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Research Article

Investigation of Structural, Electronic and Magnetic Properties of Sr_2MnMoO_6 Perovskite Using Density Functional Theory (DFT)

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Abstract – Perovskites are of great interest for optoelectronics due to their unique electronic structures and light absorption capabilities across a wide wavelength range. They exhibit unique properties that make them highly promising for applications in energy production, storage, magnetic materials, and photovoltaic technologies. These materials can potentially be used in devices such as solar cells, photodetectors, and LEDs due to their suitable photovoltaic properties. As a member of the perovskites family, $SrMnMoO_6$ stands out because the distinctive structures and characteristics of perovskites enable them to be versatile candidates for advanced technological applications.In this study, we investigated the structural, electronic, and optical properties of this compound. The calculations were performed using the full-potential linearized augmented plane-wave (FP-LAPW) method based on Density Functional Theory (DFT), employing the Wien2k package. The PBE-GGA (Perdew-Burke-Ernzerhof) functional was used for the exchange-correlation potential. The calculated structural parameters show good agreement with experimental data. Additionally, we calculated the density of states (DOS) and electronic band structure. All compounds were revealed the metallic feature. These results were also found to be in good agreement with previous studies and experimental data.

Keywords – $SrMnMoO_6$, perovskites, electronic properties, optical properties, FP-LAPW

I. INTRODUCTION

Perovskites are a class of materials with a unique crystalline structure named after the mineral perovskite, and they are characterized by the presence of an oxygen-oxygen bond, which gives them distinct chemical properties. These compounds are often formed by the reaction of oxygen with metals or other elements, leading to a wide variety of applications, from their use in industrial oxidation processes to their

role in disinfectants and bleaching agents. Due to their ability to release oxygen and facilitate reactions, peroxides are also explored for energy storage technologies and environmental cleanup solutions.

The importance of peroxides in various applications stems from their remarkable electronic, optical, and structural properties, which enable them to play a critical role in diverse fields such as materials science, environmental technology, and medicine. Peroxides have great potential, especially in the fields of developing technology and materials science [1, 2]. Their unique electronic configuration allows peroxides to act as powerful oxidizing agents, making them essential in industrial processes like polymer synthesis and wastewater treatment. Additionally, their optical properties are exploited in advanced technologies such as sensors and light-emitting devices [3-5] while their structural versatility facilitates the design of novel materials for energy storage, catalysis, and even drug delivery systems. The combination of these properties makes peroxides highly valuable in both research and practical applications [6].

These materials can play an important role in many areas such as energy production, storage, magnetic properties and photovoltaic applications [7]. $SrMnMoO_6$ attracts attention as a compound belonging to the peroxide class because the special structures and properties of peroxides make them potential materials for many Technologies [6, 8, 9]. The potential of perovskites in photovoltaic applications plays a significant role in the increasing research to design low-cost, high-efficiency energy production systems. These materials have a broader light absorption spectrum compared to traditional silicon-based solar cells, enabling them to convert more sunlight into energy [10, 11]. Additionally, perovskite solar cells have a lower environmental impact because their production processes can be carried out at lower temperatures, requiring less energy. Another important application of perovskites is in photodetectors [12]. These devices are sensors that convert light into electrical signals, and perovskites offer high light detection capabilities with great precision across a wide range of wavelengths. Perovskite materials are increasing, particularly in optoelectronic devices, sensor technologies, and the biomedical field [13].

The structural properties of perovskites also provide a significant advantage. With their high crystal quality and flexibility, perovskites are materials that can remain stable under various physical and chemical conditions. These features make them stand out as durable and long-lasting components in energy storage systems and electronic devices. Furthermore, perovskites are being researched for their promising potential in energy conversion processes such as water splitting and hydrogen production [14]. Perovskite-based catalysts for the water-splitting reactions to produce hydrogen and oxygen from solar energy can accelerate hydrogen energy production with high efficiency. This could contribute to the development of the hydrogen economy [15, 16].

The catalytic properties of peroxides stand out as a critical tool in reducing air pollution and greenhouse gas emissions. Moreover, peroxides are attracting attention as materials that can convert waste heat into electrical energy. These properties offer great potential for increasing energy efficiency, especially in industrial processes, engines and power generation systems. The use of peroxides in this area provides a more efficient energy conversion process by minimizing energy losses [17-20]. The calculation of the electronic structure of crystal structures is done using computer software packages such as ABINIT, SIESTA, CASTEP, VASP and Wien2k [21] which are based on ab initio methods that enable exact solutions of the quantum mechanical ground states of electron systems based on the Kohn-Sham equations [22].

With each new technique developed, the success of the theory is steadily increasing. In recent years, thanks to new algorithms and advanced computer hardware used in computational chemistry and materials science, it has become possible to model more complex systems. The integration of new techniques and computational tools also supports interdisciplinary research in materials science. This

enables more efficient collaborations among researchers from different fields such as physics, chemistry, engineering, and computer science.

Wien2k software offers a wide range of capabilities for performing such electronic analyses. In particular, band structure calculations provide important insights into the efficiency of perovskites for potential photovoltaic applications [23, 24]. This study investigated the structural, electronic and magnetic properties of $SrMnMoO_6$ Perovksite using the Wien2k package program based on the Density Functional theory. In the simulations, the Exchange correlation functions given by Perdew Burke and Ernzerhof (PBE) were performed using the generalized gradient approximation (GGY).

II. Materials and Method

Computational Details

The structural, electronic, and optical properties of the Sr_2MnMoO_6 perovskite materials were analyzed using the density functional theory (DFT) framework. The self-consistent full-potential linearized augmented plane wave (FP-LAPW) method was implemented for calculations with in the Wien2k software package [25]. The Perdew-Burke-Ernzerhof (PBE) taken in conjunction with the generalized gradient (GGA) functional, dependent on the material's local electron density and its gradient, has been demonstrated to extraordinarily describe the crystalline structure, lattice constants, and metallic surface energies for tightly packed solid materials. To obtain more accuracy results and electronic calculations were performed with the modified Becke-Jonhson potential (mBJLDA) within the known Wien2k [26].

In this method, the space is separated to non-overlapping muffin-tin (MT) spheres separated by an interstitial region. The basis functions are expanded into spherical harmonic functions inside the muffin-tin sphere and Fourier series in the interstitial region. The calculation began with experimental data and searched for volume's minimum energy depend. The electronic and optical calculations were performed with optimized structure data.The energy convergence of the basis set was controlled with the cut-off parameter $R_{mt}K_{max}=7$; where Rmt is the smallest of the MT sphere radii and K_{max} is the largest reciprocal lattice vector used in plane wave expansion. G_{max}, which indicates the magnitude value of the largest vector in the Fourier expansion of the charge density, was 12 (a.u.). The energy convergence is selected as 0.0001 Ry and 0.001e during self-consistency cycles. The cutoff energy, which defines the separation of valence and core states, was chosen as -7 Ryd. For accurate convergence, the k-mesh of the order $10 \times 10 \times 10$ has been used after the analysis of repeated measurement for ground state energy.

In this approach, the computational domain is divided into non-overlapping muffin-tin (MT) spheres and an interstitial region. Within the MT spheres, basis functions are expressed as spherical harmonic functions, while in the interstitial region, they are expanded into Fourier series. The process began with experimental data and involved optimizing the structure by identifying the volume corresponding to the minimum energy. Electronic and optical properties were then calculated using the optimized structural parameters.

III. Results and DISCUSSION

Structural Properties

The electronic, structural, and optical properties of the Sr_2MnMoO_6 perovskite, crystallizing in a cubic structure with space group Fm3m, were analyzed using density functional theory (DFT). These calculations were carried out employing the self-consistent full-potential linearized augmented plane wave (FP-LAPW) method implemented in the Wien2k software.

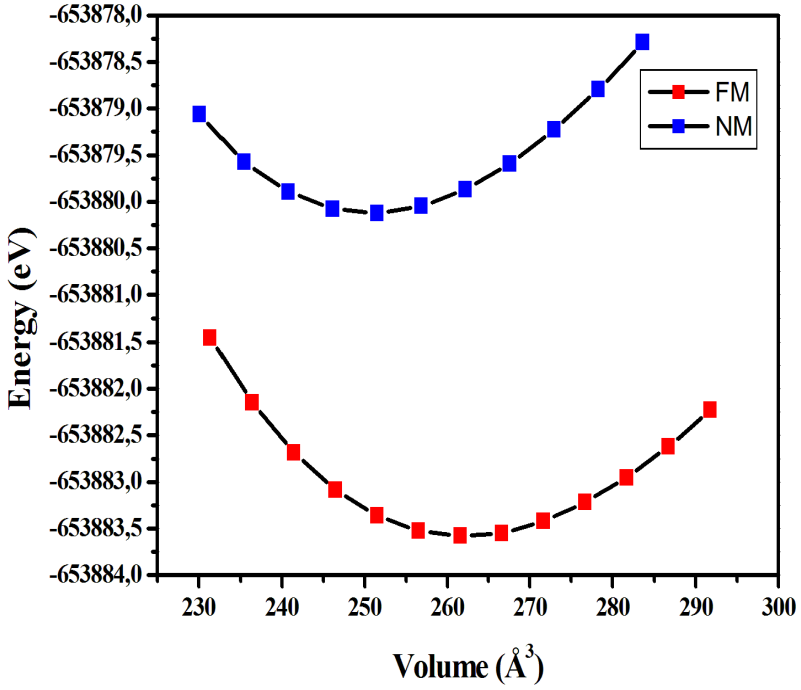

Fig. 1 Total energy dependence on unit cell volume for Sr_2MnMoO_6

The volume at which the energy reaches its minimum is identified as the ground state, with the corresponding unit cell parameters representing the optimal values.

Electronic Properties

In investigating the electronic properties of the Sr_2MnMoO_6 perovskite compound, thorough examinations of the total densities of states and the energy band structure were conducted. The total density of states (DOS) was calculated to ascertain the bonding nature and band transitions, as depicted in Fig 2. The lattice constants (a), the total energy per unit cell, the volume of the unit cell (Vo), the bulk modulus(B_0), and derivative pressure (B') for the studied structures have been calculated as 9.0337Å, -63265.169722Ry , 167.82Å ^{3}, B=102.122GPa and B'=4.89 GPa, respectively.

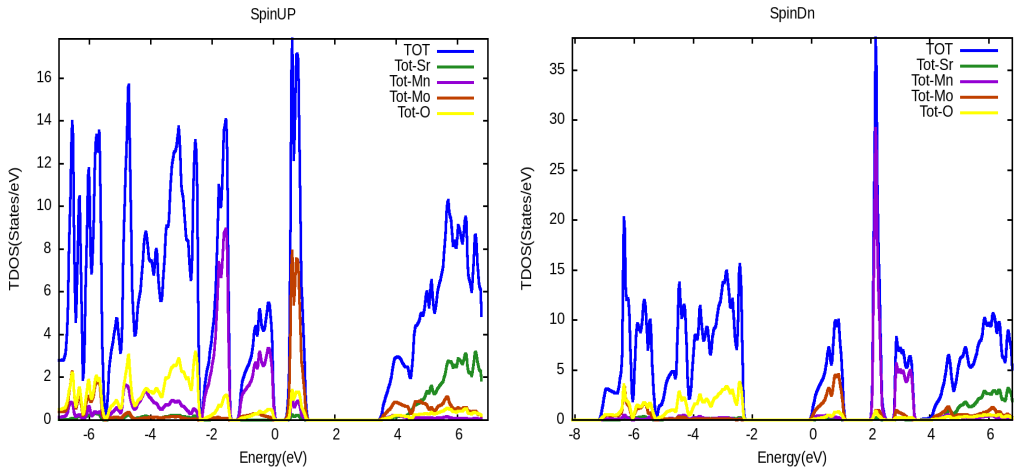

Fig. 2 Calculated total DOS of Sr_2MnMoO_6 compound with spin up and spin down configurations

Comprehensive calculations of the solid's energy bands and band gap across the Brillouin zone were conducted along the path (L–M–A–Γ–Z–V–Γ), using crystals with a relaxed structure corresponding to the minimum energy state. Band structure diagrams, covering an energy range of [−5 eV to 5 eV] and

wave vectors k, were produced to illustrate the atomic orbital distribution within a unit cell. The dotted line in Fig. 3 represents the energy level of the highest occupied state E_F.

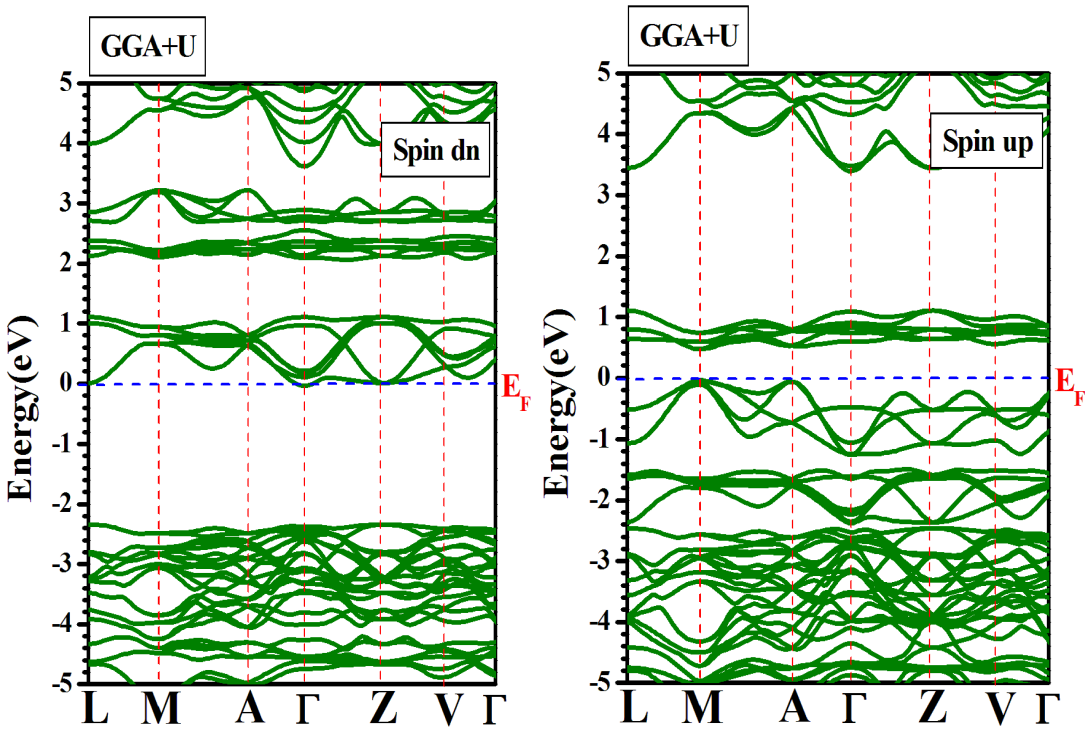

Fig. 3 Electronic band structure of Sr_2MnMoO_6 with spin up and spin down configurations

The band structure represents the permissible energy states for electrons, determined through calculations conducted at 0 K, thereby neglecting thermal effects. The highest energy level within the valence band is known as the Fermi level (E_F), which serves as the boundary between the conduction and valence bands. The conduction band is situated above E_F , while the valence band lies below it. The band gap is defined as the energy difference between the peak of the valence band and the lowest point of the conduction band.

IV. CONCLUSION

Perovskites can be used as catalysts, particularly in energy conversion and environmental technologies, to improve efficiency. Sr_2MnMoO_6 is a potential material for use in solid oxide fuel cells (SOFCs) or catalytic converters. The stability of these compounds under high temperatures and chemical reactions may make them suitable for applications in environmentally friendly energy production and pollution reduction technologies. Additionally, they could be useful in converting waste heat into electrical energy.

Sr_2MnMoO_6 perovskites, due to their unique electronic, magnetic, and catalytic properties, can be applied in a range of different fields. These compounds are expected to play an important role in future photovoltaic systems, energy efficiency applications, magnetic memories, and environmentally friendly energy production technologies. Therefore, detailed theoretical and experimental investigations of Sr_2MnMoO_6 perovskites could be a critical step toward new discoveries in materials science and advancements in their applications.

The use of perovskite materials not only enhances energy production and efficiency but also contributes to reducing environmental pollution and making energy systems more sustainable. The

advantages these materials provide across a wide range of applications, from optoelectronic devices to energy conversion systems, will significantly contribute to future technological advancements.

The theoretical and experimental investigation of Sr_2MnMoO_6 perovskites may lead to the discovery of new material classes. A detailed analysis of the electronic, structural, and magnetic properties of such compounds could lead to revolutionary developments in materials science. Furthermore, research on these materials will help us understand the properties of other perovskites and compounds, enabling the development of more efficient technologies.

The theoretical study of this compound's structural, magnetic, and electronic properties is a critical step in fully realizing the potential of these materials, optimizing their applications, and contributing to innovative technologies. Combining theoretical analyses with experimental studies could lead to more efficient and robust material designs and achieve significant progress in the technological world.

The structural and electronic properties of the Sr_2MnMoO_6 compound were studied using the full potential linearized augmented plane wave method, applying all-electron calculations based on DFT with various exchange and correlation potentials. The unit cell dimensions, total energy values, bulk modulus, and the first derivative of the bulk modulus were calculated. The density of states (DOS) and electronic band structure plots reveal that the compound exhibits metallic characteristics.

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