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Investigation of Iron-based double perovskite oxides on the magnetic phase stability, mechanical, electronic and optical properties via first-principles calculation

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HIGHLIGHTS

- Based on the DFT calculation, the Pb_2FeMO_6 (M = Mo, Re and W) compounds have been investigated.
- The ground-state properties are predicted.
- The mechanical properties reveals that these compounds are stable against any elastic deformations.
- The electronic structures reveals the half-metallic ferrimagnets (FiM-HM) for all investigated compounds.

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ABSTRACT

The main goal of the present work is to obtain report on the magnetic phase stability, mechanical, electronic and optical properties of double perovskite oxides Pb_2FeMO_6 ($M = Mo$, Re and W) by employing the *ab-initio* plane-wave method, based on the density functional theory (DFT). The exchange-correlation (XC) energy of electrons was treated using the Perdew–Burke–Ernzerhof parametrization. The ground-state electronic properties for different magnetic configurations were calculated. The formation enthalpies has been evaluated in order to determinate the stability of our compounds. The independent elastic constants and the related mechanical properties are investigated. The electronic structure calculation reveal the half-metallic ferrimagnets (FiM-HM) for all investigated compounds. The optical constants as the dielectric function, refractive index, optical reflectivity and absorption coefficient were calculated and discussed in detail. Therefore, our compounds are identified as potential candidates for spintronic applications and high performance electronic devices.

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1. Introduction

High Curie temperatures, high magnetic moments, and large spin polarization at Fermi energy E_F are indeed the most important properties which have attracted a lot of attention from scientific community in order to create spintronic device with materials exhibiting all these remarkable properties. A typical example of these materials are the half-metallic (HM) magnetic materials, they have been characterized by the coexistence of metallic behavior for one spin direction and insulating behavior for the opposite spin direction. After the discovery of the first Half-metallic ferromagnetic (HMF) compound in 1983 by de Groot et al. [1], a lot of other materials have also been theoretically predicted in many systems include spinel Fe_3O_4 [2,3], Heusler alloys [4–8] and double perovskite [9–16]. Double perovskite become one of the important materials due to their application in several research topics, such as in magnetic memory components, single-spin electron sources and high efficiency magnetic sensors [17–19]. The double perovskite compounds are usually described by the chemical formula "$A_2BB'O_6$", where A is an alkaline-earth or rare-earth ion, B and B′ are different transition metals [20]. These compounds can exhibit a large variety of crystal structure with different space groups, which the most common systems are (*Fm*-3*m*), (*R*-3), (*I*4/*m*), (*I*2/*m*) and

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($P2_1/n$) [20]. The ordered double perovskite Pb_2FeReO_6 was synthesized in 2009 by Nishimura et al. [21], who reported that this compound crystallizes in body-centered tetragonal (BCT) structure with a space group of *I*4/*m* and the lattice constants of a = b = 5.62 Å and c = 7.95 Å. Similar to Pb_2FeReO_6 the favorable crystal structure of Pb_2FeMoO_6 is body-centered tetragonal (BCT) structure with the lattice constants a = b = 5.60 Å and c = 7.94 Å [22].

In this paper we present a systematic study of structural stabilities, mechanical, electronic and magnetic properties of the double perovskite compounds Pb_2FeMO_6 (M = *Mo*, *Re* and *W*) by employing the *ab-initio* calculation using the full-potential linearized augmented plane wave (FP-LAPW) method, based on the most accurate method for the computation of the electronic structure of solids which is the density functional theory (DFT) [23–25]. The aim of the present paper is to give information on the uninvestigated properties of these compounds, which have not been recognized to date.

2. Computational methods

All calculations of this present work are carried out by means of the first-principles full-potential linearized augmented plane wave (FP-LAPW) method [26], implemented in Wien2k code [27–29], which is a quantum mechanics program that can calculate the ground state energies of atomic systems based on density functional theory (DFT) [30,31]. The exchange-correlation (XC) potentials are considered by Perdew-Burke-Ernzerhof parameterization of the generalized gradient approximations (GGA-PBE) [32,33]. The parameter $R_{MT}K_{max}$, which represent the plane wave cut-off set to 8 for all our calculations. The muffin-tin radii (MT) were chosen as 2.5, 1.84, 1.98 and 1.59 Bohr for *Pb*, *Fe*, M = (*Mo*, *Re* and *W*) and *O* atoms respectively. Within the spheres, the charge density and potential are expanded in terms of crystal harmonics up to angular momenta L = 10 and in the interstitial region a plane wave is used. The G_{max} parameter, which define in charge density Fourier expansion the magnitude of largest vector is set to 14. The Monkorst-Pack method in the Brillouin zone for our compounds are performed with 2000 special *k*-points [34]. To set up the separation of valence and core states, the cut-off energy was chosen as −7 Ry. During the self-consistency cycles we select the charge convergence as 0.0001e.

For the localized electron states such as 4*d* orbitals of the *Mo* atom and 5*d* orbitals of (*W* and *Re*) atoms for which the self-interaction is particularly large, we have also chosen the GGA+U method [35–37], to reproduces the relative energetics, magnetic ground states, and electronic structure for our systems in which GGA fails. Around-the-mean-field (AMF) [38] version was employed for the GGA+U method, we have taken the effective on site Coulomb exchange correlations U_{eff} = U -J (U and J are the Coulomb and exchange parameters, respectively). The value of J was fixed to 0 eV, hence U_{eff} was equal to U in our calculations. For transition metals the U values are lies between 2 and 6 eV [39,40], so for the present work the values were chosen to be 5 eV for *Fe*-3*d* and 2 eV for *Mo*-4*d* and (*Re*, *W*)-5*d*. The DFT method which has proven to be one of the most accurate methods for the computation of the electronic structure of solids [23,24,66–69].

3. The ground-state properties and phase stability

Pb_2FeMO_6 is a double perovskite seems to be characterized by rock-salt *Fe* and M (*Mo*, *Re* and *W*) site cation ordering within the *Fm*3*m* space group [42]. But, after comparing the calculated total energies for various probable type structure for these ordering double perovskite compounds (monoclinic, orthorhombic, tetragonal and cubic), we found that the favorable type structure is body-centered tetragonal within the *I*4/*m* space group and their crystallographic characteristics which are summarized in Table 1. Fig. 1, show a representation of the crystal structure of the considered compounds for this work.

Table 1
The crystallographic characteristics as well as the atomic positions for Pb_2FeMO_6 (M = Mo, Re and W) compounds.

	Atom	Site	x	y	z
Pb_2FeMO_6	Pb	4d	$\frac{1}{2}$	0	$\frac{1}{4}$
(M = Mo, Re and W)	Fe	2a	0	0	0
*I*4/*m*	M	2b	0	0	$\frac{1}{2}$
Z = 2	O_1	4e	0	0	O_{1Z}
	O_2	8h	O_{2X}	O_{2Y}	0

Before calculating the equilibrium ground states of our compounds, we calculated their relaxed structures in order to determinate the internal parameters of the O-atoms for different magnetic configurations (ferromagnetic (FM), ferrimagnetic (FiM) and antiferromagnetic (AFM) phases), which the latter are reported in Fig. 2. The final internal parameter of the *O*-atoms are shown in Table 2. The calculated equilibrium lattice parameters obtained from GGA and GGA+U calculations are given also in Table 2, along with the experimental and other theoretical results. We conclude that our results are in excellent agreement with that obtained from other study [21,22,41]. We can note from the results that our compounds have the highly lattice parameters in the (AFM) phases. So as to calculate the stability of our compounds, with the purpose of understanding the thermodynamic behavior of the corresponding materials. The best indicator of the stability of materials is their enthalpy of formation. The enthalpy of formation of both compounds is calculated using the following equation [43,44]:

$$\Delta H_f(Pb_2FeMO_6) = E_{tot}(Pb_2FeMO_6) - Z\,(2E(Pb) + E(Fe) + E(M) + 3E(O_2)) \qquad (1)$$

where $\Delta H_f(Pb_2FeMO_6)$ is the formation enthalpy of Pb_2FeMO_6 with (M = Mo, Re and W), E_{tot} is the total energy per unit cell of the bulk compounds, *E*(X = Pb, Fe and M), it represents the total energy per atom of the element X in pure solid state, $E(O_2)$ is the total energies

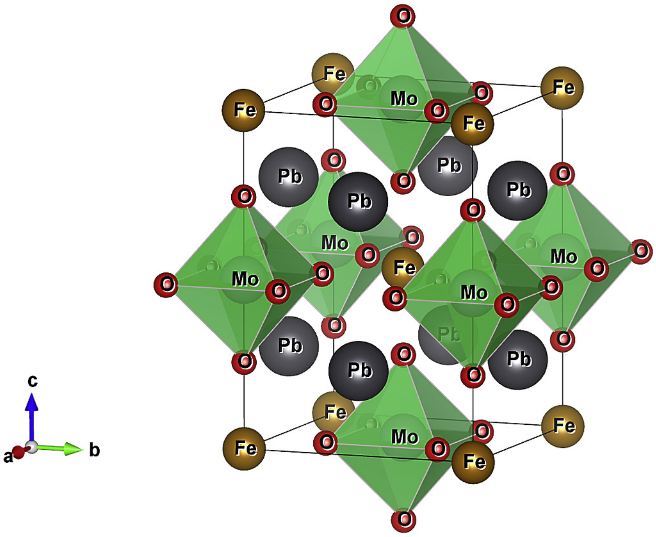

Fig. 1. A view of the crystal structure of the double perovskite Pb_2FeMoO_6 with six MoO_6 octahedron site.

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