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An ab initio study of the structural, elastic, electronic, optical properties and phonons of the double perovskite oxides Sr_2AlXO_6 ($X=\text{Ta}, \text{Nb}, \text{V}$)

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ABSTRACT

We report ab initio density functional theory calculations of the structural, elastic, electronic and optical properties of the double perovskite oxides Sr_2AlXO_6 ($X=\text{Ta}, \text{Nb}, \text{V}$). We have predicted a direct $\Gamma-\Gamma$ band gap in Sr_2AlXO_6 ($X=\text{Ta}, \text{Nb}$) and an indirect $\Gamma-X$ band gap for Sr_2AlVO_6 . The fundamental band gap increases linearly when the pressure is enhanced in the range 0–20 GPa. The frequency dependent of complex dielectric function, absorption, reflectivity and electron energy loss function were investigated in the range 0–40 eV. Features such as lattice constant, bulk modulus, elastic constants, band structure, total and local densities of states have been computed.

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1. Introduction

Double perovskite oxides have the $\text{A}_2\text{MM}'\text{O}_6$ formula and show various crystal structures. The M and M' cations present a large difference in charge or size. These double-perovskite oxides exhibit rich magnetic properties owing to the coexistence of two magnetic sites M and M'. This type of complex perovskites are the subject of enhanced scientific studies because their application in the industrial field. Double perovskite oxides exhibit interesting physical properties; in particular, their electronic structure is located from insulating to metallic, and even half-metallic with spin-polarized [1]. There are many $\text{A}_2\text{MM}'\text{O}_6$ type of double perovskite oxides reported in the literature, most of them can be elaborated under ambient pressure and others were synthesized at high-pressure. The ideal double perovskite oxides has a cubic structure with space group Fm3m. The double perovskite oxides can be obtained by a substitution of alkaline earth elements at the crystallographic site A, and transition metal or lanthanide elements at the M and M' sites [2]. For the series Sr_2AlXO_6 ($X=\text{Ta}, \text{Nb}, \text{V}$), Sr is

the best size to get a cubic space group Fm3m structure with close tolerance factor 1. These materials have various applications in technology such as dielectric resonators, voltage controlled oscillators, filters duplex in mobile phones and electrode in the magnetic junctions with tunnel effect because of their half-metallic character [3]. The tantalum complex oxides $\text{Sr}_2\text{AlTaO}_6$ shows a particular interest because of its photocatalytic activity [4,5], its ferroelectric behavior [6] and their dielectric properties [7,8]. These systems represent an important class of ceramic materials. Their catalytic properties allow a domain of very wide use in heterogeneous catalysis. It is believed that some of them would prove useful for spintronic applications. Owing to their excellent mixed-ionic and electronic conductivity and fast oxygen kinetics, double perovskite oxides exhibited excellent properties as solid oxide fuel cell oxygen electrodes [9,10].

The elaboration of Sr_2AlXO_6 ($X=\text{Ta}, \text{Nb}, \text{V}$) samples follows a mixture of SrCO_3 , Al_2O_3 , and Ta_2O_5 (Nb_2O_5 , V_2O_5) with a purity in the range 99.99 to 99.999% using a conventional solid state reaction [11]. Y.D. Li et al. [12,13] investigated by introducing intrinsic vacancies the induced magnetism in Sr_2AlXO_6 ($X=\text{Nb}, \text{Ta}$). I. Gorodea et al. studied the structural, electrical and catalytic characterization of $\text{Sr}_2\text{AlTaO}_6$ [11].

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In the present work, we applied a detailed theoretical study of the structural, elastic, electronic and optical properties of the family of double perovskite oxides Sr_2AlXO_6 ($X=\text{Ta}, \text{Nb}, \text{V}$) using the density functional theory (DFT) within LDA, LDA+U. The paper is organized as follows: The calculation method is described in Section 2. The most relevant results are reported and discussed in Section 3. Finally, the main conclusions are summarized in Section 4.

2. Calculation models and methodology

The density functional theory (DFT) calculations as implemented in the CASTEP code [14] were performed. using the local density approximation (LDA) with Teter and Pade parameterization [15] developed by Ceperly and Alder [16], LDA+U. The LDA+U method consists in a correction to the LDA energy functional to give a better description of electronic correlations. It is shaped on a Hubbard-like Hamiltonian including effective on-site interactions. It was introduced and developed by Anisimov and coworkers [17–19]. U is the unphysical curvature of the DFT total energy. We evaluate U from the DFT ground state. There is a different U for each distinct type of “Hubbard” atom, in most cases typical values are in the range $0 < U < 5$ eV. The choice of U in LDA+U requires its variation between 1 eV and 5 eV with a step of 1 eV. We noticed that the value 3 eV gives an internal parameter and a lattice constant closer to the experimental values. The interactions of valence electrons with ion cores were represented by the Vanderbilt-type ultrasoft pseudopotentials [20] for Sr, Al, Ta, Nb, V and O atoms. The data of energies and volumes obtained have been fitted to the equation of state due to Murnaghan [21] in order to obtain the minimum energy value, the bulk modulus, its pressure derivative and the equilibrium lattice parameters and associated volume. The special points sampling integration over the Brillouin zone is employed by using the Monkhorst Pack method [22] with $8 \times 8 \times 8$ k-point meshes. An energy cut-off of 360 eV was used for the calculations. The optimization of the internal coordination is a crucial task in order to have zero pressure and zero forces for correct calculations. The structural parameters were determined using the Broyden–Fletcher–Goldfarb–Shanno minimization technique [23]. The system is modeled in which the component atoms occupied the following positions: Sr (0.25, 0.25, 0.25), Al (0, 0, 0), Nb, Ta, V (0.5, 0.5, 0.5), and O (u , 0, 0).

3. Results and discussions

3.1. Structural properties

The double perovskite oxides Sr_2AlXO_6 ($X=\text{Ta}, \text{Nb}, \text{V}$) crystallize in the cubic structure with the space group Fm3m. This system

Table 1
Lattice constant, internal parameter and bulk modulus for Sr_2AlXO_6 ($X=\text{Ta}, \text{Nb}, \text{V}$).

	$\text{Sr}_2\text{AlNbO}_6$			$\text{Sr}_2\text{AlTaO}_6$			Sr_2AlVO_6	
	LDA	LDA+3	Other	LDA	LDA+3	Other	LDA	LDA+3
	{Exp}			{Exp}				
a_0 (Å)	7.8492	7.744	7.7999 [25] 7.784 [24]	7.7903	7.780	7.7839 [13] 7.7866 [24]	7.6632	7.624
u	0.2460	0.244	0.246 [25] 0.245 [24]	0.245	0.246	0.246 [13] {0.246 [24]}	0.252	249
B_0 (GPa)	164.2	168.1	172 [13]	159.7	160.8		168.8	170.2
B'	4.339	4.01	5.78 [13]	4.50	4.28		4.24	4.16

^{*} from EOS fitting.

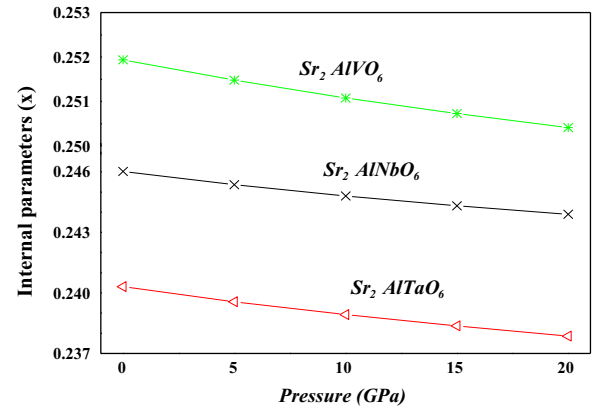


Fig. 1. The variation of internal parameter as function of hydrostatic pressure.

is characterized by two free structural parameters, the lattice constant (a) and the coordinate of the oxygen atom (u). We can see in Table 1 the obtained results for the lattice constant, the internal parameter, the bulk modulus (B) and its pressure derivative (B'), calculated by fitting the equation of state due to Murnaghan within LDA and LDA+U. Also shown for comparison are the available experimental data of lattice constant 7.7866 (7.784 Å) [24] for $\text{Sr}_2\text{AlTaO}_6$ ($\text{Sr}_2\text{AlNbO}_6$), which agree with our results and other theoretical one 7.7839 (7.7999 Å) reported in the literature [13,25]. We noticed that the LDA+U gives a lattice constant more closer to the experimental one than the LDA. The calculated equilibrium O atom positional parameter is in good agreement with the experimental value 0.246 (0.245) [24] for $\text{Sr}_2\text{AlTaO}_6$ ($\text{Sr}_2\text{AlNbO}_6$) and theoretical findings 0.246 (0.246) [13,25]. We did not find any experimental or theoretical results for Sr_2AlVO_6 , then our calculation is prediction. Under hydrostatic pressure effect in the range 0–20 GPa, the O atom parameter decreases monotonically and linearly with increasing pressure such as shown in Fig. 1. The O atom positional parameter increases in the sequence Ta → Nb → V.

3.2. Elastic constants

The predicted elastic moduli at equilibrium using LDA functional for Sr_2AlXO_6 ($X=\text{Ta}, \text{Nb}, \text{V}$) are shown in Table 2. The bulk modulus $B = \frac{1}{3}(C_{11} + C_{12})$ calculated from elastic constants has nearly the same value as obtained from the equation of state (EOS) in LDA and LDA+U cases. This may be an estimate of the reliability and accuracy of our computed elastic constants. For a cubic crystal under pressure, the generalized elastic stability criteria are [26]:

$$C_{11} + 2C_{12} + P > 0, C_{44} - P > 0, C_{11} - C_{12} - P > 0, C_{12} < B < C_{11} \quad (1)$$

The calculated elastic moduli satisfy the above criteria over the

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