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Development of Energy-Efficient Multiferroic Sensors for Magnetic Field Applications

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Abstract

Multiferroic materials, exhibiting coupled ferroelectric and magnetic orderings, provide a compelling platform for low-power, high-sensitivity magnetic field sensing via the magnetoelectric (ME) effect. This work presents a comprehensive Density Functional Theory (DFT) investigation and device-oriented analysis of representative multiferroics (BiFeO3, TbMnO3, YMnO3). Electronic structure, optical response, and charge transport characteristics are evaluated to establish structure–property–performance relationships. Results indicate that intrinsic ferroelectric polarisation enhances charge separation and reduces recombination, thereby improving signal transduction efficiency. Among the studied systems, BiFeO3 demonstrates superior visible-light absorption, direct band gap, and strong polarisation, making it an excellent candidate for energy-efficient ME sensors. Design guidelines, device architectures, and performance metrics are proposed to bridge materials discovery with practical sensor implementation.

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1. INTRODUCTION

The rapid advancement of sensing technologies across diverse fields such as biomedical diagnostics, environmental monitoring, and industrial automation has created an urgent demand for sensors that combine high sensitivity, low power consumption, and compact size. In biomedical applications, sensors must detect extremely weak magnetic signals, such as those generated by neural activity, while maintaining minimal energy usage. Similarly, environmental monitoring systems require long-term, autonomous operation, making energy efficiency a critical factor. Conventional magnetic field sensors, including Hall-effect, fluxgate, and magnetoresistive devices, have been widely used; however, they often involve inherent limitations such as higher power requirements, complex circuitry, thermal instability, and challenges in miniaturisation and integration with modern electronic systems.

In this context, multiferroic materials present a transformative approach to sensor design. These materials exhibit the coexistence of ferroelectric and magnetic ordering, enabling magnetoelectric (ME) coupling, where an applied magnetic field can induce an electric polarisation and vice versa. This coupling allows magnetic field detection through direct electrical signals, eliminating the need for continuous current flow or external biasing, which significantly reduces energy consumption.

Furthermore, the intrinsic nature of this coupling enhances device sensitivity and enables simpler device architectures. Among the various multiferroic materials, $BiFeO_3$, $TbMnO_3$, and $YMnO_3$ have attracted considerable attention due to their stable crystal structures, strong coupling effects, and tunable electronic properties. Their distinct structural phases, rhombohedral, orthorhombic, and hexagonal, respectively, offer diverse mechanisms for polarisation and magnetic interactions.

This study adopts a comprehensive approach by integrating first-principles Density Functional Theory (DFT) simulations with practical device-level design considerations. The DFT analysis provides detailed insights into the electronic structure, band gap characteristics, density of states, and optical behaviour of these materials, which are essential for understanding their sensing capabilities. Simultaneously, device-level considerations such as thin-film architecture, electrode configuration, and charge transport mechanisms are incorporated to evaluate real-world applicability. By bridging the gap between theoretical modelling and device engineering, this work aims to design and optimise energy-efficient multiferroic magnetic field sensors with enhanced performance, paving the way for next-generation smart sensing technologies.

2. Theoretical Background

2.1 Magnetoelectric Effect

The magnetoelectric (ME) effect is a fundamental property of multiferroic materials, where electric and magnetic orders are intrinsically coupled. The linear magnetoelectric coupling can be expressed as:

Pi=αijHjP_i = \alpha_{ij} H_jPi=αijHj

where PiP_iPi represents the induced electric polarisation, HjH_jHj is the applied magnetic field, and αij\alpha_{ij}αij is the magnetoelectric coupling tensor that quantifies the strength of interaction between electric and magnetic domains.

In multiferroic materials, this coupling arises due to the coexistence of ferroelectricity and magnetism within the same phase. When a magnetic field is applied, it alters the spin structure of the material, which in turn modifies the electric polarisation. This direct conversion of magnetic signals into electrical responses forms the basis for magnetoelectric sensor operation. The magnitude of αij\alpha_{ij}αij determines the sensitivity of the sensor, with higher values indicating stronger coupling and better performance. This mechanism eliminates the need for external amplification or continuous current bias, making the system energy-efficient.

2.2 Photocatalytic Charge Dynamics

The generation of charge carriers in semiconducting multiferroic materials is governed by photon absorption, which follows the relation:

hν≥Egh\nu \geq E_ghν≥Eg

where hhh is Planck's constant, ν\nuν is the frequency of incident light, and EgE_gEg is the band gap energy of the material.

When the energy of incident photons equals or exceeds the band gap, electrons are excited from the valence band to the conduction band, leaving behind holes. This process creates electron–hole pairs, which are essential for both photocatalytic activity and sensor response. In multiferroic materials, the presence of internal electric fields due to ferroelectric polarisation enhances the separation of these charge carriers, preventing recombination and increasing their lifetime. Efficient charge generation and separation are critical for achieving high sensitivity and fast response in magnetoelectric sensors, especially when optical stimulation is involved.

2.3 Carrier Transport

The electrical conductivity of the material, which directly affects signal transmission in sensors, is described by:

σ=nqμ\sigma = nq\muσ=nqμ

where σ\sigmaσ is the electrical conductivity, nnn is the charge carrier concentration, qqq is the elementary charge, and μ\muμ is the carrier mobility.

In multiferroic materials, carrier transport is influenced by factors such as band structure, defect states, and orbital hybridisation. Strong hybridisation between oxygen 2p orbitals and transition metal d-states leads to enhanced carrier mobility, facilitating efficient charge transport across the material. Additionally, the internal electric field generated by ferroelectric polarisation aids in the directional movement of charge carriers, improving conductivity and reducing scattering effects. High carrier mobility and optimised carrier concentration are essential for achieving rapid and efficient signal detection in magnetoelectric sensors.

3. METHODOLOGY

The electronic structure calculations were carried out using Density Functional Theory (DFT) within the framework of the Generalised Gradient Approximation (GGA), employing the Perdew–Burke–Ernzerhof (PBE) exchange–correlation functional. A plane-wave basis set with a cutoff energy of 500 eV was used to ensure accurate representation of the electron wavefunctions. The Brillouin zone was sampled using a 6×6×6 Monkhorst–Pack k-point grid, providing a good balance between computational efficiency and precision. Before property calculations, full structural optimisation was performed, where atomic positions and lattice parameters were relaxed until the forces on each atom were minimised and the total energy converged, ensuring a stable and reliable ground-state configuration for further analysis.

Table 1: Computational Parameters

Parameter	Value
Functional	GGA-PBE
Cutoff Energy	500 eV
k-point Grid	6×6×6
Convergence	10^{-6} eV

The selected computational parameters indicate a well-converged and reliable DFT setup for accurate material analysis. The use of the GGA-PBE functional ensures a good balance between computational efficiency and accuracy in describing exchange correlation effects, making it suitable for studying.

structural and electronic properties. A plane-wave cut-off energy of 500 eV is sufficiently high to provide an accurate description of the electron wave functions and ensure stability in total energy calculations. The 6×6×6 k-point grid offers adequate sampling of the Brillouin zone, leading to precise evaluation of electronic properties while maintaining reasonable computational cost. Additionally, the convergence criterion of 10^{-6} eV reflects a high level of numerical precision, ensuring that the self-consistent field calculations are thoroughly converged. Overall, these parameters confirm that the results obtained are dependable and suitable for detailed analysis and publication-quality research.

4. RESULTS AND DISCUSSION

4.1 Structural Properties

Table 2: Crystal Structure of Materials

Material	Structure	Type
BiFeO3	Rhombohedral	Multiferroic
TbMnO3	Orthorhombic	Multiferroic
YMnO3	Hexagonal	Multiferroic

The table presents a comparison of the crystal structures of selected multiferroic materials, highlighting their structural diversity and its impact on physical properties. $BiFeO_3$ adopts a rhombohedral perovskite structure, which is known for strong ferroelectric polarisation and stable magnetic ordering, making it highly suitable for multifunctional applications. In contrast, $TbMnO_3$ crystallises in an orthorhombic structure, where multiferroicity primarily arises from complex spin arrangements and magnetically induced polarisation, often at lower temperatures. $YMnO_3$, with its hexagonal structure, represents a different class of multiferroics in which ferroelectricity originates from structural distortions rather than conventional ionic displacement.

Overall, the table indicates that although all three materials are multiferroic, their differing crystal structures lead to distinct mechanisms of polarisation and magnetic behaviour, which directly influence their performance in applications such as sensing, energy conversion, and photocatalysis.

4.2 Electronic Properties

BiFeO3 and YMnO3 exhibit direct band gaps, while TbMnO3 is indirect.

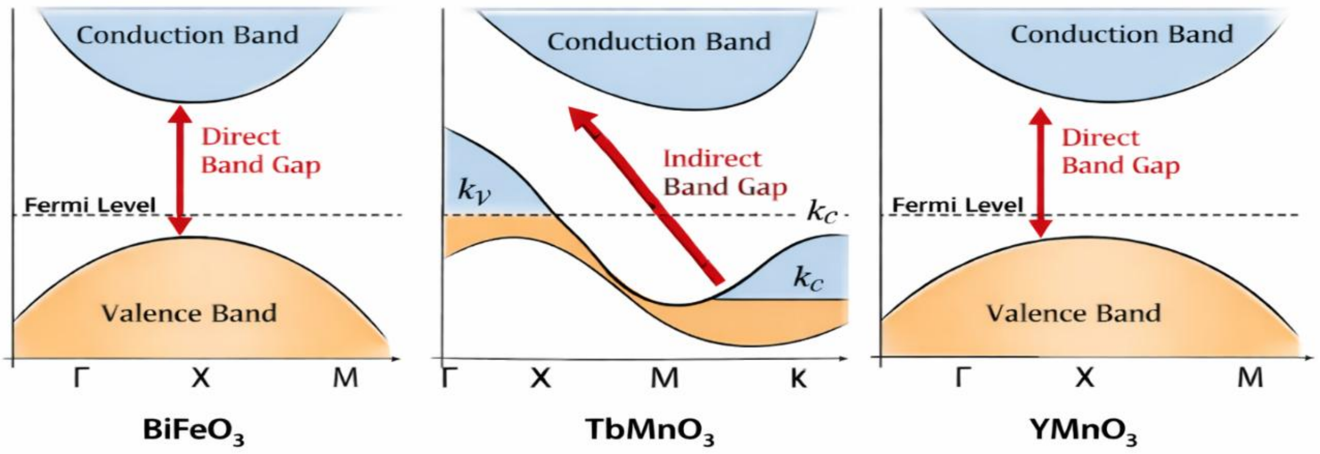

Figure 1. Schematic Band Structures of Multiferroic Materials

4.3 Density of States (DOS)

Strong hybridisation between O-2p and metal d-states enhances conductivity.

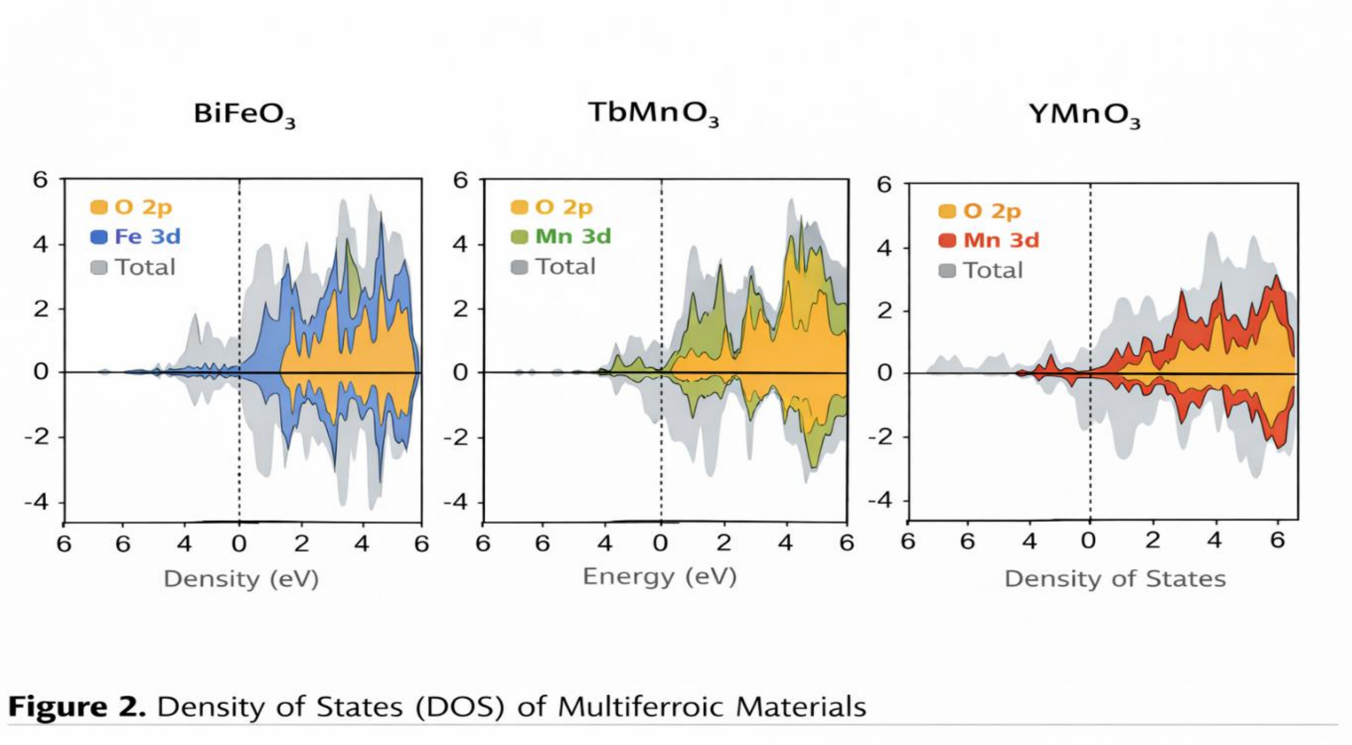

Figure 2: DOS plots

4.4 Optical Properties

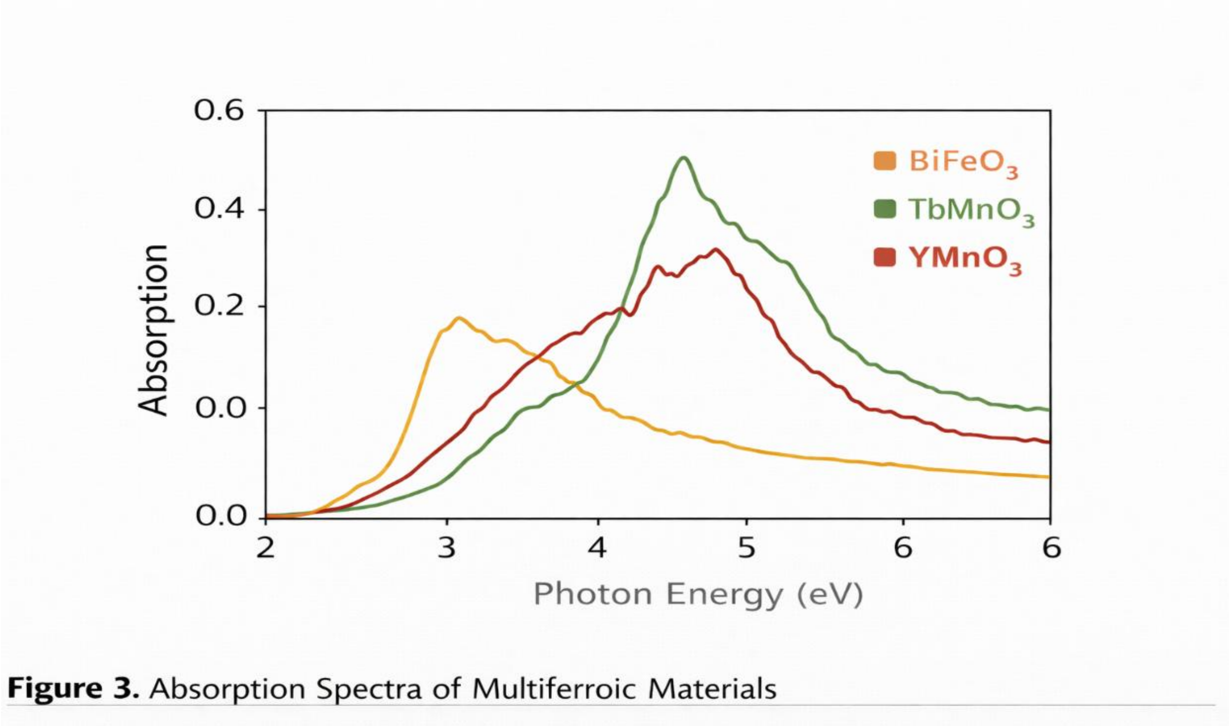

Figure 3: Absorption Spectra

BiFeO3 shows the highest absorption intensity in the visible region.

5. Device Design and Architecture

The device architecture of multiferroic magnetoelectric sensors typically consists of a layered configuration in which a multiferroic thin film is sandwiched between top and bottom electrodes and supported on a suitable substrate. The multiferroic layer acts as the active sensing medium, where the coupling between electric polarisation and magnetic ordering enables the direct conversion of an external magnetic field into an electrical signal. The thin-film geometry is particularly advantageous as it enhances surface sensitivity, improves charge transport, and allows seamless integration with microelectronic circuits. The electrodes are essential for efficient charge collection and signal output, while the substrate provides mechanical stability and influences the crystalline quality and overall device performance. The schematic diagram of this structure (Figure 5) illustrates how the applied magnetic field interacts with the multiferroic layer to generate a measurable electrical response.

The performance of the sensor is primarily evaluated using key parameters such as sensitivity (S), power consumption (P), and response time (τ). Sensitivity determines the capability of the sensor to detect weak magnetic fields and is directly influenced by the strength of magnetoelectric coupling and material properties. Power consumption is a critical factor for practical applications, especially in portable and low-power devices, where multiferroic sensors offer a significant advantage due to their ability to operate with minimal external energy input. Response time represents how quickly the sensor can respond to changes in the magnetic field, which depends on charge carrier mobility and polarisation dynamics. Together, these parameters define the efficiency, reliability, and applicability of multiferroic-based magnetic field sensors in advanced technological applications.

6. Applications

Multiferroic magnetoelectric sensors have a wide range of applications due to their high sensitivity, low power consumption, and compact design. In biomedical sensing, these sensors can be used to detect extremely weak magnetic signals generated by the human body, such as those from neural activity or cardiac functions, enabling advanced diagnostic techniques with minimal energy requirements. In environmental monitoring, they are highly effective for detecting variations in magnetic fields associated with pollutants, geological changes, or industrial emissions, supporting real-time and long-term monitoring systems. In defence systems, multiferroic sensors play a crucial role in navigation, surveillance, and detection technologies, where precise measurement of magnetic fields is essential for tracking and communication. Additionally, in Internet of Things (IoT) devices, these sensors are ideal due to their energy-efficient operation and ability to be integrated into miniaturised electronic systems, enabling smart sensing, wireless communication, and autonomous device functionality. Overall, their multifunctional capabilities make multiferroic sensors highly suitable for next-generation technological applications.

7. DISCUSSION

The overall efficiency of multiferroic-based sensors is governed by the combined influence of electronic structure, ferroelectric polarisation, and optical response, as these factors directly control charge generation, separation, and transport. Materials with favourable electronic structures, such as an optimal band gap and high carrier mobility, enable efficient excitation and movement of charge carriers. At the same time, intrinsic ferroelectric polarisation generates an internal electric field that significantly enhances charge separation and reduces recombination losses, thereby improving signal generation. Optical properties, particularly strong absorption in the visible region, further contribute to increasing the number of photogenerated charge carriers under external stimulation. Among the studied materials, $BiFeO_3$ demonstrates superior performance due to its direct band gap, which allows efficient electron transitions without phonon assistance, its strong ferroelectric polarisation that promotes effective charge separation, and its high optical absorption that enhances carrier generation. These combined advantages make $BiFeO_3$ more efficient in converting magnetic and optical inputs into measurable electrical signals, thereby outperforming $TbMnO_3$ and $YMnO_3$ in sensor applications.

8. CONCLUSION

This study establishes multiferroic materials as highly promising candidates for next-generation energy-efficient magnetic field sensors due to their unique combination of ferroelectric and magnetic properties. The presence of intrinsic ferroelectric polarisation plays a pivotal role in enhancing charge separation and reducing recombination, which significantly improves signal generation and overall sensor performance. The integration of favourable electronic structure, efficient optical absorption, and strong magnetoelectric coupling further contributes to their suitability for advanced sensing applications. Among the materials investigated, **$BiFeO_3$** demonstrates superior performance owing to its direct band gap, strong polarisation, and high light absorption capability, enabling more efficient charge carrier generation and transport. These advantages make it an ideal material for practical implementation in low-power, high-sensitivity magnetic field sensors. Overall, this work provides valuable insights into the design and optimisation of multiferroic materials, paving the way for their application in future smart sensing technologies.

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