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Unveiling the Multifaceted Nature of Sr_2FeMoO_6 Double Perovskites: Insights into Electronic and Optical Properties

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Abstract. In this study, an investigation of the intricate electronic and optical properties of the double perovskite compound Sr_2FeMoO_6 is conducted. In order to gain insight into its electronic structure, calculations are performed using the density functional theory (DFT) approach integrated into the Quantum Espresso software package. The results of these calculations reveal that the compound exhibits distinct behaviour as a direct bandgap semiconductor for both spin directions. An in-depth analysis of the dielectric function provides crucial insights into the optical absorption characteristics. At zero energy, the anticipated static dielectric constant for Sr_2FeMoO_6 is 6.16. The imaginary component, representing the energy absorbed by the compound as it is passed through by light, has a calculated maximum value of $\varepsilon_2(\omega)$ at $1.81eV$. These findings enhance our comprehension of Sr_2FeMoO_6 and facilitate the exploration of novel applications in advanced optoelectronic and thermoelectric devices. This research significantly contributes to the broader field of materials science and solid-state physics, providing valuable insights for future research endeavours.

1 Introduction

The growing demand for sustainable energy solutions has renewed interest in materials exhibiting exceptional physical properties. Double perovskites, particularly Sr_2FeMoO_6, have emerged as promising candidates due to their unique electronic and magnetic properties [1–4]. Characterized by a complex crystal structure and strong hybridization between metal orbitals, these materials offer exciting prospects for the development of innovative electronic devices.

The ongoing trend towards miniaturization of electronic devices has driven the search for multifunctional materials capable of combining multiple interesting properties. Double perovskites meet this demand, providing a platform to explore phenomena such as ferromagnetism, ferroelectricity, and superconductivity [5–7]

This study focuses on the orthorhombic phase of Sr_2FeMoO_6, a less studied phase with great potential for industrial applications. We aim to characterize in detail the structural,

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electronic, and optical properties of this phase to better understand its behavior and assess its potential applications in fields such as spintronics.

Building on previous works [8–13] , we propose an in-depth theoretical study of Sr_2FeMoO_6. We will employ ab initio calculation methods to explore the electronic structure, transport properties, and optical response of this material. The results of this study will provide a deeper understanding of the underlying mechanisms governing the properties of Sr_2FeMoO_6 and identify new avenues for the design of functional materials.

2 Computational Details

To delve into the intricate electronic interactions within Sr_2FeMoO_6 perovskites, we performed electronic structure calculations using the Quantum Espresso code [14] . DFT calculations were employed to generate the material's absorption spectrum. Atomic positions were optimized through the BFGS algorithm [15], and electron-electron interactions were modeled using the $PBE - GGA$ with norm-conserving pseudopotentials [16] . The SCF procedure was initiated with a $2 \times 2 \times 2$ k-point mesh, which was subsequently refined to a $4 \times 4 \times 3$ mesh for more precise DOS and PDOS calculations. Given the orthorhombic crystal structure, electronic structure calculations were converged to stringent thresholds of 47 R_y for kinetic energy and 489 R_y for charge density. Gaussian smearing with a Degauss value of $0.01R_y$ and an electron convergence criterion of 10^{-6} R_y ensured accurate results. These computational settings were meticulously selected to provide a comprehensive understanding of the electronic properties and behavior of Sr_2FeMoO_6 perovskites in their orthorhombic phase.

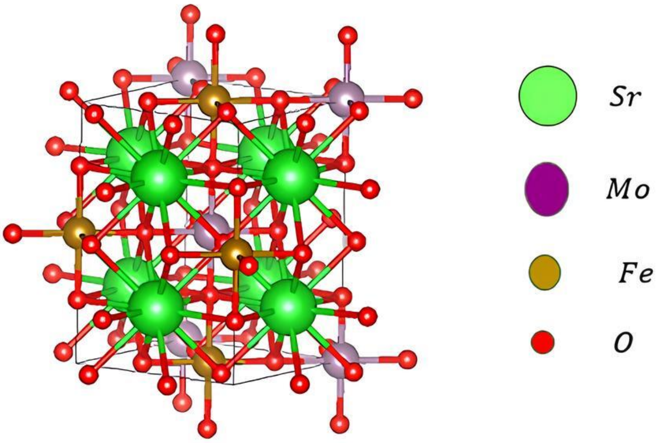

Figure 1. The double perovskite Sr_2FeMoO_6

3 Discussion of Results

3.1 Electronic properties

Understanding the electronic properties of solids is crucial because they heavily influence a material's ability to interact with light and heat. In particular, the electronic band structure plays a central role. This knowledge is essential for designing materials used in various devices, such as solar cells, thermoelectric converters, and transistors [17]. To examine the electronic structure and band distribution in Sr_2FeMoO_6, we employed the GGA approximation within density functional theory (DFT). Before these analyses, the crystalline structure underwent optimization to its lowest-energy equilibrium state, as depicted in Fig 1. This optimization process, coupled with the examination of elemental and orbital contributions, provides an enriched understanding of the electronic structures.

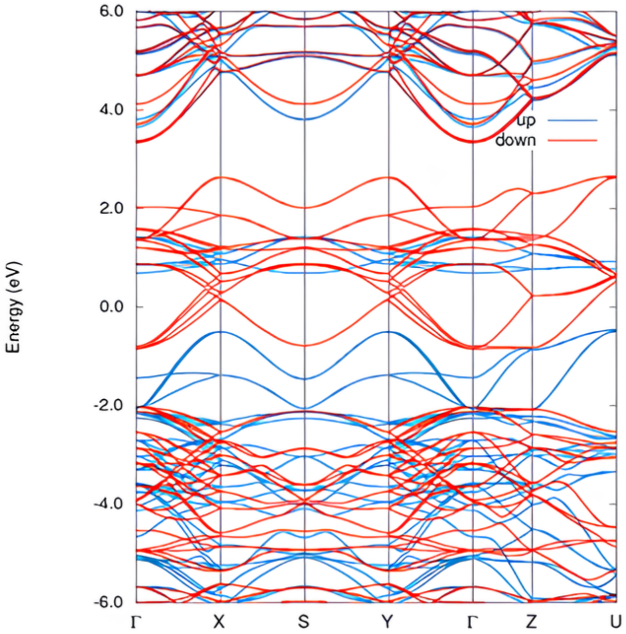

Figure 2. The band structure for Sr_2FeMoO_6 (Spin-Up/Down)

Our analysis encompasses the band structure, the density of electronic states (DOS), and the projected density of states (PDOS). By examining these properties, we can gain insights into the intricate electronic behavior of Sr_2FeMoO_6 and the specific contributions of its constituent elements. To understand the electronic band structures and band gaps, we performed calculations along high-symmetry directions within the first Brillouin zone, focusing on locating the conduction band minimum (CBM) and the valence band maximum (VBM) Fig 2. presents the spin-polarized electronic band structures of Sr_2FeMoO_6, highlighting high-symmetry points in the Brillouin zone ($\Gamma, X, S, Y, \Gamma, Z, U$). The Fermi level, set at $0eV$, serves as a reference. The spin-down channel exhibits a clear overlap between the valence and conduction bands, indicating strong metallic behavior for the minority spin. In contrast, the spin-up channel displays a distinct energy gap of approximately $0.8eV$ between the valence band (VB) and the conduction band (CB), suggesting semiconducting behavior for the majority spin. [18, 19]

To further elucidate the nature of the valence and conduction bands, we calculated the total density of states (TDOS) Fig 3 and the projected density of states (PDOS) Fig 4 . The lowest valence band is predominantly composed of oxygen $2p$ states, located around $[-6, -2]eV$. The spin-up configuration exhibits a narrow band gap, while the spin-down configuration remains metallic. This distinct electronic behavior confirms the half-metallic character of Sr_2FeMoO_6.

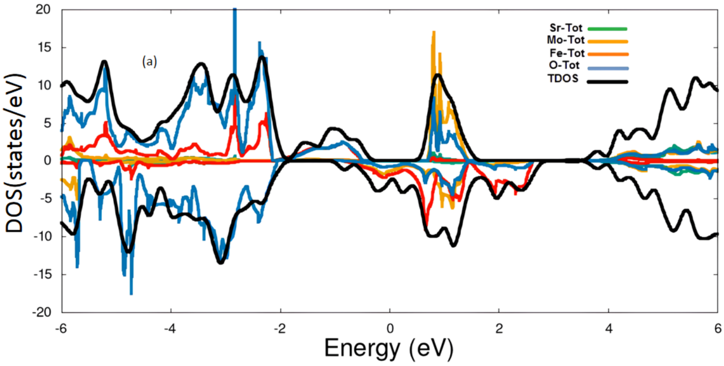

Figure 3. The total density of states TDOS for Sr_2FeMoO_6

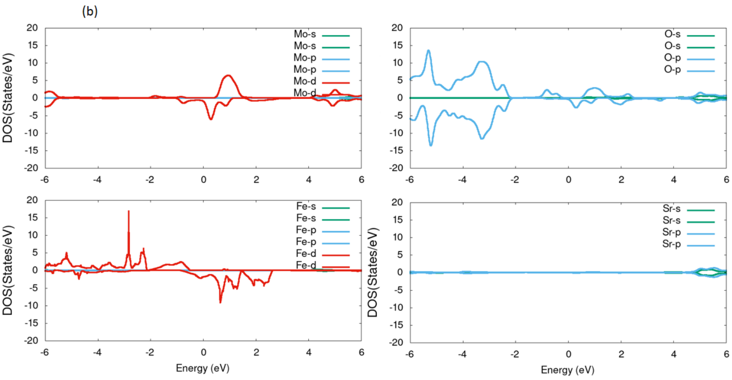

Figure 4. The projected density of states PDOS for Sr_2FeMoO_6

By analyzing the PDOS, we can observe the hybridization between $Fe\ 3d - orbitals$ and $Mo\ 4d - orbitals$ with oxygen $2p - orbitals$. This hybridization significantly influences the electronic states near the Fermi level, contributing to the unique electronic properties of Sr_2FeMoO_6.

3.2 Optical properties

Our intricate optical properties for Sr_2FeMoO_6 are described by the complex dielectric function, represented as: $\varepsilon = \varepsilon_1 + i\varepsilon_2$.

This formulation incorporates both the real (ε_1) and imaginary (ε_2) parts of the dielectric constant, which are crucial for understanding the material's interaction with light. The imaginary part (ε_2) is particularly intertwined with the electronic band structure, as it dictates the material's absorption properties. Through the application of the Kramers-Kronig relation, we can derive the real part from its imaginary counterpart [20]. As a result, the material's optical behavior is expected to closely resemble the anticipated electronic structures and density of states. The calculation of both real and imaginary dielectric functions was meticulously

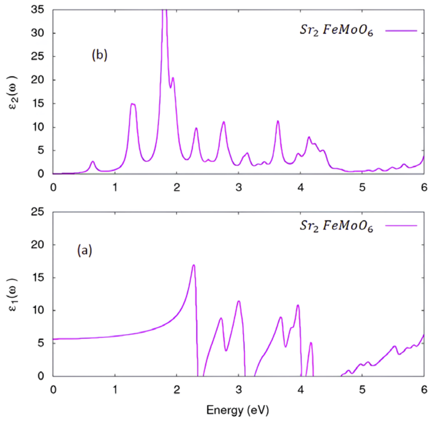

Figure 5. The Dielectric Function (real (a) and imaginary part (b)) for Sr_2FeMoO_6

performed within the energy range of $0to6eV$. The dielectric constant of Sr_2FeMoO_6 is depicted in Fig 5 as a function of photon energy. The figure separates the real and imaginary parts for clarity. At zero energy, the anticipated static dielectric constants for Sr_2FeMoO_6 is 6.16 Fig 3(a) . Notably, the prominent peaks in the real dielectric constant for the compound is strategically positioned within the visible spectrum.
The imaginary component signifies the energy input when light traverses through the compounds. Sr_2FeMoO_6 exhibits a calculated maximum value of $\varepsilon_2(\omega)$ at $1.81eV$ Fig 5(b). These findings underscore the nuanced optical properties of the materials, particularly within the visible spectrum, offering valuable insights for potential applications in optoelectronic devices.

4 Conclusion

The investigation into the electronic and optical properties of Sr_2FeMoO_6 has yielded valuable insights into the fundamental physics of these materials. The calculated electronic structure reveals that it exhibits distinct behaviour as a direct bandgap semiconductor for both spin directions. Moreover, the calculated dielectric function indicates substantial optical absorption in the visible range. These findings, when considered alongside the material's stability and the abundance of its constituent elements, suggest that Sr_2FeMoO_6 may be a promising candidate for photovoltaic and optoelectronic applications. Further research could include the development of synthesis techniques capable of efficiently producing high-quality Sr_2FeMoO_6 thin films and nanostructures on a large scale.

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