly from the contributions of V (3d) and Cr (3d) elements. Ba_2MnWO_6 was found to be semiconductor, agreement with the results of J. Cheng and Z. Q. Yang. The ground magnetic phases for the first two compounds were found to be ferromagnetic while, the third was found to be antiferromagnetic material. These caused the hybridization between the V/Cr (3d) t_{2g} spin up and Hf/Ta (5d) t_{2g} spin up, and between Mn (3d) t_{2g} spin up and W (5d) t_{2g} spin down orbitals. The magnetic moments were found to be 1.39 μ_B for V^{4+}, 0.35 μ_B for Hf^{4+}, 2.79 μ_B for Cr^{3+}, -0.46 μ_B for Ta^{5+}, 4.41 μ_B for Mn^{2+} and -0.42 μ_B for W^{6+}.

Keywords: Double perovskite oxides; Transition-metals; LMTO-ASA method.

1. Introduction

Since, the observation of the room-temperature colossal magnetoresistance (CMR) phenomena in Sr_2FeMoO_6 [1] and Sr_2FeReO_6 [2], intensive research efforts have been devoted to understand the crystal structure, electronic and magnetic properties of double perovskites [3]. The properties such colossal magnetoresistance [4], half-metallic [5], high magnetic ordering temperature [6], magnetodielectric [7] and other functional properties, make these materials ideal for many applications [4,8]. The physical origin of magnetoresistance (MR) in Sr_2FeMoO_6 and mixed-valance manganese oxides is half-metallicity, i.e., the material is an insulator in one of the spin direction while, is metallic in the other direction [8,9]. This leads to a complete, 100% spin polarization of the conduction electrons at the Fermi level. In addition, this in turn results in strongly spin-dependent scattering of the charge carriers and thus a possibility to influence the resistance using relatively weak magnetic fields [6].

Double perovskite oxide structures are a broad family of complex materials with high technological potential in spintronics devices [4]. The general chemical formula of double perovskite oxides is $A_2BB'O_6$, takes the rock-salt crystal structure. This structure, as seen in Fig.(1), has an ordered one of the alternate perovskite units ABO_3 and $AB'O_3$ along three crystallographic axis [6]. Site A in $A_2BB'O_6$ can be an alkali metal such as Sr^{2+}, Ca^{2+}, Ba^{2+}, or La^{3+} [4] and B–B′ sites are usually occupy by different transition-metals [8]. In this study, the pairs B–B′ have a multivalent of 8+, i.e., V^{4+} (3d)–Hf^{4+} (5d), Cr^{3+} (3d)–Ta^{5+} (5d), and Mn^{2+} (3d)–W^{6+} (5d). Each transition-metal site is surrounded by an oxygen octahedron and the A atoms are situated in the holes produced by eight adjacent oxygen octahedral [10]. The main objective of this study is systematic comparison study of the structures, electronic and magnetic properties of a new series of cubic crystalline double perovskite oxides Ba_2VHfO_6, Ba_2CrTaO_6 and Ba_2MnWO_6. In this study the first-principle linear muffin-orbital within atomic sphere approximation (LMTO-ASA), based on the density functional theory (DFT), has been used to calculate the electronic and magnetic structures.

2. Calculation method

The self-consistent band structure calculations presented in this study have performed within the local spin density approximation (LSDA) in the framework of density functional theory (DFT). Linear muffin-tin orbital (LMTO) method functioning within atomic sphere approximation (ASA) [11], executed by LmtArt code [12], was used. Spin-orbit coupling and spin-polarization were included in the calculations. The Hartree potential was expanded in term of spherical harmonic $L_{max} = 6$, and an exchange correlation potential of von Barth–Hedin type was adopted [8]. Thus, the basis set consists of Ba (6s 5p 5d 4f), V/Cr/Mn (4s 4p 3d), Hf/Ta/W (6s 6p 5d) and O (2s 2p) linear muffin-tin orbitals (LMTOs) were taken as valance states. The Ba (5s), V/Cr/Mn (3p) and Hf/Ta/W (5p 4f) were taken as semicore states. It has verified that the structures were close enough that no empty spheres were needed to introduce in the unit cells [7]. The on-site Coulomb interaction *U*, or (LDA+*U*) method [13], has been considered in the calculations for Ba_2VHfO_6, Ba_2CrTaO_6 and Ba_2MnWO_6 compounds. The screened Coulomb and exchange parameters *U* and *J* were used for calculating the correlation interaction [14]. For 3d electrons, ($U = 8.0$ eV, $J = 0.89$ eV) for Ba_2VHfO_6, ($U = 8.0$ eV, $J = 0.89$ eV) for Ba_2CrTaO_6 and ($U = 4.0$ eV, $J = 0.90$ eV) for Ba_2MnWO_6, while, ($U = 1.0$ eV, $J = 0.90$ eV) was used for 5d electrons.

3. The crystal structure of $Ba_2BB'O_6$

The electronic structure of double perovskite oxides Ba_2VHfO_6, Ba_2CrTaO_6 and Ba_2MnWO_6 were studied. Each of 3d and 5d orbits in transition-metals steps up on their atomic number by adding an electron to the d orbit. These compounds were considered to have a cubic crystal structures with space group Fm-3m (No. 225), such as shown schematically in Fig.(1). The valance states of the three pairs of transition-metals in the unit cell have the forms: V^{4+} ($3d^1$) – Hf^{4+} ($5d^0$), Cr^{3+} ($3d^3$) – Ta^{5+} ($5d^0$) and Mn^{2+} ($3d^5$) – W^{6+} ($5d^0$). The d^0-ions were formed in the configurations of the 5d elements in all compounds. First, for these three compounds the lattice parameters and atoms positions were calculated by using the SPuDS program. SPuDS accepts the formula $A_2MM'O_6$ of the rock salt B–cation ordered perovskite with space group of face-centered cubic (Fm-3m). Thus, the lattice parameters $a = b = c$, their ratio $b/a = 1$ and $c/a = 1$, and $\alpha = \beta = \gamma = 90°$ [11]. The angle of the exchange interaction B – O – B′ obtained from SPuDS was 180°. The optimized crystal structure, lattice parameters and oxygen positions (*u*), is listed in Table (1). Second, the generated data from SPuDS calculations is used as input file, structure data, in BandLab program. The BandLab code is used to calculate the charge densities, densities of states (DOSs) and band structures (Fat Bands). The configurations of the transition-metal ions and their valance states in the unit cells, are V^{4+} / Cr^{3+} / Mn^{2+} (3d 4s) and Hf^{4+} / Ta^{5+} / W^{6+} (4f 5d 6s), the semi cores are V/Cr/Mn (3p) and Hf/Ta/W (5s 5p). According to the space group, ten atoms and five sorts were used to build the unit cells. In the face-centered cubic (fcc), the setting of atomic positions in the unit cells of the three compounds are: Ba at (¼,¼,¼) and (¾,¾,¾), V/Cr/Mn at (0,0,0), Hf/Ta/W at (½,0,0), O_1 at $(0,\pm u,0)$ and O_2 at $(0,0,\pm u)$. General, for the three compounds the sorts of atoms, atomic sites, atomic positions and occupancies tabulated in table (2). These were obtained from the output file of SPuDS program, and using the international crystallographic table to calculate the full positions of Ba and O atoms [15]. The u coordinate of the oxygen atom varied during the substitution of B and B′ transition-elements. They were calculated and found to be ($u = 0.2413$) in Ba_2VHfO_6, ($u = 0.2496$) in Ba_2CrTaO_6, and in Ba_2MnWO_6 it was found to be ($u = 0.2670$), which is very close to the value 0.2654 found in ref. [11]. The structure of the unit cells in double perovskite oxide compounds can be regarded as a combination of cubic $BaBO_3$ (B = V, Cr, Mn) and $BaB'O_3$ (B′ = Hf, Ta, W) single perovskites in superlattice. The atoms B and B′ have layers stacked, thus no empty spheres in the unit cells. The mixed transition-metal ions B (3d) and B′ (5d) can coupled to each other in the layers either in ferromagnetic (FM) or antiferromagnetic (AFM) order [4,11].

Table (1). The space group, lattice parameters and oxygen position for $Ba_2BB'O_6$ compounds.

Crystal	Space group	*a* (Å)	*u*
Ba_2VHfO_6	Fm-3m	8.0010	0.2413
Ba_2CrTaO_6	Fm-3m	7.9215	0.2494
Ba_2MnWO_6	Fm-3m	8.2270	0.2670

Table (2). The general atomic positions and occupancies of $Ba_2BB'O_6$ compounds in the fcc structures. The O position is varied and depends on the B-B′ elements.

Atom	Site	x	y	z	Occup.
Ba	8c	1/4	1/4	1/4	1
B (3d)	4a	0	0	0	1
B′ (5d)	4b	1/2	0	0	1
O	24e	*u*	0	0	6

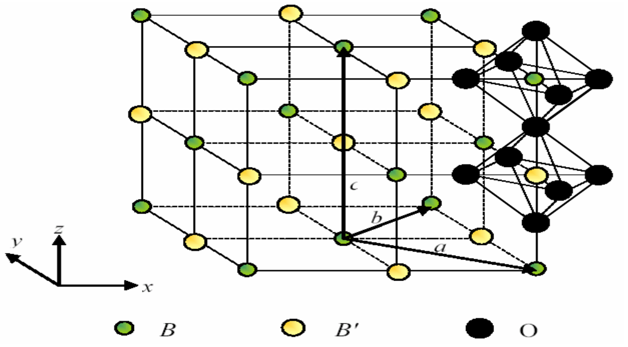

Fig. (1). The face-centered cubic (Fm-3m) double perovskite oxide $A_2BB'O_6$ crystallizes in the rock-salt structure. It was depicted as BO_6 and $B'O_6$ octahedra surrounding the A-site cation.

4. Results and discussion

4.1 The electronic structure of $Ba_2BB'O_6$

The electronic and magnetic structures of three double perovskite oxides were calculated. The total and partial densities of states (DOSs) were obtained from the BandLab calculations. Fig.(2) shows the total density of states (Total DOS) as a function of Energy (in eV) for the 3d – 5d mixed double perovskite oxides Ba_2VHfO_6 (BVHO), Ba_2CrTaO_6 (BCTO) and Ba_2MnWO_6 (BMWO) in the fcc crystal structures. In addition, Figs.(3, 4 and 5) illustrate the total and partial densities of states (DOSs) of the three double perovskite oxides Ba_2VHfO_6, Ba_2CrTaO_6 and Ba_2MnWO_6, respectively. The up and down parts of each panel represents the spin up and spin down bands, respectively. The energy zero is set at the Fermi level (E_F). From the densities of states of Ba_2VHfO_6 and Ba_2CrTaO_6 in Fig. (3) and Fig. (4), it seen that the conduction is to be through the contributions of V 3d (t_{2g}) and Cr 3d (e_g) bands, which are crossing the E_F. While there are no contributions from the Hf (5d) and Ta (5d) bands, as show in panels (a) in Fig. (3 and 4). Because the 5d orbits in the Hf^{4+} and Ta^{5+} ions contains no electrons ($5d^0$) and this is clearly reflected in bands below E_F, the majority of the bands are located above E_F, between +2.0 eV and +4.0 eV.

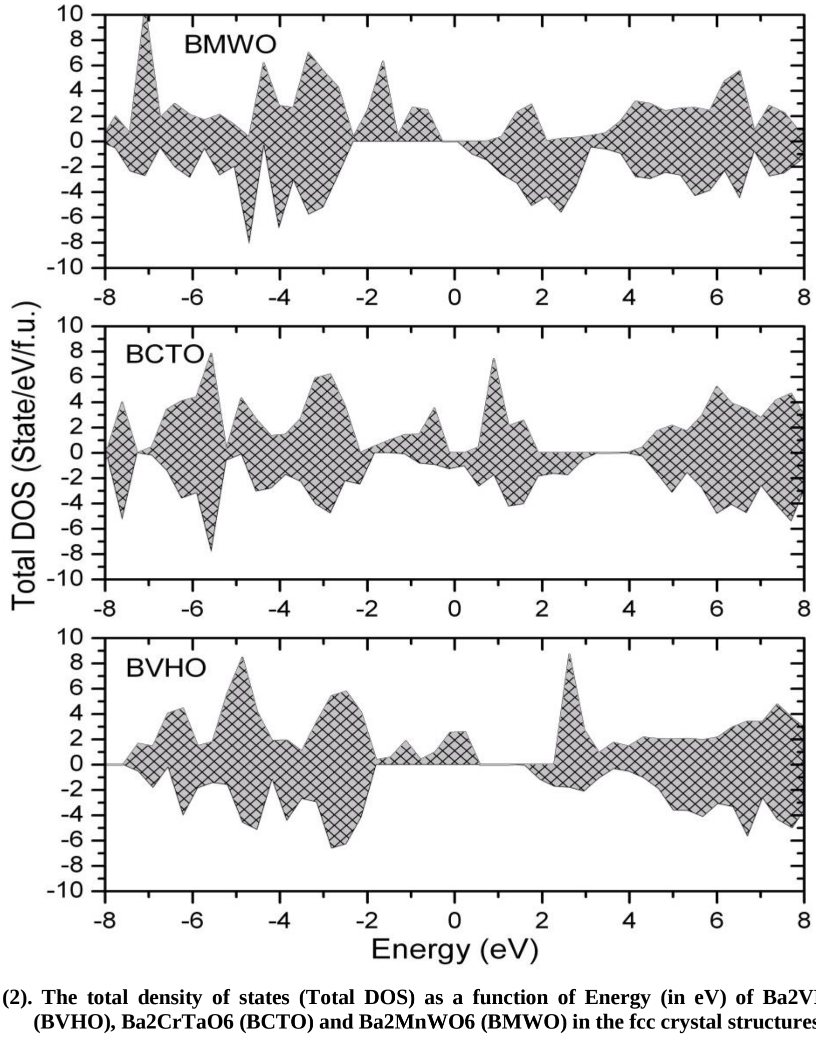

Fig. (2). The total density of states (Total DOS) as a function of Energy (in eV) of Ba2VHfO6 (BVHO), Ba2CrTaO6 (BCTO) and Ba2MnWO6 (BMWO) in the fcc crystal structures.

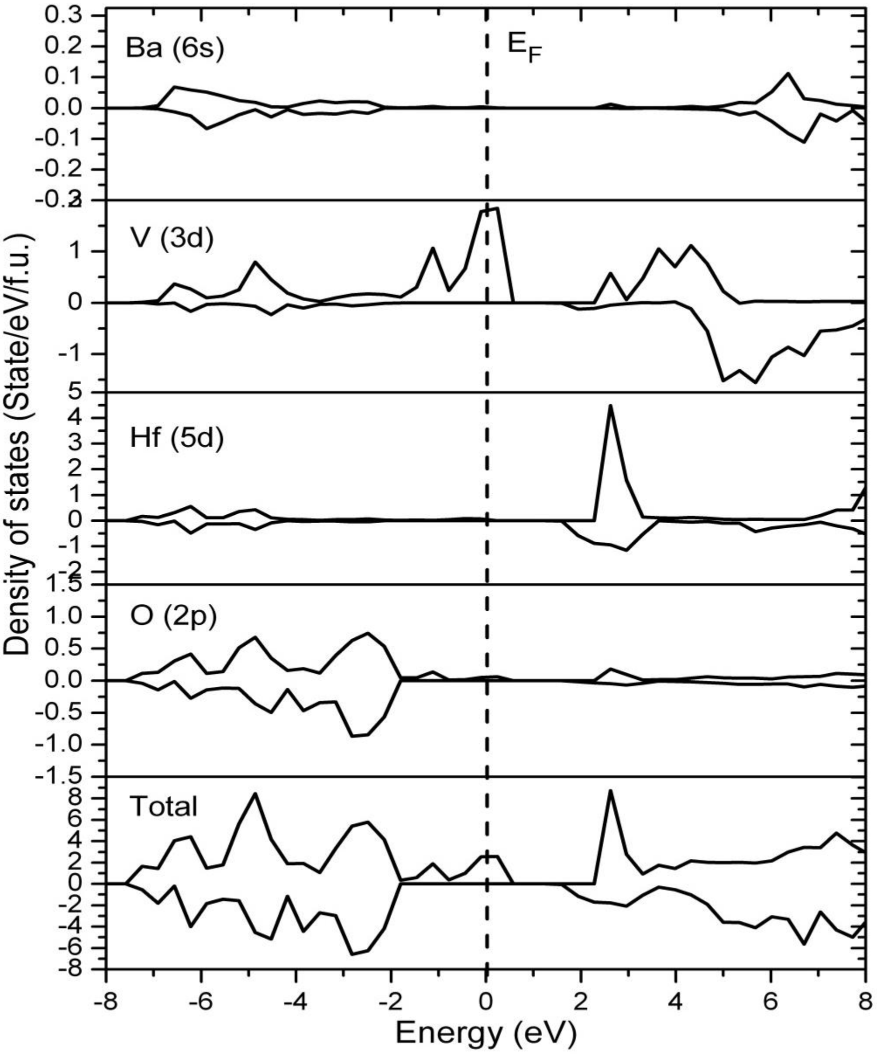

Fig. (3). The total and partial densities of states of Ba2VHfO6 in the fcc structure.

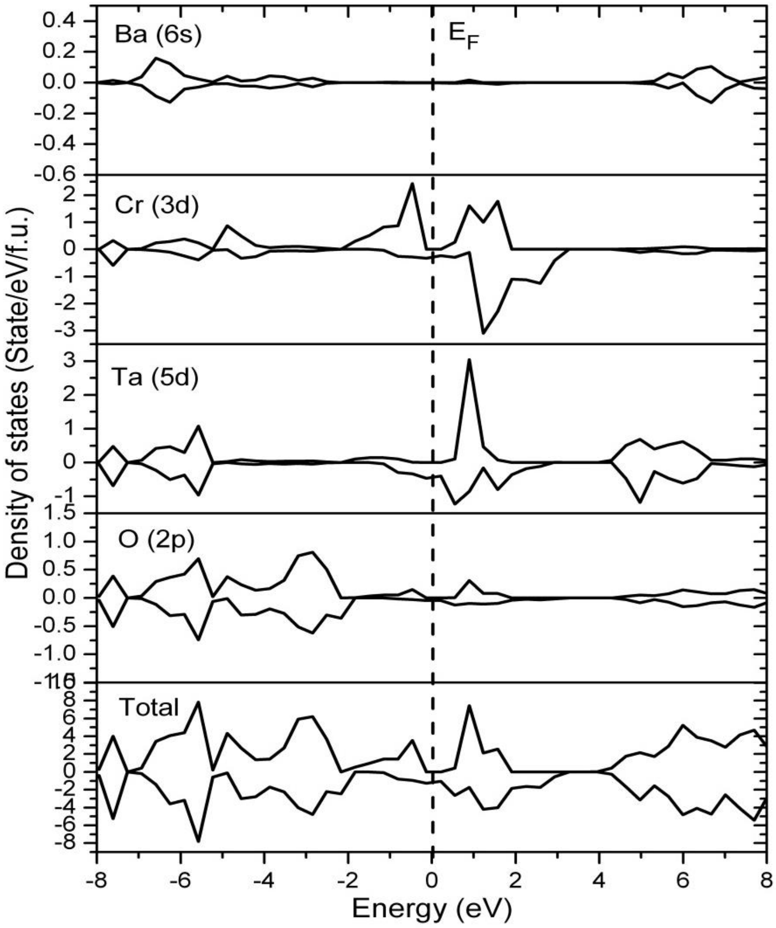

Fig. (4). The total and partial densities of states of Ba2CrTaO6 in the fcc structure.

On the other hand, the V^{4+} and Cr^{3+} ions are seen to be affected by the crystalline field where clear splitting of their bands are seen below and above E_F. The bands of V^{4+} and Cr^{3+} ions are almost equally distributed between the valence and conduction band which indicates the near half-filling state of the 3d bands. Further, it seen that in panels (b) and (d) in Fig. (3 and 3), the V^{4+} 3d (t_{2g}) spin up and Cr^{3+} 3d (e_g) spin up bands hybridized with the O 2p bands resulting the conducting bands of these two compounds. Half-metallic (HM) property is appeared in the compound of Ba_2VHfO_6. From the PDOS of V 3d in panel (b) in Fig. (3), the spin up V 3d (t_{2g}) band cross the E_F while the V 3d (t_{2g}) spin down band make a gap with the E_F, and this similarly of HM found in La_2VCuO_6 and La_2VMnO_6 [16].

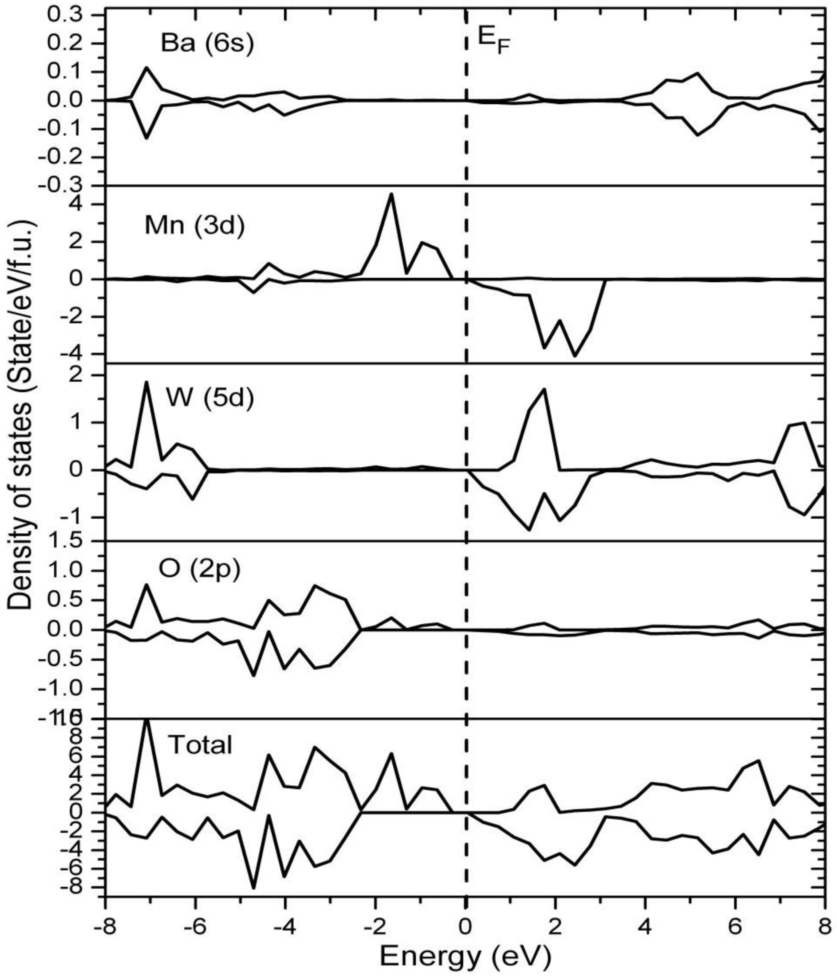

Fig. (5). The total and partial densities of states of Ba2MnWO6 in the fcc structure.

Fig.(5) illustrates the total and partial densities of states of the compound Ba_2MnWO_6. From the TDOS, there was an energy gap, about 0.75 eV, between E_F and the filled orbit. This classifies Ba_2MnWO_6 as a semiconductor material, which agree with J. Cheng and Z. Q. Yang results, obtained and published in Ref. [11]. The PDOS showed that, there were hybridization between the Mn 3d (e_g) and O (2p) orbits, which resulted as band emerged at E_F, indicating the half-filling of Mn 3d orbits (d^5). The contribution of W (5d) ion is very small, a weakly bands appears below the E_F, this reflects the empty 5d orbit in W^{6+} ($5d^0$) ion and populated 5d orbit in W^{5+} ($5d^1$) ion. This explained the effect of exchange interaction between Mn – O

– Mn magnetic ions in semiconductor Ba2MnWO6 double perovskite. Because the ion W^{5+} contains one electron 5d (d^1), there are some bands above the E_F as W 5d (t_{2g}) spin up and down as seen in panel (a), also there are a very small band occupation below the E_F, and W 5d hybridizes with O 2p between -6.0 eV and -3.0 eV, and at +2.0 eV above the E_F. From the PDOS of Mn^{3+} ion, panel (b), the splitting of the 3d bands, t_{2g} and e_g, indicates that Mn^{3+} is affected by crystalline field about 1.9 eV between the Mn 3d (t_{2g}) and Mn 3d (e_g) peaks, and the exchange energy is about 6.8 eV between the Mn 3d (t_{2g}) spin up and Mn 3d (t_{2g}) spin down peaks. The Mn^{2+} (e_g) spin up bands was hybridized with O 2p, which results bands emerged at E_F.

4.2 The magnetic structure of $Ba_2BB'O_6$

In double perovskite oxides $Ba_2BB'O_6$ with a B (3d) magnetic transition ion with less localized states, the magnetic exchange is dominated by the hopping of electrons between the different B-sites. This process can result either in ferromagnetic (FM) or in antiferromagnetic (AFM) electron coupling. Antiferromagnetic superexchange via the long range B – O – B′ – O – B exchange path [9,11,14], usually dominant for B′ ions with delocalized 5d electrons such as Hf^{4+}, Ta^{5+} or W^{6+} ions. The hybridizations between B′ (5d) and B (3d) states, result in a kinetic energy driven mechanism causing strong ferromagnetic exchange interaction between the B-sites [11]. From the PDOS of the $Ba_2V^{4+}Hf^{4+}O_6$ system, Fig.(3), it seen at energy about -4.5 eV that there is weak hybridization between the V 3d e_g spin up and Hf 5d e_g spin up states. There is no additional hybridization between the other remaining bands. The type of the half-metallic property appears in this compound is similar to that of CrO_2 [17]. This shows that this compound is a weak ferromagnetic (FM) material. As a result, a ferromagnetic coupling between V-sites is obtained. The local magnetic moments is calculated for V^{4+} $3d^3$ (S = 3/2) and Hf^{4+} $5d^0$ (S = 0) ions, they are found to be 1.39 and 0.35 μ_B, see Fig.(6).

In double perovskite oxide Ba_2CrTaO_6, the Cr 3d is a magnetic transition ion with strong localized states (t_{2g}^3), so, the magnetic exchange is dominated by hopping of electrons between the t_{2g} levels. This process can result in ferromagnetic (FM) coupling via the Cr – O – Ta – O – Cr exchange path that usually dominant for Ta^{5+} ($5d^0$) ions with noble gas configuration ions [13]. From the PDOS of $Ba_2Cr^{3+}Ta^{5+}O_6$ system, Fig.(4), it seen that at energy -1.5 eV there is strong hybridization between the Cr 3d t_{2g} spin up and O 2p, and Cr 3d e_g – Ta 5d e_g spin up and O 2p at E_F. There is Cr – Ta bands hybridization at energy of -7.5 eV. This shows that this compound is a ferromagnetic (FM) material, see Fig.(6). As a result, a ferromagnetic coupling between Cr-sites is obtained. The local magnetic moments are calculated and found to be 2.79 for Cr^{3+} 3d (S = 3/2) and -0.46 μ_B for Ta^{5+} 5d (S = 0).

The PDOS of $Ba_2Mn^{2+}W^{6+}O_6$ system in Fig.(5), shows that there are weak hybridizations between the W 5d e_g spin up and Mn 3d e_g spin up bands at E = -5.5 eV, where the W 5d t_{2g} spin up and Mn 3d t_{2g} spin up bands hybridize at E = -4.2 eV. These hybridizations Mn (3d) – O (2p) – W (5d) cause an antiferromagnetic

(AFM) exchange state, see Fig.(6). This is consistent with that obtained in reference [10,11]. These computations revealed that the valence bands are mainly formed from Mn 3d – O 2p states, while the conduction bands are derived from W 5d – O 2p states. The local magnetic moment on Mn^{2+} 3d (S = 5/2) ions is calculated and found to be 4.41 μ_B. This is not consistent with 4.42 μ_B**,** the value that obtained by J. Cheng et al for Ba_2MnWO_6 [11]. J. Cheng et al. were explained that due to antiferromagnetic structure, there is another kind of Mn^{2+} (3d) ions with the magnetic moment of 4.41 μ_B, whereas, the magnetic moment on W^{6+} 5d (S = 2) ions was -0.42 μ_B.

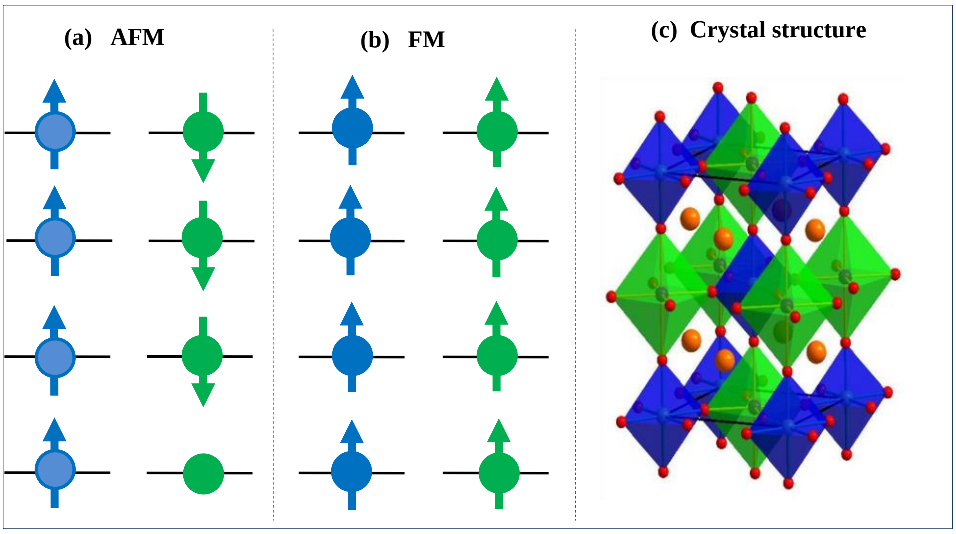

Fig. (6). Schematics show the favorite magnetic phases in transition metal cubic double perovskite oxides Ba2BB'O6; (a) AFM and (b) FM phases, in B (3d) – O (2p) – B' (5d) 1800-superexchange chains. B (3d) and B' (5d) ions are represented by blue and green spheres, and arrows ↑ and ↓ represent the spin-up and spin-down, respectively. (c) 3D arrangement of BO6 and B'O6 octahedra causes 180o bond-angle in B (blue octahedra) – O (small red spheres) – B' (green octahedra), while the large red spheres in caves between the BO6 – B'O6 octahedra be Ba2+ (6s) ions.

Table (3). Magnetic order and spin magnetic moments for Ba2BB'O6 compounds.

Compound	**Magnetic order**	m_B	$m_{B'}$	m_{Total}
Ba_2VHfO_6	FM	1.39	0.35	2.0
Ba_2CrTaO_6	FM	2.79	–0.46	3.0
Ba_2MnWO_6	AFM	4.41	–0.42	4.0

5. Conclusion

Using ab-initio linear muffin-tin orbital with atomic sphere approximation (LMTO-ASA) density functional method, a systematical study was carried out on the structural, electronic and magnetic properties of a series include three members of double perovskite oxides Ba_2VHfO_6, Ba_2CrTaO_6 and Ba_2MnWO_6. The total and partial densities of states were calculated with LSDA+U method. The compound Ba_2VHfO_6 are found to be a half-metallic conductor results of the contribution of spin up V 3d (t_{2g}) bands, the second member Ba_2CrTaO_6 found to be a conductor through the competition of the spin up and down of Cr 3d (t_{2g}) bands. While the third compound Ba_2MnWO_6 was found to be a semiconductor. Ferromagnetism (FM) order is observed in both double perovskite oxide structures Ba_2VHfO_6 and Ba_2CrTaO_6. These results was due to the V 3d (t_{2g}) spin up orbital hybridized with the Hf 5d (t_{2g}) spin up orbital and hybridization between the localized Cr 3d (t_{2g}) spin up and delocalized Ta 5d (t_{2g}) spin up orbitals. Antiferromagnetic (AFM) is observed in the third compound of Ba_2MnWO_6. The local magnetic moments in the unit cells of the crystals of three compounds are found to be: 1.39 μ_B for V^{4+} ion, 0.35 μ_B for Hf^{4+}, 2.79 μ_B for Cr^{3+}, -0.46 μ_B for Ta^{5+}, 4.41 μ_B for Mn^{2+}, and -0.42 μ_B for W^{6+}.

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التراكيب الكهربية والمغناطيسية لأكاسيد البيروفسكيت الثنائي $Ba_2BB'O_6$ (BB'=V-Hf, Cr-Ta, Mn-W) المكون من خليط من العناصر الانتقالية (3d–5d) باستخدام طريقة (LMTO-ASA)

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قسم الفيزياء، كلية العلوم، جامعة القصيم، بريدة ٥١٤٥٢، المملكة العربية السعودية

ملخص البحث. التراكيب الكهربية والمغناطيسية لسلسلة من أكاسيد البيروفسكيت الثنائي $Ba_2BB'O_6$
تم حسابها باستخدام المبادئ الأولية لطريقة الجهد الخطي الكعكي المداري مع تقريب الكرات الذرية (LMTO-ASA). تم إجراء الحسابات باستخدام أسلوب تقريب كثافة السبين المحلية بالإضافة إلى طاقة تفاعل كولومب (LSDA+U) على خلفية نظرية كثافة الدالة (DFT). أوضحت النتائج أن Ba_2VHfO_6 له خاصية نصف موصل وBa_2CrTaO_6 هو موصل. شرائط التوصيل في هذين المركبين تتشكل بصورة رئيسية من إسهامات عناصر V (3d) وCr (3d). المركب Ba_2MnWO_6 وجد أن له خاصية شبه موصل، وهذا يتفق مع النتائج التي تحصل عليها J. Cheng وZ. Q. Yang. الحالات المغناطيسية الأرضية للمركبين الأولين وجدت أنها مغناطيسية-موازية بينما المركب الثالث وجد أنه مادة مغناطيسية-مضادة. هذه الخواص ناتجة عن التهجين المداري بين V/Cr (3d) t_{2g} وHf/Ta (5d) t_{2g} ذات السبين الأعلى وبين مدارات Mn (3d) t_{2g} ذات السبين الأعلى وW (5d) t_{2g} ذات السبين الأسفل. العزوم المغناطيسية الجزئية في هذه المركبات وجد أنه يساوي $1.39\ \mu_B$ لـ V^{4+}، $0.35\ \mu_B$ لـ Hf^{4+}، $2.79\ \mu_B$ لـ Cr^{3+}، $0.46\ \mu_B$ لـ Ta^{5+}، $4.41\ \mu_B$ لـ Mn^{2+} و $-0.42\ \mu_B$ لـ W^{6+}.