

An AI-Driven Roadmap for the Development of Alkali Metal-Modified BiFeO₃ Multiferroics

Om Prakash Hota¹ and Sudhansu Sekhar Hota^{2,*}

¹Dept. of Teacher Education, Rajendra University, Prajna Vihar, Balangir, Odisha-767002, India

²Department of Physics, ITER, Siksha 'O' Anusandhan Deemed to be University, Bhubaneswar-751030, India

Abstract: Bismuth ferrite (BiFeO₃) is one of the most promising single-phase multiferroic materials because it coexists with ferroelectric and antiferromagnetic ordering at room temperature. Nevertheless, it has intrinsic limitations for practical applications, including high leakage current, poor magnetization due to cycloidal spin structures, and phase instability. This review is a detailed discussion of the basic physics behind BiFeO₃, its crystal structure, the origin of ferroelectricity, magnetic ordering, as well as the magnetoelectric coupling mechanism. The alkali metal (Li, Na, K, Rb, Cs) substitution is of particular interest, as it has been found to be a useful approach to design structural distortion, defect chemistry, polarization behavior, and magnetic interactions. In addition, the shortcomings of traditional experimental methods in the optimization of dopant content and processing are mentioned. To address these problems, new artificial intelligence (AI) and machine learning (ML) methods are pointed out as effective means to speed up the exploration of materials, forecast structure-property correlations, and design high-performance multiferroics. Lastly, a roadmap for the systematic creation of alkali metal-modified BiFeO₃ systems is suggested, which offers perspectives on the subsequent generation of versatile materials and applications in devices.

Keywords: BiFeO₃, Multiferroics, Alkali metal doping, Ferroelectricity, Magnetoelectric coupling, Spin structure, Machine learning, Artificial intelligence, Perovskite oxides, Materials informatics.

1. INTRODUCTION

Multiferroic materials Multiferroic materials that use two or more order parameters of ferroic type have, e.g., ferroelectricity, ferromagnetism, or ferroelasticity, attracted significant interest because of their multifunctional capabilities in the development of spintronics, sensors, actuators, and non-volatile memory devices [1-3]. The interaction of the electric and magnetic order parameters of such materials allows magnetic properties to be externally controlled by applying electric fields, which provides energy-saving solutions to the next generation of electronic devices [1, 2].

BiFeO₃ has been one of the most promising materials amongst the other multiferroic materials due to its distinctive capability of coexisting in a state of both ferroelectric and antiferromagnetic orderings at room temperature [4, 5]. BiFeO₃ crystallizes in a rhombohedrally distorted perovskite structure with R3c space group, and has a large Curie temperature (~1100 K) and Neel temperature (~640 K), and is thus a useful device material [4-6]. The latest developments have shown that it can be used in a wide variety of applications, including photocatalysis, energy harvest, and multifunctional electronic devices [5, 6]. Moreover, continuous researches have been conducted in structural engineering and compositional developments

to develop functional characteristics within the engineering [7].

The multiferroicity in BiFeO₃ has essentially been determined by its distinctive electronic structure and its magnetic interactions. This is mainly due to the fact that the ferroelectric behavior is attributed to the stereochemically active 6s² lone pair electrons of the Bi³⁺ ions, which cause a non-centrosymmetrical distortion in the lattice, thus causing spontaneous polarization [4, 5]. Alternatively, G-type antiferromagnetism with Fe³⁺-O-Fe³⁺ super exchange interaction forms magnetic ordering in BiFeO₃ [4, 6]. Nevertheless, the appearance of a long-wavelength cycloidal spin structure (~62 nm) cancels the macroscopic magnetization and in this way restricts its magnetic response [4]. This spin cycloid is either suppressed by chemical substitution or external perturbation to achieve an enhanced weak ferromagnetism and an enhanced magnetoelectric coupling [7, 8]. Thus, these natural physical processes are important in understanding and regulating physical mechanisms to enhance the multifunctional characteristics of BiFeO₃-based systems.

These attractive properties notwithstanding, pure BiFeO₃ has a number of intrinsic weaknesses that inhibit its extensive technological use. These are high leakage currents as a result of oxygen vacancies, low magnetization as a result of the existence of a cycloidal spin structure, as well as difficulty in making phase-pure synthesis [4, 5]. These problems severely impair its ferroelectric and magnetoelectric functionality,

*Address correspondence to this author at the Department of Physics, ITER, Siksha 'O' Anusandhan Deemed to be University, Bhubaneswar-751030, India; E-mail: sudhansusekhar405@gmail.com

thus compelling it to employ suitable measures to improve its property [4, 8].

Chemical doping is one of the most efficient methods to break these drawbacks, especially by replacing the A-site or B-site of the perovskite lattice [7, 8]. In this regard, alkali metal doping with such elements as lithium (Li⁺), sodium (Na⁺), and potassium (K⁺) receives more and more interest because of the possibility to adjust the structural, electrical, and magnetic characteristics of BiFeO₃ [9, 10]. Introduction of the alkali metal ions into the lattice can result in lattice deformation, altering defect chemistry, and preventing oxygen vacancy formation, which in turn reduces leakage current and enhances the performance of ferroelectrics [9]. Moreover, these types of doping have the capability of increasing magnetization by interrupting the spiral spin structure and encouraging spin canting, which is an essential step towards augmenting magnetoelectric coupling [8].

It has also been noted that alkali metal modification can also have a significant effect on the electronic structure and band gap of BiFeO₃, and hence its usability in optoelectronics and energy-related applications [10]. Also, the changes in behavior of charge transport and polarization dynamics produced by doping add to the better performance of the device [6, 7]. Nevertheless, the issue of the type and concentration of dopants optimization is a complicated task because of the multicollinear interaction of various structural and electronic aspects. Conventionally, the design and optimization of doped multiferroic materials are heavily dependent on time-consuming, resource-intensive, and inefficient experimental trial and error studies [11, 12]. These traditional processes restrict the high-speed exploration of large compositional design spaces and interfere with the process of finding high-performance materials with customized characteristics. Consequently, the increased necessity has arisen for other methods capable of speeding up the process of materials discovery with minimal costs of experimentation.

Over the past few years, AI and ML have become potent instruments in the field of materials science, facilitating the data-driven design of improved materials as well as rapid discovery of novel materials [11, 13, 14]. Information on large datasets, the possibility to detect hidden trends, and high-precision prediction of material properties can be efficiently analyzed using AI-based methods, which greatly simplifies the situation of having to conduct a lot of experiments [11, 12]. In predicting important properties, including bandgap, polarization, and magnetic ordering of complex oxide systems, techniques of supervised

learning, neural networks, and high-throughput screening have proven effective [15, 16].

Moreover, machine learning has been very promising to inform the development of multiferroic materials through the establishment of optimal compositions and processing regimes [17, 18]. As an example, ML-based systems have been used to hasten the identification of new ferroelectric and multiferroic systems, which can be used to identify promising materials with improved functional characteristics [16, 17]. Besides, the combination of AI and high-throughput computational techniques has also enabled the sampling of large compositional space, thus offering new perspectives on structure-property relationships in complex materials [12]. In the recent progress that materials informatics has made, autonomous research workflows have been developed, in which AI algorithms drive experimental design and optimization in a closed-loop fashion [12]. These are especially useful in the case of multi-parameter systems, such as alkali metal-doped BiFeO₃, the ultimate properties of which depend on many different parameters. With the help of the AI-based methods, the optimization of doping strategies can be dramatically accelerated, and the overall performance of the multiferroic materials can be improved.

In spite of these remarkable achievements, no in-depth studies have been undertaken that combine alkali metal doping plans with AI-based plans to develop BiFeO₃-based multiferroics in a systematic manner. The majority of the existing literature priorities lie either on experimental studies of doped systems or on isolated studies of computations and do not afford a single framework to unify the two fields [8, 11]. The identified gap indicates that there is a need to conduct a thorough review integrating experimental knowledge with AI-based approaches.

Therefore, the present review is projected to have a profound and methodical overview of the alkali metal-modified BiFeO₃ multiferroics with a particular emphasis on AI-based design solutions. The review discusses the fundamentals of BiFeO₃, its properties and limitations, along with the influence of alkali metal doping on the structural and functional performance of the material and the role of machine learning in the speedy discovery of materials. Finally, a roadmap given by an AI is recommended to guide further research on the path of efficient design and optimization of next-generation multiferroic materials.

2. FUNDAMENTAL PHYSICS OF BIFEO₃ MULTIFERROICS

BiFeO₃ is a single-phase multiferroic material, which is amongst the most researched materials owing

to its simultaneous ferroelectric and antiferromagnetic ordering at room temperature. BiFeO_3 is a multifunctional material, and the crystal structure, electronic configuration, and magnetic interactions inherently regulate the ferroic properties and the coupling mechanism [19-22]. These basic dimensions need to be thoroughly known as a means of modelling their performance via compositional engineering and by exterior perturbation [23, 24].

It has been indicated that the symmetry and phase stability and domain structure of BiFeO_3 can be altered significantly by means of structural changes, *i.e.*, cation exchange and defect engineering, and consequently, the ferroelectric and magnetic properties of BiFeO_3 can be affected in a tremendous way [19-22]. In addition, the lattice distortion, charge distribution, and spin ordering interaction are also critical in the determination of the multiferroic properties of this material. Specifically, the structural and electronic degrees of freedom are particularly coupled, which allows the coexistence of various ferroic orders, making BiFeO_3 an exemplary model system to study the phenomenon of magnetoelectricity.

Furthermore, the recent developments in nanoscale engineering and thin-film creation have also shown that the intrinsic properties of BiFeO_3 can be enhanced by the dynamics and strain effects of domain walls [25]. These results emphasize the significance of learning the basic physics of its multiferroicity that can be used as a basis for designing better materials with the help of doping techniques and AI-based methods, which are discussed in further subtopics.

2.1. Crystal Structure and Symmetry

At room temperature, BiFeO_3 crystallizes in a perovskite structure, rhombohedrally distorted in space group $R3c$. This is a structure with a network of corner-sharing FeO_6 octahedra, and Bi^{3+} ions in the A-site of the perovskite lattice. The geometry defect of the ideal cubic perovskite structure is caused by the stereochemical activity of the lone pair electrons of Bi^{3+} that results in a non-centrosymmetric geometry necessary to be ferroelectric [23, 24].

Structural investigations have demonstrated that phase transitions and compositional changes can be caused by doping and modification of the structure, leading to changes in the symmetry of BiFeO_3 , which in turn affects its physical characteristics [19, 20]. As an example, various crystallographic phases can be stabilized by substituting rare-earth and forming solid solutions, which leads to an improved dielectric and magnetic behaviour [21, 22]. In addition, the lattice parameters and domain structures can also be varied using thin-film engineering and strain, which further gives control of the functionality of the material [25].

Of special interest is the connection between crystal symmetry and functional properties because breaking of symmetry is a requirement for the occurrence of ferroelectricity and magnetoelectric coupling. Thus, accurate regulation of the crystal structure is the key to the optimization of the performance of BiFeO_3 -based systems.

2.2. Origin of Ferroelectricity

BiFeO_3 ferroelectricity is based on the stereochemically active $6s^2$ lone pair electrons of Bi^{3+}

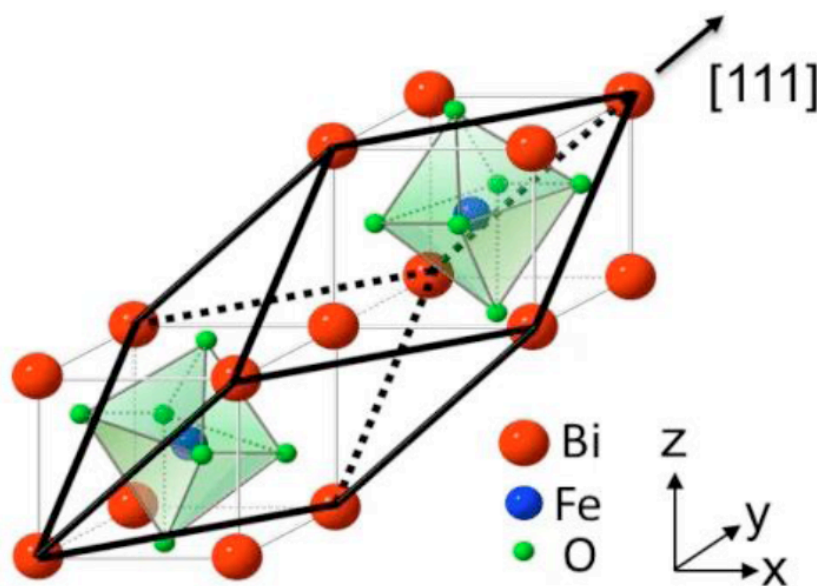


Figure 1: Crystal structure of BiFeO_3 showing rhombohedral ($R3c$) symmetry with Bi, Fe, and O atomic positions. Reproduced from Mejia *et al.*, Journal of Physics: Conference Series, 2016, with permission (OPEN ACCESS C.C BY 3.0) [26].

ions, which give rise to an off-center displacement in the perovskite lattice, leading to spontaneous polarization. This dislocation discontinuity of the symmetry of the crystal inversion, as well as the large polarization value (up to 90-100 $\mu\text{C}/\text{cm}^2$) of the substance, is what makes BiFeO₃ one of the most promising ferroelectric substances [27].

The stoichiometry of the cation, distortion of the lattice, and the concentration of the defects are some of the important factors that establish the amount of polarization and also its stability [27]. It has also been shown in recent years that external influences like strain, electric field, and compositional tuning can have a big effect on ferroelectric properties, and analogous structure-property connections have been identified in doped perovskite systems [28-30]. These are also in line with previous reports in which compositional control is instrumental in adjusting ferroic properties [29]. Polarization is also important in applications like photocatalysis and conversion of energy, where polarization promotes the separation and transmission of charge [31].

Moreover, by having polarization and other order parameters coupled, multifunctional behavior can be realized, and such behavior can be controlled by doping and nanoscale engineering. These properties make it important to know how the concept of ferroelectricity in BiFeO₃ came into existence in order to maximize its functionality.

2.3. Magnetic Ordering and Spin Structure

BiFeO₃ has G-type antiferromagnetic ordering. In this type, the magnetic moments of neighboring Fe³⁺ ions are antiparallel due to the superexchange interaction between oxygen atoms. This Fe³⁺-O-Fe³⁺ bond causes the long-range magnetic ordering observed in the material [32].

One of the unique characteristics of BiFeO₃ is a long-wavelength cycloidal spin structure (c. 62 nm) that is able to modulate the antiferromagnetic order and effectively delocalize the net macroscopic magnetization [33, 34]. This spin cycloid imposes a practical scale on the magnetic response of the material, but it may be suppressed by doping, strain, or

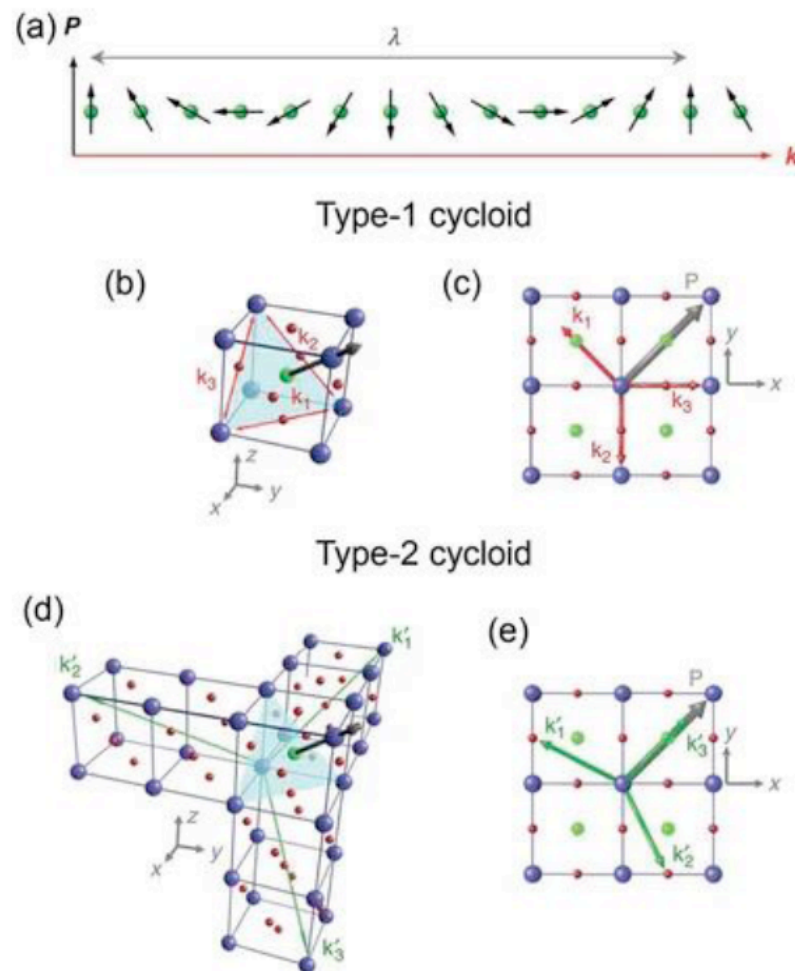


Figure 2: Representation of spin cycloids in BiFeO₃, illustrating type-1 and type-2 cycloidal spin structures and their propagation vectors.

Reproduced from Burns *et al.*, Advanced Materials, 2020, under CC-BY 4.0 license [34].

an external field of the material, resulting in weak ferromagnetism.

Recent work also includes the development of magnetic symmetry and transport of magnon systems in BiFeO₃-based systems, including the discovery of complex interactions and spin dynamics [32, 33]. These results highlight the necessity to comprehend spin structure and magnetic ordering in order to enhance magnetoelectric performance.

2.4. Magnetoelectric Coupling Mechanism

The magnetoelectric coupling between the ferroelectric and the magnetic orderings in BiFeO₃ can occur due to the coexistence of both. This results in the ability of the electric polarization to interact with the magnetic moments. Spin-orbit interactions and considerations of symmetry dominate this type of coupling, as is the case with the Dzyaloshinskii-Moriya interaction, which is also important to connect magnetic and electric order parameters.

Magnetoelectric coupling can be greatly increased through structural and compositional changes to change both the lattice symmetry and electronic structure [35, 36]. As an illustration, co-substitution and strain engineering have been demonstrated to enhance both ferroelectric response and magnetic response at the same time, resulting in enhanced coupling effects [35].

More recent theoretical work has also demonstrated the potential of using electric-field control of magnetic states in complex multiferroic systems, which are new avenues to spintronic applications [37]. This kind of development suggests that BiFeO₃ has the potential to be used as a platform in multifunctional devices.

2.5. Limitations of Pristine BiFeO₃

Pristine BiFeO₃ possesses good characteristics; there are also a few limitations in its use. The high

leakage current, primarily attributed to oxygen vacancies and non-stoichiometry, is a significant problem [38, 39]. These weaknesses lead to augmented conductivity and corrosion of the ferroelectric properties.

The second weakness is low net magnetization due to the cycloidal spin structure that suppresses macroscopic magnetism. Besides, the lack of phase-pure synthesis and structural stability also makes it difficult to use in practice [40-42]. Some of the ways that have been used to overcome these challenges include doping, strain engineering, and controlled methods of synthesis. Particularly, defect engineering and compositional tuning have proven to have immense potential in the removal of leakage current and the general performance [39].

The following limitations are essential in the design of superior materials based on BiFeO₃, as later on in the paper.

3. ALKALI METAL DOPING IN BIFEO₃

This alkali metal doping is among the most helpful techniques of structurally, electrically, and magnetically engineering perovskite oxides, more so BiFeO₃. Introduction of monovalent alkali ions such as Li⁺, Na⁺, and K⁺ into the A-site of the perovskite lattice results in severe lattice deformation, alteration of charge compensation mechanisms, and defect chemistry. These effects are very fundamental in the elimination of the natural limitations of pure BiFeO₃, including high leakage current, low magnetization, and phase instability.

Modifications to internal electric fields and manipulation of charge transport behavior in perovskite have been observed in recent years to be controllable by alkali metal insertion, and this results in overall functional performance [43]. Such modifications can easily be made in BiFeO₃ to achieve polarization,

Table 1: Intrinsic Structural and Ferroic Properties of BiFeO₃

Property	Value	Reference
Crystal Structure	Rhombohedral (R3c)	[23, 24]
Curie Temperature (T _c)	~1100 K	[23]
Néel Temperature (T _N)	~640 K	[23, 32]
Polarization	~90–100 $\mu\text{C}/\text{cm}^2$	[28, 30]
Magnetic Ordering	G-type Antiferromagnetic	[32, 33]
Spin Structure	Cycloidal (~62 nm)	[34]
Magnetization	Weak (suppressed by spin cycloid)	[34]
Leakage Behavior	High due to oxygen vacancies	[38, 39]

stabilization of ferroelectric domains, and enhancement of magnetoelectric coupling, which presents a viable route to the tuning of polarization. Besides this, ionic size discrepancy between alkali ions and Bi³⁺ is caused as well, and these can be regulated to induce structural distortion, which is significant in regulating phase transitions and ferroic properties.

3.1. A-site Alkali Doping (Li, Na, K)

One of the best studied methods of manipulating the properties of BiFeO₃ is A-site substitution with alkali metals. Charge imbalance caused by the substitution of Bi³⁺ ions by monovalent ions (Li⁺, Na⁺, and K⁺) is usually balanced by either the oxidation state of Fe ions or oxygen vacancies. This form of compensation contributes greatly to the conductivity of the electrical properties of the material, the polarization characteristic, and the magnetism of the material.

In the case of perovskite systems, A-site alkali doping has been demonstrated to improve ionic mobility and electrochemical performance by changing the lattice structure and electrochemical charge transport pathways [44]. Likewise, the synergistic effects between dopants and alkali metals in oxide systems cause a better structural stability and improved functional properties of the oxide systems when co-doped [45]. Multi-element substitution plans have been reported to enhance compositional engineering by causing structural evolution and enhancing magnetoelectric coupling in the case of BiFeO₃ [46].

Moreover, alkali metal doping has the capability of impacting the electronic band structure that facilitates bandgap-tuning and enhanced photocurrent response that are essential in optoelectronic and energy-related applications [47]. Though others are on transition metal doping (e.g., Cu), they also prove that compositional modification can have a significant impact on structural, magnetic, and ferroelectric properties, and this is in support of the overall idea of having property improvement because of doping [48].

However, there are integrated doping approaches like (La, K)-modified BiFeO₃ system that have demonstrated simultaneous improvement of both the ferroelectric and magnetic characteristics as a result of enhanced domain orientation and prohibition of spin cycloidal structures [49]. These data make it evident that A-site alkali doping is a promising pathway to the targeted adjustment of multifunctional properties in BiFeO₃ by means of controlled lattice distortion and defect engineering.

3.2. Structural and Phase Transition Behavior

The alkali metal doping has an important effect on the structural evolution and the phase transition behavior of BiFeO₃. Introduction of dopant ions in the lattice can change lattice parameters, strain and alter symmetry that may produce phase transitions between crystallographic phases, including rhombohedral, orthorhombic and tetragonal.

The morphotropic phase boundary (MPB), where various phases exist, is one of the most important concepts in the study of such transitions and results in improved functional properties. Research on doped BiFeO₃ systems has demonstrated that the existence of MPB has a considerable effect in amplifying ferroelectric and piezoelectric reactions owing to amplification in the polarization rotation and domain motion [50]. The same phase transition phenomenon is also seen in other perovskite systems, where doping of the material causes structural modifications that are accompanied by changes in magnetic and dielectric properties [51].

The A-site or B-site substitution in the BiFeO₃-based materials can lead to a change of the rhombohedral R3c phase to a different symmetry phase in order to alter the ferroic properties [52, 53]. Such structural transitions can be related to the change in the domain structure, polarization dynamics, and magnetoelectric coupling. Additionally, the distortion of the lattice through doping can have an effect on the angles of the bonds as well as the bond lengths, which have a direct impact on the electronic structure and magnetic interactions.

Phase stability is also largely contributed to by defect engineering. Defects can be introduced or blocked by the incorporation of a dopant to cause local distortions of the lattice that can impact further phase changes and functionality. Defect-induced modifications, such as those that increase piezocatalytic and ferroelectric performance against doped BiFeO₃ systems, have been demonstrated [54].

In general, the power to regulate the structural evolution and phase changes by means of doping of alkali metals is essential to the multifunctional character of BiFeO₃. Such structural changes are the basis of further changes in electrical, magnetic, and magnetoelectric properties.

The emergence of a morphotropic phase boundary (MPB) plays a crucial role in enhancing the ferroelectric and magnetic properties of doped BiFeO₃ systems by stabilizing coexisting phases and facilitating polarization rotation [50-54]. This phenomenon is schematically illustrated in Figure 3.

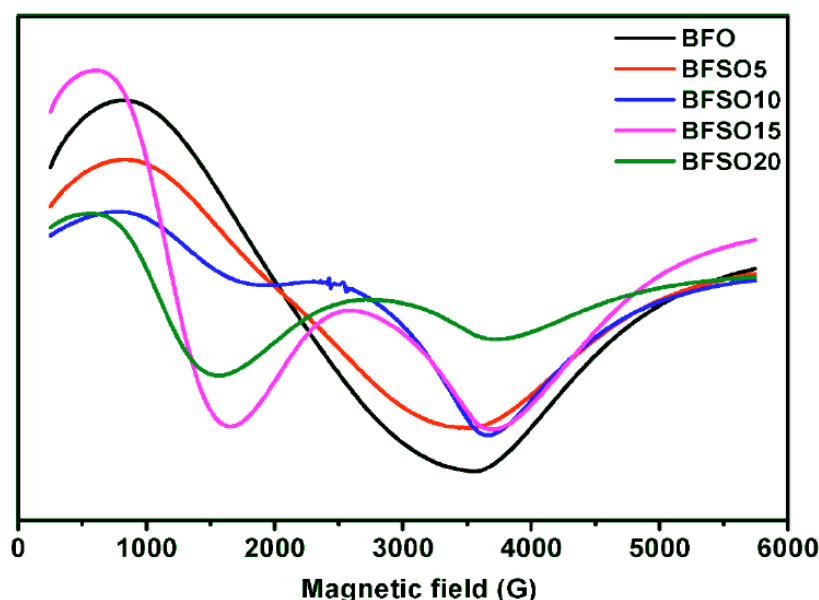


Figure 3: Morphotropic phase boundary (MPB) concept in doped BiFeO₃ illustrating phase coexistence and enhanced functional properties.

Reproduced from F.F. Orudzhev *et al.*, *Molecules*, 2022, 27, 7029. <https://doi.org/10.3390/molecules27207029> (CC BY 4.0 license) [55].

Table 2: Effect of Alkali Metal Doping on Structural and Functional Properties of BiFeO₃

Dopant	Structural Effect	Electrical Effect	Magnetic Effect	Ref
Li	Lattice contraction	Leakage ↓	Slight ↑	[44]
Na	Phase stability	Polarization ↑	Moderate ↑	[47]
K	Larger distortion	Resistivity ↑	Strong ↑	[49]

3.3. Electrical and Magnetic Properties

Electrical and magnetic properties of materials include the ability to conduct and retain a magnetic field (in the presence of a magnetic field). Intrinsic defects, compositional tuning, and structural distortions induced by dopants play a crucial role in dictating the electrical and magnetic characteristics of BiFeO₃, which in turn can be regarded as the determinants of the multifunctional performance of this material. High leakage current is one of the severe constraints of pristine BiFeO₃, and it is mainly caused by oxygen vacancies and mixed valence of Fe²⁺/Fe³⁺ ions. These defects entrap localized electronic states in the band gap, which enables charge transport via hopping conduction and therefore suppresses ferroelectric hysteresis behaviour. This means that its stability to polarization is lower and therefore restricts its use in real-life devices. Recent research has shown that leakage current may be suppressed well using a controlled process of defect engineering and doping. Indicatively, Liu *et al.* indicated that leakage current suppression yields a great deal of improvement in both the temperature stability and the performance of bismuth ferrite-based lead-free piezoceramics [56].

On the same note, Gao *et al.* have demonstrated that non-stoichiometric control and variation of processing atmosphere have a strong impact on leakage current behavior, as well as ferroelectric behavior by changing defect density and charge transport processes in BiFeO₃ thin films [57]. Besides that, Ahn and Son showed that Cr-modified BiFeO₃ thin films have an outstanding ferroelectric property and a high energy storage capacity because leakage current is effectively suppressed, and domain switching properties are also improved [58].

Simultaneously, the magnetic characteristics of BiFeO₃ are dictated by its inherent G-type antiferromagnetic arrangement, which is disturbed by a long-wavelength cycloidal spin arrangement of about 62 nm. This cycloidal spin spacing efficiently removes the net macroscopic magnetization, thus restricting its magnetic reaction. Nevertheless, chemical substitution has been demonstrated to make a remarkable improvement in magnetization by breaking this spin cycloid. As an example, Salamatin *et al.* have shown that Tb doping increases the magnetic properties by changing the microstructure and phonon interactions and suppressing the cycloidal spin structure partially [59].

Besides chemical substitution, post-synthesis treatments can also affect the magnetic properties of BiFeO₃-based thin films. Kostishyn *et al.* studied the magnetic properties of nanoscaled BiFeO₃, (BiLa)FeO₃, and (BiNd)FeO₃ multiferroic films after corona treatment [60]. Their research shows that corona treatment can serve as an alternative processing method to tune the magnetic response of BiFeO₃-based materials. In the case of multi-functional-property optimization, it is important to note that the magnetic properties of BiFeO₃ are affected by chemical composition and lattice distortion as well as the processing and post-treatment conditions [60].

Similarly, in another study by Palchaev *et al.*, it was revealed that Sm doping causes phase evolution and defect-induced characterization of BiFeO₃ ceramics, which enhances magnetic ordering and general functional behaviour [61]. Weak ferromagnetism and the enhancement of magnetization are facilitated by the suppression of the spin cycloid, which leads to the spin canting. Such effects can also be explained by the distortion of the lattice and changes in the angle between Fe-O-Fe bonds that change superexchange interactions and enhance magnetoelectric coupling. Therefore, the performance of doped BiFeO₃ systems as both electrical and magnetic materials is enhanced synergistically, and this is the reason why they can be potential candidates in the application of spintronics and multifunctional memory devices.

3.4. Defect Chemistry and Oxygen Vacancies

The elementary part of the chemistry of defects in BiFeO₃ that guides the electrical, magnetic, and

dielectric characteristics has oxygen vacancies as the largest inherent defect that influences the functional conduct of the material. Such vacancies are normally created as a result of volatilization of Bi³⁺ ions in the course of high-temperature synthesis, charge imbalance brought by aliovalent doping, and non-stoichiometric processing conditions. Its existence in the form of oxygen vacancies causes the formation of states that are donor-like in the band gap, contributing to the electron hopping conduction and making the leakage current much larger. This not only weakens ferroelectric properties but also lowers the reliability of the devices. Thus, it is necessary to control the concentration of oxygen vacancy to optimize the BiFeO₃-based materials.

Recent studies have concentrated on the strategies with an aim of controlling oxygen vacancies by controlling synthesis and engineering defects. Reis *et al.* have shown that pyrolysis temperature and oxygen annealing conditions provide a viable way of controlling the oxygen vacancy concentration in BiFeO₃ thin films, resulting in enhanced dielectric and ferroelectric properties [63]. Equally, Ajmal *et al.* have indicated that vacancies of oxygen are important towards modulating dielectric, magnetic, and optical properties in Sm and Ti co-doped BiFeO₃ systems, especially at the morphotropic phase boundaries, multifunctional properties are optimized [64].

In addition to vacancy control, defect chemistry in perovskite multiferroics is a complicated process that requires cations, vacancies, and distortions of the lattice. Kumar and Gupta have also focused on the fact that defect-dipole interactions and sustainable defect engineering methods are required to achieve

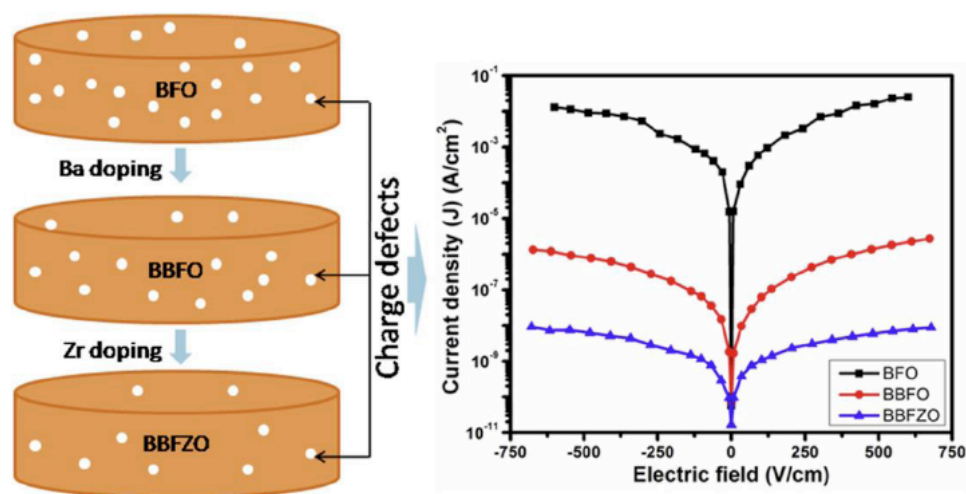


Figure 4: Schematic illustration of defect modulation in BiFeO₃ through Ba substitution (BBFO) and Ba-Zr co-substitution (BBFZO) (left), along with the corresponding leakage current density (J) as a function of applied electric field (E) (right), demonstrating significant suppression of leakage current upon co-doping due to controlled defect states and structural distortion. Reproduced from A. Sasmal, S. Sen, and P. Sujatha Devi, Materials Chemistry and Physics, vol. 254, 2020, Art. no. 123362, with permission from Elsevier. License Number: 6238141366436. [62].

Table 3: Effect of Doping and Defect Engineering on Electrical and Magnetic Properties of BiFeO₃

Strategy	Mechanism	Property Improved	Ref
Alkali metal doping	Lattice distortion & charge compensation	Polarization enhancement	[44-49]
Leakage current control	Suppression of oxygen vacancies & defects	Reduced leakage current	[56-58]
Rare-earth doping	Spin cycloid suppression & spin canting	Enhanced magnetization	[59, 61]
Oxygen vacancy control	Vacancy regulation via annealing & co-doping	Improved dielectric & ferroelectric stability	[63, 64]
Defect engineering	Defect–dipole interaction & cation tuning	Enhanced polarization & coupling	[65, 66]

customization of multifunctional characteristics in perovskite systems [65].

Also, Yoshida *et al.* showed that vacancy and cation engineering can give rise to switchable polarization in perovskite materials, which also indicated how defect chemistry can be vital in the regulation of ferroic behavior [66]. Moreover, the experience of similar perovskite systems like LaMnO₃ suggests that the universal practice of defect-mediated mechanisms in the tuning of electrical transport and magnetic properties, as mentioned in earlier research [29].

Overall, the controlled defect engineering not only minimizes the leakage current but also enhances polarization stability, magnetoelectric coupling, and functional performance of BiFeO₃ in general. It is with such a comprehensive understanding of the behavior

of oxygen vacancy and defect interactions that the rationality of the design of high-performance multiferroic materials is justified.

4. AI/ML IN MATERIALS

This has resulted in the recent faster rate of art AI and ML, which has fundamentally altered the area of materials science in that it allows the discovery and optimization of complex materials systems with regard to the data. ML-based methods are of great benefit to perovskite oxides, in particular BiFeO₃, which show multifaceted interactions between structure, defects, and multifunctional properties. Those allow one to observe the hidden associations in broad data sets and also facilitate the forecast of the material characteristics, thereby sound enough to overcome the shortcomings of the ancient conventional approaches,

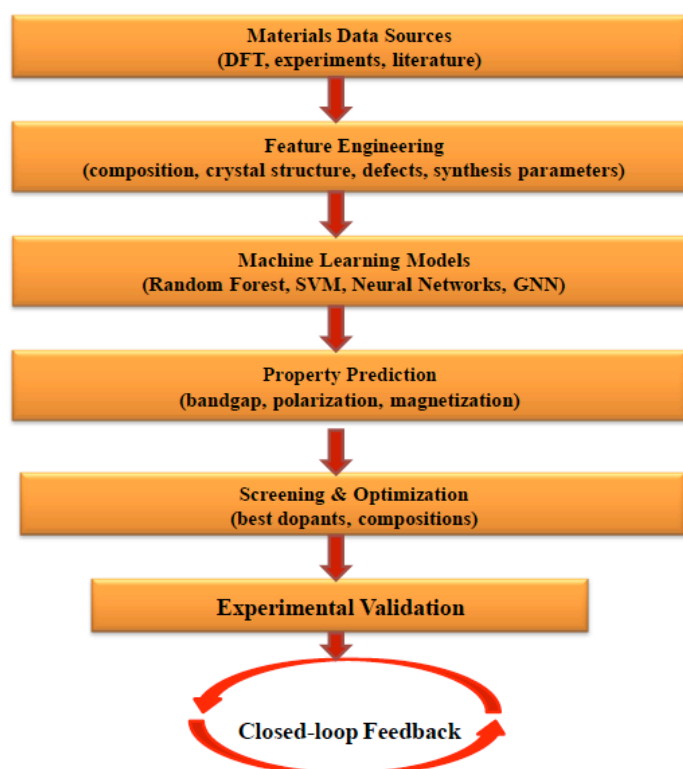


Figure 5: AI-driven workflow for accelerated discovery and optimization of BiFeO₃-based multiferroic materials, illustrating the integration of materials data sources, feature engineering, machine learning models, property prediction, screening and optimization, and experimental validation within a closed-loop framework.

where the experimental activity is performed by trial and error. Integrating ML with materials informatics has enhanced the investigation of the correlation between structure and properties and has also enabled the formation of materials with desired electrical, magnetic, and optical features rationally [67-71].

4.1. Properties Prediction Machine Learning

Machine learning has been demonstrated as a powerful predictor of significant properties of perovskite materials, in particular bandgap and polarization, relevant in electronic and energy applications. Combative data enable one to construct predictive models between compositional and structural features and electronic properties. Indicatively, ML-based models have sufficiently demonstrated the capability to predict the values of band gaps of an exceptionally large range of perovskite materials with high precision in a process that can be repeated many times using materials and reduces the cost of computing by a factor of many times [67-69]. These models adopt such descriptors as atomic radii, electronegativity, and crystal symmetry as a tool for defining strong relationships between composition and electronic structure.

Other applications of ML have also been effective in the study of ferroelectric properties, including polarization behaviors as well as the prediction of band gaps. The complex approaches that employ theoretical frameworks, such as Landau theory, have enabled engineering of ferroelectric materials with multifunctional behaviour that is optimised, such as

enhanced polarization and stability [69]. Moreover, they have used graph neural network methods to make local electric polarization predictions, wherein the intricate interactions at the atomic level in the crystal lattices are captured, making such predictions more accurate [71].

Recent reports have also shown the application of ML in the identification of perovskite substances with extremely high polarization and the potential to control the creation of the next generation of multiferroic systems [72, 73]. These developments demonstrate the critical position of ML in rapid prediction of the property and rational design of high-performance materials.

4.2. High-throughput & Autonomous Discovery

High-throughput and Autonomous Discovery: This method is mostly employed to identify variations in the target protein's subcellular localization and catalytic activity caused by crystalline inhibitors or agonists, for example, through the use of affinity tagging techniques. High-Throughput and Autonomous Discovery: The technique is typically used to detect changes in the subcellular localization and catalytic activity of the target protein in response to crystalline inhibitors or agonists, such as affinity tagging technology.

Combining machine learning with the application of high-throughput computational techniques has made it possible to explore huge compositional and structural spaces in materials science. High-throughput screening with AI capabilities can be used to simultaneously screen a large number of material

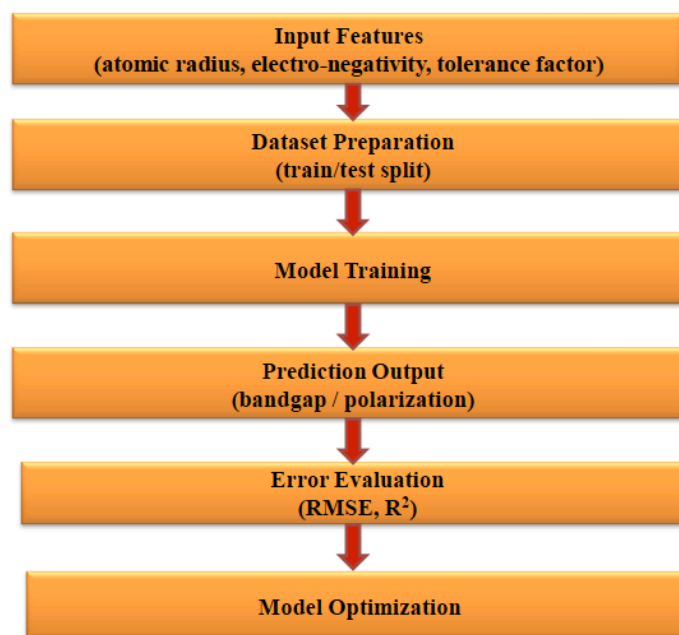


Figure 6: Machine learning framework for prediction of bandgap and polarization in perovskite materials, highlighting feature selection, model training, and performance evaluation [67-72].

Table 4: Summary of Machine Learning Approaches and Predicted Properties in Perovskite Materials

ML Method	Target Property	Material System	Key Outcome	Ref
Random Forest	Bandgap	Perovskites	Accurate bandgap prediction	[67-69]
Neural Networks	Polarization	Ferroelectrics	Enhanced polarization prediction	[70]
Graph Neural Network	Local polarization	Oxides	Atomic-scale prediction	[71]
ML Screening	High polarization	Perovskites	Discovery of new materials	[72]
AI + HT	Materials optimization	Multi-systems	Accelerated discovery	[73-76]

candidates, and thus, the time taken to discover the most suitable compositions with the desired properties is highly minimized. Recent advances in AI-induced materials discovery have shown that simulation data, experimental results, and predictive models can be combined into one framework to produce accelerated materials design and optimization [73]. Such methods are especially useful with highly nonlinear parameter space complex oxide systems, which have a large parameter space.

Along with the development of computing, self-driving labs have also revolutionized materials research as they allow experiments to be conducted autonomously. These systems combine robotics, real-time data collection, and machine learning algorithms and conduct experiments with little human intervention. This enables closed-loop systems to provide continuous feedback between prediction and experimentation, which results in fast optimization of synthesis parameters and material properties [75, 76]. In addition, high-throughput approaches have already been implemented successfully in other interconnected

directions, which suggests information on the structure-property relationships and assists in designing superior functional materials [74]. All of these methods and strategies are a paradigm shift to automated and faster materials discovery.

4.3. Multiferroics: Machine Learning

The use of machine learning on multiferroic materials has created a fresh perspective on coupled ferroic properties and optimization. The systematic search for compositional and structural variations is possible using ML-driven approaches, which results in the finding of materials with improved magnetoelectric coupling. To highlight the point, machine learning was used to study ferromagnetic-ferroelectric multiferroics, enabling the discovery of promising candidate materials by efficiently exploring substitutional effects and phase stability [77]. On the same note, ML-based experiments on rare-earth doping in oxides have shown synergistic influences on magnetism, providing more insight into the importance of compositional tuning [78].

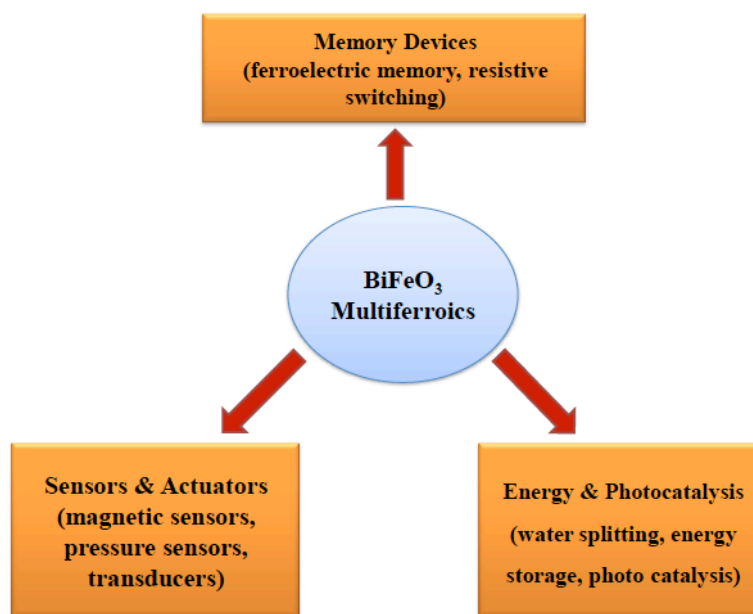


Figure 7: Schematic overview of major applications of BiFeO₃-based multiferroic materials, including memory devices, sensors, actuators, and energy-related applications [80-88].

In addition, new AI models have been trained to predict phase diagrams and stability of ferroelectric material, thus allowing the discovery of new functional materials with a specific set of properties [79]. The principle of AI has also been applied to decide the stability of phases and determine the most suitable dopants in ferroelectric systems, which continues to improve the creation of high-performance materials [80]. The developments underscore how machine learning can be transformative in the future of multiferroic research and the speed at which next-generation multifunctional materials can be created.

5. APPLICATIONS

Multiferroic materials obtained using BiFeO₃ have been of much interest in the near past as they offer a combination of both ferroelectric and magnetic characteristics, thus offering a broad spectrum of applications in high-tech electronic and energy-related equipment. These materials are very convenient to use in multiple applications since they have the capability of concurrently controlling both electric and magnetic order parameters, which are used in memory devices, sensors, actuators, and energy-related technologies. Innovations in doping and defect engineering have also been made within the past and have consequently improved the performance of BiFeO₃, rendering it a good future candidate for the application of next-generation devices.

5.1. Memory Devices

The property of BiFeO₃ makes the material highly suited for non-volatile memory applications because of its good ferroelectric and resistive switching characteristics. Combining BiFeO₃ with other perovskite systems has made the creation of advanced memristive devices, which are better in performance, possible. In the example of composite thin films, Bi₄Ti₃O₁₂-BiFeO₃ has yielded better electrical characteristics and applications in memristor applications by improving the ferroelectric characteristics and minimizing leakage current [81]. Likewise, triphasic nanocomposite architectures that are integrated with BiFeO₃ have demonstrated good magnetoelectric coupling and low-leakage properties, which make them suitable for providing reliable non-volatile memory storage [82]. Moreover, the BiFeO₃ thin films with resistive switching have been used to implement multi-bit storage, whose potential in high-density memory has been noted [83].

5.2. Sensors and Actuators

The versatility of BiFeO₃ also allows an extended variety of applications in sensor and actuator

applications, in which the interrelation between electrical and magnetic characteristics can be used to the benefit of increased functionality. Multiferroic materials are highly sensitive to external stimuli, including electric fields, magnetic fields, and mechanical stress, and therefore, they are the most suitable among other materials in sensing and adopting higher sensing technology. Recently, the application of BiFeO₃-based materials in sensors and transducers has been emphasized, showing an enhanced level of sensitivity and a high level of operational efficiency [84]. Besides, the BiFeO₃-based sensor technologies have come a long way, and they are currently used in environmental monitoring and in biomedical equipment [85]. BiFeO₃'s inherent properties enhance the process of multifunctionality and room-temperature operation of the material, and the degree of functionality is further enhanced by the inherent nature of the BiFeO₃ material, enhancing its application in actual smart sensing and actuation systems [86].

5.3. Energy and Photocatalysis

BiFeO₃ is also not an exception, as it has been presented as a promising material in any energy-related application, particularly in photocatalysis and energy storage. It has a small bandgap, and ferroelectric polarization is high, which is a good charge separator required during photocatalytic reactions. Recent studies have determined that engineered materials containing BiFeO₃ are more photocatalytic in terms of environmental remediation and energy usage [87].

Also, BiFeO₃ was investigated as a future generation photocatalyst that can help fill the gap between material design and the actual facet of the environment [88]. The introduction of nanoparticles of metal and hybridization has additionally enhanced the performance of the BiFeO₃ in the field of energy storage and photocatalytic systems, and this has underscored the fact that it is applicable in sustainable energy systems [89].

6. AI-BASED ROADMAP TO THE DESIGN OF ALKALI METAL-MODIFIED BIFEO₃ MULTIFERROICS

The introduction of AI into materials science has made it possible to make a paradigm shift from the traditional trial-and-error methods to the data-driven and predictive design method. Within the paradigm of BiFeO₃-based multi-ferroics, in which material performance is determined by the multifunctional interplay of structural, electronic, and magnetic degrees of freedom, AI-inspired algorithms can provide a systematic structure in accelerating the discovery and optimization. The most recent developments in

AI-based materials discovery have shown that it is possible to integrate computationalization, experimental data, and machine learning algorithms into cohesive data processes and identify high-performance materials with customized properties in a short amount of time [90, 91].

The development of processes of materials design based on large-scale materials databases and contemporary ML approaches is one of the key characteristics of this change. Projects like Materials Project have enabled large data sets to be generated and analyzed, and it is now easy to predict material behavior and guide it to experimentation [92]. Such frameworks enable researchers to explore compositional and structural spaces effectively, select good candidates, and decrease the amount of time and cost involved in developing materials. In addition, according to systematic reviews of data-driven design, the opportunities and challenges of applying AI in the materials design process include problems regarding data quality, interpretability of models, and scalability [93].

The last research has also shown how AI can be used in the synthesis of complex functional materials, such as catalysts and architected materials, where data-intensive techniques allow optimization of structural and functional properties concomitantly [94, 95]. Using the same approach, important parameters of the multiferroic system, including polarization, magnetization, and leakage current, can be optimized through finding the best doping solution and defect geometry. In addition to that, AI-based design has been effectively implemented on programmable and adaptive materials, which demonstrates how AI-based design can create next-generation smart materials with tunable functions [96].

A recent development in this area is the idea of closed-loop materials optimization, in which machine learning models are refined via feedback of experimental results. This method allows predictive models to be refined in real-time and thus hastens the discovery process as the predictive model becomes more and more accurate and reliable. This paradigm is also facilitated by the construction of the integrated digital infrastructures and workflow management systems that allow the smooth data exchange and cooperation between various phases of materials research [97].

In general, the AI-inspired roadmap of multiferroic materials focuses on the ability to bring together data science, computational modeling, and experimental validation into one system that will facilitate faster materials discovery. Through these strategies, the

current issues in BiFeO₃-based systems, such as leakage current, weak magnetization, and structural instability, can be mitigated, and novel materials with improved multifunctional capabilities can be developed. This paradigm causes faster evolution of advanced multiferroic materials, as well as gives a base for the next generation of intelligent and autonomous materials studies.

High-performance BiFeO₃-based multiferroics require the simultaneous control of structural, electrical, magnetic, optical, defect parameters, and processing parameters. The identity, concentration, defect chemistry, lattice distortion, phase stability, and synthesis conditions all contribute to the compositional space in which alkali-metal modification occurs, a space that is multidimensional. The traditional trial-and-error approach is thus suboptimal for investigating the wide design space of modified BiFeO₃ systems. Recent advances in AI, ML, high-throughput screening, and data-driven materials design offer a means to speed the process by correlating material descriptors with experimental properties [98, 99]. AI-driven methods are now being increasingly employed for functional and ferroelectric materials to establish structure–property relationships, speed up the candidate identification process, and enable optimization in complex processing space [98]. Furthermore, a new approach to the identification of physically significant relationships in multiferroic perovskite systems using interpretable ML and HTS has recently been shown to be successful [99].

A seven-stage roadmap is proposed to systematically design and optimize the alkali metal-modified BiFeO₃ multiferroics based on the above developments. The roadmap combines data collection, pre-processing, feature engineering, AI/ML model development, high-throughput candidate screening, experimental validation, and closed-loop iterative optimization. The framework is meant to be used in conjunction with experimental materials research, not as a replacement for it. The ultimate goal is to create a workflow that continuously improves through the integration of experimentally validated results as part of the database, and then applying these to generate predictions of the next generation of BiFeO₃ materials.

6.1. Stage I: Data Acquisition and Dataset Construction

The first stage of the proposed roadmap involves constructing a sufficiently broad and reliable dataset for alkali metal-modified BiFeO₃. The predictive capability of any AI/ML model is strongly dependent on the quality, diversity, and physical relevance of the data

supplied to it. Therefore, data should be collected from multiple complementary sources, including published experimental studies, density functional theory (DFT) calculations, established materials databases, and, where available, internally generated experimental measurements [100, 101].

For the BiFeO₃ system, the dataset should contain compositional variables such as alkali-metal identity (Li, Na, K, Rb, and Cs), dopant concentration, substitution site, and overall chemical composition. Structural information should include lattice parameters, crystal symmetry, phase purity, unit-cell volume, strain, crystallite size, and relevant bond lengths and bond angles. Electronic and magnetic descriptors obtained from DFT calculations may include band gap, formation energy, magnetic moment, magnetic ordering, and defect-related energetics. Experimental measurements should include polarization, coercive field, leakage current, dielectric constant, dielectric loss, magnetization, coercive magnetic field, and other application-specific properties.

Processing information should also be incorporated because synthesis and post-treatment conditions can significantly affect the final properties. Variables such as synthesis route, precursor conditions, calcination temperature, annealing temperature, atmosphere, film thickness, and post-treatment conditions should therefore be recorded whenever available. The integration of DFT predictions with experimental and database information can provide a broader computational foundation for materials discovery and reduce dependence on isolated experimental datasets [101]. The resulting database would serve as the primary knowledge base for subsequent preprocessing, descriptor construction, prediction, and candidate selection.

6.2. Stage II: Data Cleaning, Harmonization and Preprocessing

Raw materials data obtained from different publications and computational sources are rarely directly comparable because of variations in measurement conditions, reporting formats, units, composition notation, and experimental procedures. The second phase is then to transform the heterogeneous information into a homogeneous and machine-readable data set. In deep-learning research on perovskite materials, it is clear that only consistent and reliable data can be used to make meaningful predictions about properties [102].

The preprocessing should involve removing duplicates, identifying missing values, converting units, normalizing composition, and flagging anomalous and

physically implausible observations. If the data are categorical (like synthesis method, atmosphere, or measurement technique), then it is possible to make appropriate numerical representations.

The reported experimental uncertainties should be kept and not thrown away since uncertainty is important to model reliability. To prevent data leakage, it is important to keep training, validation, and independent test sets separated prior to model development. The result of this step should be a harmonized and quality-controlled dataset that can be used for the generation of the descriptors and for the modelling using AI/ML.

6.3. Stage III: Feature Engineering and Target Selection

To connect the chemical and structural properties of alkali metal-modified BiFeO₃ with numerical input to an AI/ML model, feature engineering is needed. Therefore, the descriptors should capture the key factors that influence the structure–property–performance relationships of the material. Recent efforts on perovskites focus on the need for crystal structure, microstructure, composition, and stability to be expressed in useful, meaningful numerical parameters that are interpretable for ML analysis [104]. Therefore, there is a growing trend towards integrating physically meaningful representations with sophisticated predictive and generative methods in materials studies, which are also leading to the use of AI for materials research and properties prediction [105].

Chemical descriptors can include ionic radius, electronegativity, atomic mass, oxidation state, valence characteristics, and dopant concentration for the alkali metal-modified BiFeO₃. The structural descriptors may be lattice parameters, unit-cell volume, symmetry or space group, Fe–O–Fe bond angle, bond lengths, tolerance factor, strain, or structural distortion. Descriptors for defects should include oxygen-vacancy concentration, Fe²⁺/Fe³⁺ ratio, Bi-site vacancies, defect concentration (where available), and defect formation energy (where available). The processing descriptors ought to contain synthesis route, calcination (annealing) temperature, processing atmosphere, film thickness, and post-treatment conditions.

The selected variables are dependent on the application. The structural targets could be phase purity, lattice distortion, and phase stability. The electrical properties that can be targeted include leakage current, dielectric constant, polarization, and coercive field. Examples of magnetic targets include those that have been saturated or permanently magnetized, are magnetically ordered, or have

indicators related to spin-cycloid suppression. Optical targets can be band gap or photocurrent. Multi-target modelling could then be employed to produce trade-offs between these properties. These descriptor-based representations can also help in interpretability of the model by connecting the properties predicted to the physically meaningful chemical, physical, and processing factors [104, 105].

6.4. Stage IV: AI/ML Model Development and Validation

The fourth step is the predictive element of the roadmap. After the dataset is cleaned, physically meaningful descriptors are generated, and then the different AI/ML algorithms are evaluated based on the size, structure, and complexity of the available dataset. Recently, the combined use of compositional, structural, and electronic descriptors with machine-learning techniques, high-throughput calculations, and experimental databases for the prediction of magnetic properties was emphasized in the context of AI-driven magnetic-material discovery [106]. More comprehensive evaluations of AI materials-by-design also illustrate the shift from traditional materials informatics to deep learning, generative methods, and increasingly automated materials design processes [107].

Initial evaluation of conventional supervised-learning models like random forest (RF), the support vector machine (SVM), gradient boosting methods, and artificial neural networks can be done for alkali metal-modified BiFeO₃. These models can be used to make baseline predictions of properties like leakage current, polarization, dielectric response, magnetization, or band gap. If such large, structurally representative datasets become available, then deep-learning approaches and graph neural networks (GNNs) can be considered as models because they can explicitly take into account the structural relations. The model selected should not simply be based on model complexity but on model predictive performance, data size, model interpretability, computational cost, and, of course, the nature of the object property to be measured [106, 107].

Model development should include: suitable training, validation, hyperparameter optimization, and independent testing. For continuous properties, regression metrics like coefficient of determination (R^2), mean absolute error (MAE), and root mean square error (RMSE) may be used, while for categorical properties, classification metrics can be used, e.g., phase stability, phase purity classes. Also, feature importance analysis or interpretable ML should be included to find out which of the chemical, structural,

defect, and/or processing variables has the most significant effect on the predicted response. Importantly, the present roadmap does not presume that any one model will be the overwhelming best. Rather, a series of models should be compared systematically and the best model chosen for each desired property.

6.5. Stage V: High-Throughput Screening and Candidate Selection

Once a model is validated, it can be used to explore a much larger design space than can be explored in the usual way by experimentation. To minimize the number of candidate materials that need to be synthesized and characterized, a strategy of high-throughput (HT) ML screening has been adopted [108, 109]. Recent research has shown how interpretable ML can be used in conjunction with high-throughput screening to specifically target the multiferroic perovskite systems and thus offer a close methodological connection to the proposed BiFeO₃ roadmap [99].

The candidate compositions in the proposed framework will be derived by systematically varying the alkali-metal species (Li, Na, K, Rb, and Cs), doping concentration, and selected processing variables. The model can then predict the structural, electrical, magnetic, and optical responses that can be expected from these candidates. The selection of candidates must be done using a set of previously determined performance criteria, not the optimum that exists for everyone. For instance, in one screening objective, it is necessary to have low leakage current, high polarization, high magnetization, and phase stability. Other limitations like chemical feasibility, synthesis availability, and thermal stability can also be used. Multi-objective screening would thus produce a ranked list of candidate compositions for experimental testing specifically a list of “best” candidates rather than a single “best” composition.

6.6. Stage VI: Experimental Validation and Characterization

The sixth stage involves AI predictions in real-world materials research. Candidates produced by AI need to be validated before their predicted properties are verified by experiments. AI search and discovery are recently recognized as a key strategy to rapidly develop materials by combining computational prediction with materials synthesis, characterization, and experimental trials [110, 111].

The selected compositions of alkali metal-modified BiFeO₃ materials require a controlled and reproducible synthesis. Structural characterization methods are: X-ray diffraction (XRD), Rietveld refinement, and microscopic analysis (scanning or transmission

electron microscopy, if applicable). Polarization–electric field (P-E) measurements, dielectric properties, leakage-current analysis, and coercive-field determination are among the measurements that should be performed to electrically characterize the material. The following magnetic measurements should be performed as part of the magnetic characterization: Magnetization–magnetic field (M–H) measurements and, if necessary, magnetic measurements as a function of temperature. Band gap characterization or photocurrent characterization may also be performed when it is a desired objective of the measurement.

The experimental values obtained should then be compared with the values from the AI. Prediction–experiment deviations should be measured and analysed instead of just identified as a failure of the model. Variations can be caused when the processing variables are not represented, when there is some uncertainty in the measurements, when there are defects, phase impurities, or when there is some limitation in the training data. These newly generated experimental observations should then be added to the database, which will then form the basis of the closed-loop optimization stage.

6.7. Stage VII: Closed-Loop Feedback and Iterative Optimization

The final step upgrades the roadmap from a one-shot prediction tool to an iterative materials-discovery system. A closed-loop workflow involves feeding the experimental results back into the dataset at the end of every validation round and updating the predictive model with the feedback. This is especially well suited to the use of Bayesian optimization and active-learning strategies, which can choose new experiments from a small (or noisy, or expensive) set of experiments, and can exploit promising regions while exploring poorly understood regions. It has been shown recently that literature-derived data, predictive modelling, constrained candidate generation, and experimental feedback can all be combined together for iterative materials discovery in a closed-loop, active-inverse learning approach [113].

For alkali metal-modified BiFeO₃, the process can therefore be represented as:

Initial dataset → preprocessing → feature engineering → AI/ML prediction → candidate screening → synthesis → characterization → prediction–experiment comparison → dataset update → model-retraining → next candidate selection.

The model can be updated to recognize that regions of the compositional and processing space will be more

likely to benefit from measured additions of additional experiments, not just ones chosen at random. Bayesian optimization is also suitable to include multiple objectives and experimental constraints, for instance when polarization, leakage current, magnetization, phase stability, and processing feasibility are to be optimized simultaneously [112]. Therefore, every experimental cycle adds new data to further enhance the predictive power and the physical insight of the BiFeO₃ system. This is an iterative approach that can lead to more efficient and maybe semi-autonomous materials optimization [112, 113].

6.8. Integrated AI-Driven Roadmap for Alkali Metal-Modified BiFeO₃

The whole roadmap consists of the combination of all seven steps into one materials design workflow. The process starts with the creation of a multimodal database that includes data from literature sources, experimental studies, computer simulations, and databases. Further on, the data is cleaned and standardized, and physical descriptors of the composition, crystal structure, defects, and processing conditions are generated. Machine Learning/AI models are built in order to define the relationships between these descriptors and desired properties (structural, electrical, magnetic, and optical).

The models are further utilized for high-throughput screening of alkali-metal-containing compositions of BiFeO₃ as well as processing conditions. Candidates are chosen among the selected ones according to certain multifunctional criteria and are synthesized and experimentally characterized. Experimental data are compared to model predictions and included in the database. The database is further used for retraining the model or making adjustments to it, which starts the new optimization loop.

Although the described roadmap is meant to offer an approach to transition from the traditional method of empirical optimization to a more systematic process of material design based on alkali metal doping of BiFeO₃ multiferroics, its use will still require adequate data availability, reproducibility of experiments, physical descriptors, modelling techniques that take into account uncertainties, and reproducibility of synthesis and characterization. Therefore, AI should be seen as a framework for decision-making and knowledge generation but not as a replacement for materials physics.

Below, Table 5 outlines the key steps in the proposed AI-driven roadmap, where the inputs, activities, outputs, and goals for each step are

Table 5: Stages, Inputs, Operations, Outputs, Objectives, and Supporting References of the Proposed AI-based Roadmap

Stage	Major Inputs	Main Operation	Expected Output	Primary Objective	Refs.
I. Data acquisition and dataset construction	Literature data, DFT calculations, materials databases, experimental measurements	Data collection, integration and organization of compositional, structural, electronic, magnetic and processing information	Initial multimodal BiFeO ₃ dataset	Establish a comprehensive knowledge base for model development	[100, 101]
II. Data cleaning, harmonization and preprocessing	Raw heterogeneous materials data	Duplicate removal, missing-value handling, unit conversion, normalization, harmonization and uncertainty management	AI-ready standardized dataset	Improve data consistency, quality and reliability	[102]
III. Feature engineering and target selection	Composition, crystal structure, defects and processing conditions	Generation and selection of chemical, structural, defect and processing descriptors; definition of target properties	Physically meaningful feature matrix and target variables	Establish quantitative structure–property relationships	[104,105]
IV. AI/ML model development and validation	Feature matrix and target properties	Model training, validation, hyperparameter optimization, performance evaluation and interpretability analysis using RF, SVM, ANN/DNN and GNN approaches	Validated predictive models	Predict structural, electrical, magnetic and optical properties	[106, 107]
V. High-throughput screening and candidate selection	Candidate alkali-metal compositions, dopant concentrations and processing conditions	ML-based prediction, high-throughput screening and multi-objective candidate prioritization	Ranked/prioritized candidate materials	Reduce the experimental search space and identify promising candidates	[99, 108, 109]
VI. Experimental validation and characterization	AI-prioritized candidate materials	Synthesis followed by XRD, microscopic, electrical, magnetic and optical characterization	Experimentally validated property dataset	Verify predictions and identify prediction–experiment deviations	[110, 111]
VII. Closed-loop feedback and iterative optimization	AI predictions, experimental results and updated dataset	Active learning, Bayesian optimization, model updating and iterative candidate selection	Updated dataset, refined model and next-generation candidates	Continuously improve prediction and material performance through feedback	[112, 113]

presented. This roadmap starts with the assimilation of the literature, computational, database, and experimental data and continues with the data preprocessing step, followed by the feature engineering phase and the development of the AI/ML models. Further on, the shortlisted formulas and processing conditions go through experimental testing, and the acquired results are added to the dataset for retraining and updating of the models. Hence, this table offers a step-by-step overview of the roadmap that is proposed to develop optimized alkali metal-doped BiFeO₃ multiferroics.

7. FUTURE PERSPECTIVES

Further work on the investigation of BiFeO₃-based multiferroics in the future must aim at the defect chemistry and atomic-scale control of doping so that functional properties can be improved further. It is predicted that the combination of artificial intelligence

and high-throughput screening, data-driven workflow, and autonomous experimentation will greatly expedite the process of discovering optimized materials with enhanced performance [90–93]. Also, recent developments in materials design with AI assistance and programmable functional systems demonstrate the prospect of creating next-generation smart and adaptive materials [94–96]. The development of combined digital infrastructure and closed-loop optimization systems will also help to facilitate effective materials development and integration of devices, creating a viable usage [97].

8. CONCLUSION

It is important to note that there has been a major advancement in BiFeO₃-based multiferroic materials in this review, with doping and defect engineering playing a significant role in addressing major limitations of the materials, including high leakage current and poor magnetization. Modulation of oxygen vacancy and

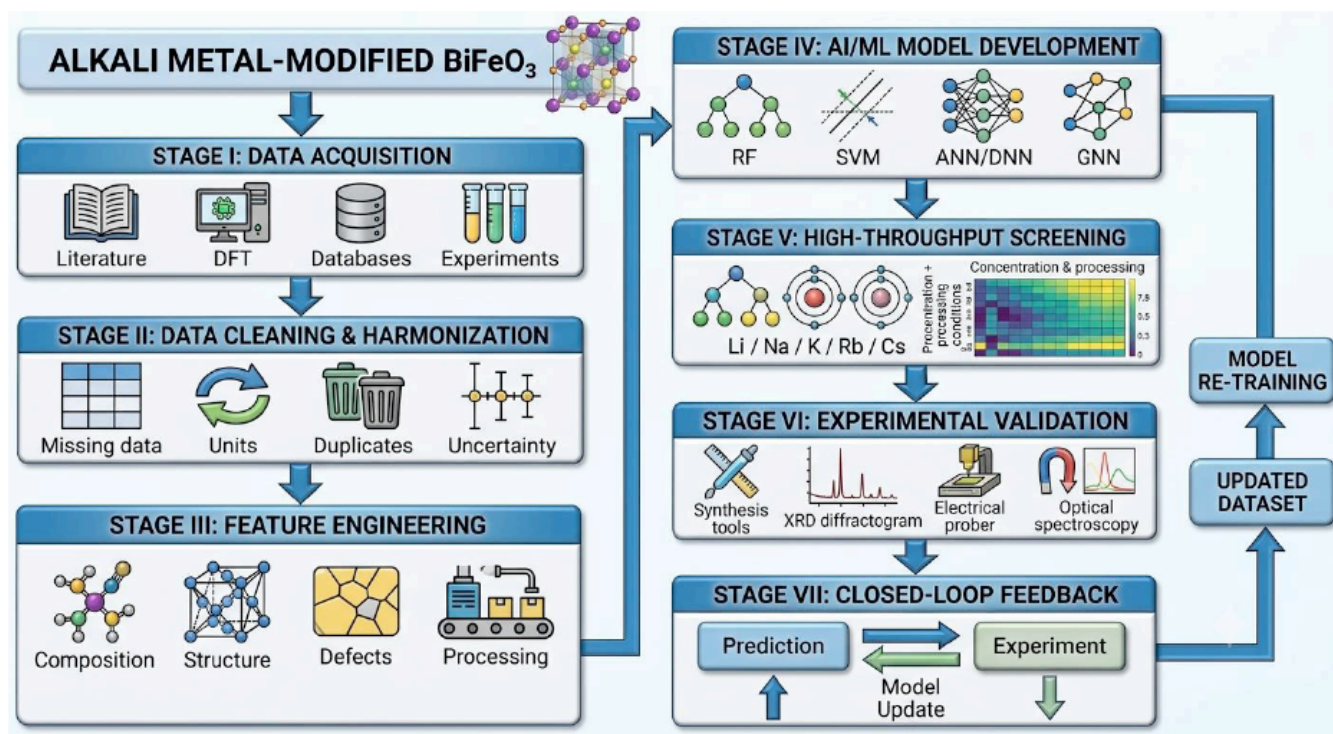


Figure 8: AI-powered roadmap towards the design and optimization of BiFeO₃ multiferroics modified with alkali metals. The roadmap includes seven interconnected steps starting from the collection of experimental, computational, database, and literature data, proceeding through data cleansing and integration, feature engineering, development of AI/ML models, and high-throughput screening of alkali-metal compositions and processes. Afterward, the AI/ML-prioritized compositions are experimentally synthesized and characterized structurally, electrically, magnetically, and optically. The experimental data are then included in an updated dataset to retrain the model, creating a closed-loop cycle for materials optimization.

controlled substitution are useful in improving electrical and magnetic performance. The combination of machine learning and artificial intelligence also hastens the process of materials discovery by allowing the rapid prediction and optimization of important properties. Also, BiFeO₃ has a promising technology through the variety of its applications in memory devices, sensors, and energy systems. In general, a joint effort of defect engineering and AI solutions is a promising direction towards creating high-performance multifunctional materials.

DATA AVAILABILITY

The data supporting the findings of this study are available within the article. Additional data related to this work can be obtained from the corresponding author upon reasonable request.

CONFLICT OF INTEREST

The authors declare that they have no conflict of interest.

FUNDING

The authors did not receive any specific funding for this work.

ACKNOWLEDGMENTS

The authors acknowledge the Siksha 'O' Anusandhan Deemed to be University, Bhubaneswar, for providing academic support and research facilities.

AUTHOR CONTRIBUTIONS

Om Prakash Hota: Conceptualization, literature review, writing - original draft, visualization. Sudhansu Sekhar Hota: Supervision, validation, reviewing and editing.

REFERENCES

- [1] W. Sun, *et al.*, "A unified symmetry framework for spin-ferroelectric coupling in altermagnetic multiferroics," *Nature Communications*, 2026. <https://doi.org/10.1038/s41467-026-69635-2>
- [2] X. Jiang, *et al.*, "Non-Volatile Electric-Field Control of Ferro- and Antiferroelectric States in Multiferroic Oxides," *Advanced Functional Materials*, 2026: e29056. <https://doi.org/10.1002/adfm.202529056>
- [3] M. Kumar and S. Dabas, "Multiferroic and Magnetoelectric Materials: Fundamentals and Properties," *Multiferroic and Magnetoelectric Materials: Applications and Emerging Green Technologies*. Singapore: Springer Nature Singapore, 2026, pp. 1-30. https://doi.org/10.1007/978-981-95-4391-5_1
- [4] S. Sharma, *et al.*, "Phase transition driven enhancements of multiferroic properties in doped BiFeO₃: a comprehensive review," *Materials Science in Semiconductor Processing*, vol. 195, 2025, p. 109613. <https://doi.org/10.1016/j.mssp.2025.109613>

- [5] A. Jain, *et al.*, "BiFeO₃-based lead-free materials: Recent breakthroughs and their multifunctional applications," *Journal of Alloys and Compounds*, vol. 1010, 2025, p. 177170. <https://doi.org/10.1016/j.jallcom.2024.177170>
- [6] D. Lu, *et al.*, "Strategic material engineering of BiFeO₃-based piezo-photocatalysts for environmental and energy applications," *Journal of Alloys and Compounds*, 2025, p. 185828. <https://doi.org/10.1016/j.jallcom.2025.185828>
- [7] S. Dutta, *et al.*, "Computational and experimental approach to La₃₊ doping at the B-site of BiFeO₃: Insights into BiFeO₃ 90La0.10O₃ multiferroic," *Chemical Engineering Journal Advances*, vol. 22, 2025, p. 100742. <https://doi.org/10.1016/j.ceja.2025.100742>
- [8] X. Wang, *et al.*, "Phase Transition Regulation and Concurrent Ferroelectric and Magnetic Improvement in BiFeO₃ via Rare-Earth Multi-substitution Strategy," *Ceramics International*, 2026. <https://doi.org/10.1016/j.ceramint.2026.03.315>
- [9] M. O. Moysa, *et al.*, "Dielectric relaxation, crystal structure and magnetic phenomena in solid solutions based on alkali metal niobates and bismuth ferrite in a wide range of external influences," *Ceramics International*, vol. 51, no. 4, 2025, pp. 5208-5216. <https://doi.org/10.1016/j.ceramint.2024.11.494>
- [10] B. Agrawal, *et al.*, "Structure-controlled electronic structure and electrochemical energy storage mechanisms in Bi-rich BiFeO₃-based asymmetric supercapacitor devices," *Journal of Energy Storage*, vol. 147, 2026, p. 120230. <https://doi.org/10.1016/j.est.2025.120230>
- [11] M. Cheng, C. L. Fu, R. Okabe, A. Chottrattanapituk, A. Boonkird, N. T. Hung, and M. Li, "Artificial intelligence-driven approaches for materials design and discovery," *Nature Materials*, 2026, pp. 1-17. <https://doi.org/10.1038/s41563-025-02403-7>
- [12] T. Lookman, Y. Liu, and Z. Gao, "Materials informatics: Emergence to autonomous discovery in the age of ai," *Advanced Materials*, 2026, p. e15941. <https://doi.org/10.1002/adma.202515941>
- [13] X. Bai, and X. Zhang, "Artificial intelligence-powered materials science," *Nano-micro letters*, vol. 17, no. 1, 2025, p. 135. <https://doi.org/10.1007/s40820-024-01634-8>
- [14] L. Goswami, M. K. Deka, and M. Roy, "Artificial intelligence in material engineering: A review on applications of artificial intelligence in material engineering," *Advanced Engineering Materials*, vol. 25, no. 13, 2023, p. 2300104. <https://doi.org/10.1002/adem.202300104>
- [15] Y. Liu, *et al.*, "Generative artificial intelligence and its applications in materials science: Current situation and future perspectives," *Journal of Materials*, vol. 9, no. 4, 2023, pp. 798-816. <https://doi.org/10.1016/j.jmat.2023.05.001>
- [16] W. Hu, *et al.*, "Accelerated discovery of supertetragonal perovskites with giant polarization via machine learning," *npj Computational Materials*, 2026. <https://doi.org/10.1038/s41524-026-01970-w>
- [17] X. Huang, *et al.*, "Machine learning-accelerated exploration of ferromagnetic-ferroelectric multiferroics in element substituted 2D transition metal dichalcogenides," *Physical Review Materials*, vol. 9, no. 12, 2025, p. 124417. <https://doi.org/10.1103/r417-h8nc>
- [18] T. Wang, *et al.*, "PU-learning-guided discovery of synthesizable multiferroic nitride perovskites with altermagnetic order," *npj Computational Materials*, 2025. <https://doi.org/10.1038/s41524-025-01876-z>
- [19] M. A. M. Teixeira, *et al.*, "Pathways to obtain high-entropy BiFeO₃-based thin films modified by rare earth cations," *Ceramics International*, 2026. <https://doi.org/10.1016/j.ceramint.2026.01.401>
- [20] D. K. Palchav, *et al.*, "Phase evolution, defect chemistry and functional properties of Sm-doped BiFeO₃ synthesized by solution combustion," *Ceramics International*, 2026. <https://doi.org/10.1016/j.ceramint.2026.03.218>
- [21] A. Varshney, *et al.*, "BiFeO₃ Nanoparticles Doped with Ca-Ho and Having Tunable Magnetism and Band Gap Modulation for Photocatalysis," *ACS Applied Nano Materials*, 2026.
- [22] I. V. Lisnevskaya, *et al.*, "Multiferroic solid solutions BiFe_{1-kh}(Ni, M) xO₃ (M= Ti, Nb, W): phase and structural analysis, comparison of dielectric and magnetic properties," *Ceramics International*, 2026. <https://doi.org/10.1016/j.ceramint.2026.01.273>
- [23] N. Ma, *et al.*, "Recent Progress in BiFeO₃-Based Sensor Technologies: Fundamentals, Performance Metrics, and Diverse Applications," *Advanced Materials*, 2026: e20682.
- [24] N. Jahangeer, P. Mitra, and B. H. Venkataraman, "Tailoring Dielectric and Multiferroic Properties in BiFeO₃-SrTiO₃ Solid Solution Synthesised via Molten Salt Route for Capacitor-Based Storage Applications," *IET Nanodielectrics*, vol. 9, no. 1, 2026: e70025. <https://doi.org/10.1049/nde2.70025>
- [25] A. Tariq, *et al.*, "Large-area engineering of ferroelectric charged domain walls in (110)-oriented BiFeO₃ thin films," *Scripta Materialia*, vol. 276, 2026: 117196. <https://doi.org/10.1016/j.scriptamat.2026.117196>
- [26] J. Mejia, C. Canaria, R. Burgos, C. Ortiz, G. Supelano, and C. Vargas, "Structural study of yttrium substituted BiFeO₃," *Journal of Physics: Conference Series*, vol. 687, 2016: 012091. <https://doi.org/10.1088/1742-6596/687/1/012091>
- [27] R. L. Palomino-Resendiz, *et al.*, "Analysis of the effect of cationic ratio Bi³⁺/Fe³⁺ on the magnetic and multiferroic properties of BiFeO₃ nanoparticles synthesized using a sonochemical-assisted method," *Ceramics International*, vol. 48, no. 10, 2022, pp. 14746-14753. <https://doi.org/10.1016/j.ceramint.2022.02.011>
- [28] Hu, Wenguang, *et al.* "Accelerated discovery of ferroelectric perovskites with giant polarization via machine learning." (2025). <https://doi.org/10.21203/rs.3.rs-5623186/v1>
- [29] O. P. Hota, P. Mohanty, and R. Mahapatra, "Future Research Direction on Rare-Earth and Alkaline-Earth Metal-Doped LaMnO₃ Perovskites," *Brazilian Journal of Physics*, vol. 55, no. 6, 2025: 272. <https://doi.org/10.1007/s13538-025-01898-4>
- [30] J.-Y. Wu, *et al.*, "Enhancement of Photocatalytic Activity in BiFeO₃ Nanoparticles through Electrical Polarization," *Advanced Energy and Sustainability Research*, vol. 6, no. 7, 2025: 2400285. <https://doi.org/10.1002/aesr.202400285>
- [31] Z. Yang, *et al.*, "Ferroelectric Bi₂Fe₄O₉ for efficient peroxydisulfate activation: The overlooked role of spontaneous polarization," *Separation and Purification Technology*, vol. 374, 2025: 133787. <https://doi.org/10.1016/j.seppur.2025.133787>
- [32] S. Husain, and R. Ramesh, "Magnon transport in multiferroic antiferromagnet," *npj Spintronics*, vol. 3, no. 1, 2025: 36. <https://doi.org/10.1038/s44306-025-00099-8>
- [33] C. A. Crawford, *et al.*, "Evolution of Magnetic Symmetry through the BiFeO₃-Ca₂Fe₄/3W₂/3O₆ Phase Diagram," *Inorganic Chemistry*, vol. 64, no. 30, 2025, pp. 15413-15423.
- [34] S. R. Burns, O. Paull, J. Juraszek, N. Valanoor, and D. Sando, "The Experimentalist's Guide to the Cycloid, or Noncollinear Antiferromagnetism in Epitaxial BiFeO₃," *Advanced Materials*, 2020. <https://doi.org/10.1002/adma.202003711>
- [35] K. Komadera, *et al.*, "Structure, magnetic properties, and cycloidal spin ordering in Nd-doped BiFeO₃ synthesized by sol-gel method," *Ceramics International*, vol. 51, no. 6, 2025, pp. 7208-7216. <https://doi.org/10.1016/j.ceramint.2024.12.155>
- [36] V. Venkidu, *et al.*, "Structural, electronic, and magnetic correlations governing multiferroic and magnetoelectric response in charge-compensated La-Nd co-substituted BiFeO₃ with DFT insights," *Ceramics International*, 2026.
- [37] S. Long, *et al.*, "Enhanced ferroelectric and magnetoelectric properties of BiFeO₃-based ceramics modified by SrTiO₃," *Ceramics International*, vol. 51, no. 18, 2025, pp.

- 26702-26710.
<https://doi.org/10.1016/j.ceramint.2025.03.352>
- [38] G. Wang, *et al.*, "Electric field switching of altermagnetic spin-splitting in multiferroic skyrmions." arXiv preprint arXiv: 2601.06738, 2026.
- [39] Q. Gao, *et al.*, "Leakage current and ferroelectric behavior of non-stoichiometric BiFeO₃ thin films prepared at different atmospheres." Journal of Alloys and Compounds, vol. 1017, 2025: 178982.
<https://doi.org/10.1016/j.jallcom.2025.178982>
- [40] T. Yang, *et al.*, "Design of oxygen vacancy in BiFeO₃-based films for higher photovoltaic performance." Applied Surface Science, vol. 575, 2022: 151713.
<https://doi.org/10.1016/j.apsusc.2021.151713>
- [41] S. S. Das, G. Egawa, and S. Yoshimura, "Pulsed DC Reactive Sputtering Using a Conducting Target: A Strong Method to Produce High-Quality BiFeO₃-based Multiferroic Thin Films." Chemical Physics Impact, 2026: 101004.
<https://doi.org/10.1016/j.chphi.2026.101004>
- [42] S. Panda, and S. K. Parida, "Influence of lower Gd concentration and temperature in BiFeO₃: microstructure, electrical, and infrared properties for device application." Journal of Materials Science: Materials in Electronics, vol. 37, no. 1, 2026: 44.
<https://doi.org/10.1007/s10854-025-16380-9>
- [43] Lili Song, *et al.*, "Rational Construction and Modulation of Built-In Electric Field for High-Efficiency Alkali Metal-Based Batteries." Angewandte Chemie, 2026: e6795880.
<https://doi.org/10.1002/ange.6795880>
- [44] Yi Li, *et al.*, "Unlocking the intrinsic mechanisms of A-site K/Na doped perovskite fluorides pseudocapacitive cathode materials for enhanced aqueous zinc-based batteries." Energy Storage Materials, vol. 57, 2023, pp. 334-345.
<https://doi.org/10.1016/j.ensm.2023.02.020>
- [45] Xian Pan, Gurong Lin, and Kaiping Peng, "Preparation and characterization of Ta and monovalent alkali metals (Li, Na, K) co-doping on Sr11Mo4O23 electrolyte for solid oxide fuel cells." Journal of Alloys and Compounds, vol. 938, 2023, p. 168482.
<https://doi.org/10.1016/j.jallcom.2022.168482>
- [46] Lu Liu, *et al.*, "Structural evolution and improved magnetoelectric coupling effect in BiFeO₃ ceramics based on the multi-element co-substitution." Journal of Magnetism and Magnetic Materials, 2026: 173944.
<https://doi.org/10.1016/j.jmmm.2026.173944>
- [47] Mingqiang Zhong, *et al.*, "Photocurrent Densities and Bandgap Engineering in A/B-site Co-substituted Bi0.5Na0.5TiO₃ Ferroelectric Semiconductors." Journal of Alloys and Compounds, 2026: 186311.
<https://doi.org/10.1016/j.jallcom.2026.186311>
- [48] Janmejaya Mishra and Bibekananda Sundaray, "Influence of copper doping on structural, magnetic, and ferroelectric properties of bismuth ferrite nanofibers." physica status solidi (b), vol. 263, no. 1, 2026: e202500267.
<https://doi.org/10.1002/pssb.202500267>
- [49] Anurak Prasatkhetragarn, *et al.*, "Investigation on ferromagnetic and ferroelectric properties of (La, K)-doped BiFeO₃-BaTiO₃ solid solution." Ceramics International, vol. 39, 2013, pp. S249-S252.
<https://doi.org/10.1016/j.ceramint.2012.10.071>
- [50] Srihari N. Venugopalrao, Jyothilakshmi Rudresh, and Kodihalli K. Nagaraja, "Panoptic overview of morphotropic phase boundary in improving ferroelectric properties of Gd doped bismuth ferrite." Journal of Physics and Chemistry of Solids, 2025: 113228.
<https://doi.org/10.1016/j.jpcs.2025.113228>
- [51] Sandeep Kumar Singh Patel, *et al.*, "Structural and magnetic properties of Dy³⁺-doped BaTiO₃ nanorods: A study of the tetragonal-to-cubic phase transition and emergent diluted magnetism." Journal of Magnetism and Magnetic Materials, 2025: 173658.
<https://doi.org/10.1016/j.jmmm.2025.173658>
- [52] Ubaid Ur Rehman, *et al.*, "Enhanced Ferroelectric and Piezoelectric Properties of BiFeO₃-SrTiO₃ Ceramics through Subtle Al³⁺ Doping." Ceramics International, 2025.
<https://doi.org/10.1016/j.ceramint.2025.10.271>
- [53] K. Krishna Rao, *et al.*, "Effect of La substitution on the structural, optical, ferroelectric, and electrical properties of BiFeO₃." Journal of the Korean Ceramic Society, vol. 62, no. 4, 2025, pp. 810-823.
<https://doi.org/10.1007/s43207-025-00513-1>
- [54] Jiejun Zhu, *et al.*, "Efficient Piezocatalysis of BiFeO₃ Achieved via Defect Introduction through Doping." Journal of Alloys and Compounds, 2026: 187044.
<https://doi.org/10.1016/j.jallcom.2026.187044>
- [55] F. F. Orudzhev, N. M.-R. Alikhanov, S. M. Ramazanov, D. S. Sobola, R. K. Murtazali, E. H. Ismailov, R. D. Gasimov, A. S. Aliev, and Ş. Tâlu, "Morphotropic Phase Boundary Enhanced Photocatalysis in Sm Doped BiFeO₃." Molecules, vol. 27, 2022, p. 7029.
<https://doi.org/10.3390/molecules27207029>
- [56] J. Liu, X. Yan, and Z. Yang, "Improved temperature stability in bismuth ferrite-based lead-free piezoceramics by leakage current suppression." Ceramics International, 2026.
<https://doi.org/10.1016/j.ceramint.2026.02.234>
- [57] Q. Gao *et al.*, "Leakage current and ferroelectric behavior of non-stoichiometric BiFeO₃ thin films prepared at different atmospheres." Journal of Alloys and Compounds, vol. 1017, p. 178982, 2025.
<https://doi.org/10.1016/j.jallcom.2025.178982>
- [58] Y. Ahn and J. Y. Son, "High-efficiency energy storage in Cr-modified BiFeO₃ thin films with suppressed leakage current and improved ferroelectricity." Journal of the Korean Ceramic Society, vol. 62, no. 5, pp. 1057-1067, 2025.
<https://doi.org/10.1007/s43207-025-00533-x>
- [59] D. A. Salamatin *et al.*, "Enhanced magnetic properties, phonon and microstructure effects by Tb in the high-pressure synthesized BiFeO₃-based ceramics." Journal of Materials Science: Materials in Electronics, vol. 36, no. 12, p. 752, 2025.
<https://doi.org/10.1007/s10854-025-14744-9>
- [60] Kostishyn, V. G., *et al.* "Effect of corona treatment on magnetic properties of nanoscaled multiferroic films BiFeO₃, (BiLa) FeO₃ and (BiNd) FeO₃." Solid State Phenomena 233: 388-391, 2015.
<https://doi.org/10.4028/www.scientific.net/SSP.233-234.388>
- [61] D. K. Palchaev *et al.*, "Phase evolution, defect chemistry and functional properties of Sm-doped BiFeO₃ synthesized by solution combustion." Ceramics International, 2026.
<https://doi.org/10.1016/j.ceramint.2026.03.218>
- [62] A. Sasmal, S. Sen, and P. Sujatha Devi, "Significantly suppressed leakage current and reduced band gap of BiFeO₃ through Ba-Zr co-substitution: Structural, optical, electrical and magnetic study." Materials Chemistry and Physics, vol. 254, p. 123362, 2020.
<https://doi.org/10.1016/j.matchemphys.2020.123362>
- [63] Reis, Saulo P., *et al.* "Controlling Oxygen Vacancies in BiFeO₃ Thin Films via Pyrolysis Temperature and O₂ Annealing." Nanomaterials 16.7 (2026): 395.
<https://doi.org/10.3390/nano16070395>
- [64] S. Ajmal *et al.*, "Effect of oxygen vacancies on dielectric, magnetic and optical properties of Sm and Ti co-doped bismuth ferrite ceramics with morphotropic phase boundary." Ceramics International, 2025.
<https://doi.org/10.1016/j.ceramint.2025.10.145>
- [65] M. Kumar and K. Gupta, "Concluding remarks, future outlook, and emerging ideas on the sustainable perovskite multiferroic materials," in Sustainable Perovskite Multiferroic Materials: A Plethora of Applications. Singapore: Springer, 2025, pp. 305-313.
https://doi.org/10.1007/978-981-96-7419-0_12
- [66] S. Yoshida *et al.*, "Switchable polarization in an A-site deficient perovskite through vacancy and cation engineering." Journal of the American Chemical Society, vol. 148, no. 4, pp. 4557-4567, 2026.
<https://doi.org/10.1021/jacs.5c19790>
- [67] S. Wang *et al.*, "From formability to bandgap: machine learning accelerates the discovery and application of

- perovskite materials," *ACS Nano*, vol. 19, no. 32, pp. 29049-29072, 2025.
<https://doi.org/10.1021/acsnano.5c07494>
- [68] F. Gou *et al.*, "Machine learning-assisted prediction and control of bandgap for organic-inorganic metal halide perovskites," *ACS Applied Materials & Interfaces*, vol. 17, no. 12, pp. 18383-18393, 2025.
<https://doi.org/10.1021/acsami.5c00218>
- [69] A. Sabagh Moeini, F. S. Tehrani, and A. Naeimi-Sadigh, "Machine learning-driven band gap prediction/classification and feature importance analysis of inorganic perovskites," *International Journal of Energy Research*, 2025, Art. no. 9974355.
<https://doi.org/10.1155/er/9974355>
- [70] R. Yuan *et al.*, "Machine learning-enabled design of ferroelectrics with multiple properties via a Landau model," *Acta Materialia*, vol. 286, p. 120760, 2025.
<https://doi.org/10.1016/j.actamat.2025.120760>
- [71] Y. Ma *et al.*, "Prediction of local electric polarization using graph neural networks," *Physical Review B*, vol. 111, no. 18, p. 184105, 2025.
<https://doi.org/10.1103/PhysRevB.111.184105>
- [72] Li, Menglu, *et al.* "Supertetragonal BaZrS₃: A promising perovskite sulphide with giant ferroelectricity and low band gap." *Science China Physics, Mechanics & Astronomy* 67.8 (2024): 287011.
<https://doi.org/10.1007/s11433-024-2394-1>
- [73] B. Madika *et al.*, "Artificial intelligence for materials discovery, development, and optimization," *ACS Nano*, vol. 19, no. 30, pp. 27116-27158, 2025.
<https://doi.org/10.1021/acsnano.5c04200>
- [74] K. Song *et al.*, "New directions for thermoelectrics: A roadmap from high-throughput materials discovery to advanced device manufacturing," *Small Science*, vol. 5, no. 3, p. 2300359, 2025.
<https://doi.org/10.1002/smssc.202300359>
- [75] A. K. Y. Low *et al.*, "Self-driving laboratories: translating materials science from laboratory to factory," *ACS Omega*, vol. 10, no. 28, pp. 29902-29908, 2025.
<https://doi.org/10.1021/acsomega.5c02197>
- [76] R. B. Canty *et al.*, "Science acceleration and accessibility with self-driving labs," *Nature Communications*, vol. 16, no. 1, p. 3856, 2025.
<https://doi.org/10.1038/s41467-025-59231-1>
- [77] X. Huang *et al.*, "Machine learning-accelerated exploration of ferromagnetic-ferroelectric multiferroics in element substituted 2D transition metal dichalcogenides," *Physical Review Materials*, vol. 9, no. 12, p. 124417, 2025.
<https://doi.org/10.1103/PhysRevMaterials.9.124417>
- [78] G. Xu *et al.*, "Synergistic effects of rare-earth doping on the magnetic properties of orthochromates: a machine learning approach," *AAPPS Bulletin*, vol. 35, no. 1, p. 30, 2025.
<https://doi.org/10.1007/s43673-025-00175-5>
- [79] C. Zhang and X. Chen, "FerroAI: a deep learning model for predicting phase diagrams of ferroelectric materials," *npj Computational Materials*, vol. 11, no. 1, p. 282, 2025.
<https://doi.org/10.1038/s41524-025-01778-0>
- [80] S. Yan *et al.*, "Artificial intelligence-driven phase stability evaluation and new dopants identification of hafnium oxide-based ferroelectric materials," *npj Computational Materials*, vol. 11, no. 1, p. 2, 2025.
<https://doi.org/10.1038/s41524-024-01510-4>
- [81] P. Mitra *et al.*, "Physical properties of multiferroic (1-x) Bi₄Ti₃O₁₂-x BiFeO₃ composite thin film fabricated by pulsed laser deposition technique for memristor devices: A comparative study," *Journal of Magnetism and Magnetic Materials*, vol. 629, p. 173303, 2025.
<https://doi.org/10.1016/j.jmmm.2025.173303>
- [82] I. Sagheer *et al.*, "Triphasic BiFeO₃-BaTiO₃-CoFe₂O₄ nanocomposite architectures elucidating efficient magnetoelectric coupling and low-leakage non-volatile memory storage," *Materials Science in Semiconductor Processing*, vol. 206, p. 110383, 2026.
<https://doi.org/10.1016/j.mssp.2025.110383>
- [83] S.-H. Chen *et al.*, "Resistive switching behavior of perovskite BiFeO₃ thin films and their two-bit-per-cell applications," *Journal of Materials Science: Materials in Electronics*, vol. 36, no. 8, p. 478, 2025.
<https://doi.org/10.1007/s10854-025-14436-4>
- [84] S. D. Nair *et al.*, "Perovskite multiferroic materials for sensors and transducers applications," in *Sustainable Perovskite Multiferroic Materials: A Plethora of Applications*. Singapore: Springer, 2025, pp. 227-252.
https://doi.org/10.1007/978-981-96-7419-0_9
- [85] N. Ma *et al.*, "Recent progress in BiFeO₃-based sensor technologies: Fundamentals, performance metrics, and diverse applications," *Advanced Materials*, 2026, Art. no. e20682.
- [86] A. Varshney *et al.*, "Room-temperature perovskite multiferroic material bismuth ferrite (BiFeO₃): A highly investigated material among various perovskite multiferroic materials," in *Sustainable Perovskite Multiferroic Materials: A Plethora of Applications*. Singapore: Springer, 2025, pp. 85-125.
https://doi.org/10.1007/978-981-96-7419-0_4
- [87] D. Lu *et al.*, "Strategic material engineering of BiFeO₃-based piezo-photocatalysts for environmental and energy applications," *Journal of Alloys and Compounds*, 2025, Art. no. 185828.
<https://doi.org/10.1016/j.jallcom.2025.185828>
- [88] D. Jalandhara *et al.*, "BiFeO₃ as a next-generation photocatalyst: Bridging material design with environmental remediation," *ChemPhysChem*, vol. 26, no. 10, p. e202401092, 2025.
<https://doi.org/10.1002/cphc.202401092>
- [89] A. ur R. Khan *et al.*, "Eco-friendly fabrication of metal@BiFeO₃ for synergistic energy storage and photocatalytic applications," *Journal of Sol-Gel Science and Technology*, vol. 116, no. 2, pp. 1730-1747, 2025.
<https://doi.org/10.1007/s10971-025-06967-3>
- [90] B. Madika *et al.*, "Artificial intelligence for materials discovery, development, and optimization," *ACS Nano*, vol. 19, no. 30, pp. 27116-27158, 2025.
<https://doi.org/10.1021/acsnano.5c04200>
- [91] H. Xin *et al.*, "Roadmap for transforming heterogeneous catalysis with artificial intelligence," *Nature Catalysis*, 2026.
<https://doi.org/10.1038/s41929-026-01479-x>
- [92] M. K. Horton *et al.*, "Accelerated data-driven materials science with the Materials Project," *Nature Materials*, vol. 24, no. 10, pp. 1522-1532, 2025.
<https://doi.org/10.1038/s41563-025-02272-0>
- [93] J. C. Quinones-Gomez, E. Mor, and J. Chacon, "Data-driven design in the design process: A systematic literature review on challenges and opportunities," *International Journal of Human-Computer Interaction*, vol. 41, no. 4, pp. 2227-2252, 2025.
<https://doi.org/10.1080/10447318.2024.2318060>
- [94] X. Chen *et al.*, "Recent advances in data-driven design of dual-atom catalysts," *Advanced Functional Materials*, vol. 36, no. 2, p. e10647, 2026.
<https://doi.org/10.1002/adfm.202510647>
- [95] J. Yeo *et al.*, "Hybrid TPMS-based architected materials for enhanced specific stiffness using data-driven design," *Materials & Design*, vol. 249, p. 113523, 2025.
<https://doi.org/10.1016/j.matdes.2024.113523>
- [96] A. C. Karacakol *et al.*, "Data-driven design of shape-programmable magnetic soft materials," *Nature Communications*, vol. 16, no. 1, p. 2946, 2025.
<https://doi.org/10.1038/s41467-025-58091-z>
- [97] S. Bekemeier *et al.*, "Advancing digital transformation in material science: The role of workflows within the materialdigital initiative," *Advanced Engineering Materials*, vol. 27, no. 8, p. 2402149, 2025.
<https://doi.org/10.1002/adem.202402149>
- [98] Ali, Faizan, *et al.* "Artificial Intelligence for Fluorite Ferroelectric Materials: From Discovery to Optimization." *Advanced Electronic Materials* (2026): e70492.
<https://doi.org/10.1002/aelm.70492>

- [99] Wang, Yuezhu, *et al.* "Interpretable ML-Driven High-Throughput Screening Reveals Orbital-Site-Spin Synergy for Cross-Field-Enhanced Multiferroic Perovskite Photocatalyst Design." *ACS Catalysis* 16.17 (2026): 16994-17010.
<https://doi.org/10.1021/acscatal.6c03756>
- [100] GP, Jeslin Jebish. "Integration of density functional theory and machine learning for materials discovery in energy applications." *Discover Chemistry* 3.1 (2026): 531.
<https://doi.org/10.1007/s44371-026-00985-y>
- [101] Patel, Rutu, Mayankumar L. Chaudhary, and Ram K. Gupta. "Data-driven and computational insights into borophene: integrating machine learning with DFT and AI." *Coordination Chemistry Reviews* 550 (2026): 217385.
<https://doi.org/10.1016/j.ccr.2025.217385>
- [102] Wang, Beibei, and Juan Wang. "Formation Energy Prediction and Feature Analysis of Lead-Free Double Perovskites Based on Deep Learning." *Molecules* 31.18 (2026): 3175.
<https://doi.org/10.3390/molecules31183175>
- [103] Moore, H. L., *et al.* "Data collection and harmonization in preterm respiratory research: recommendations and insights from PELICAN." *Pediatric Pulmonology* 61.9 (2026): e71812.
<https://doi.org/10.1002/ppul.71812>
- [104] Su, Yu, *et al.* "Machine Learning Descriptors for Mapping Structure-Property-Performance Relationships of Perovskite Solar Cells." *Advanced Energy Materials* 16.7 (2026): e05294.
<https://doi.org/10.1002/aenm.202505294>
- [105] Zhao, Long, and Hongxiang Zong. "AI-Driven Decoding of Material Dynamics: From Machine Learning Potentials and Interpretability to Generative Prediction." *Advanced Materials* 38.29 (2026): e14626.
<https://doi.org/10.1002/adma.202514626>
- [106] Elilarassi, R., *et al.* "Artificial intelligence-driven magnetic property prediction and materials discovery for next-generation spintronics." *RSC advances* (2026).
<https://doi.org/10.1039/D6RA02308H>
- [107] Gupta, Kritesh Kumar, *et al.* "Artificial Intelligence in Materials by Design: Critical Review And Perspectives on Materials Informatics to Generative and Agentic Intelligence." *Archives of Computational Methods in Engineering* 33.4 (2026): 6015-6045.
<https://doi.org/10.1007/s11831-025-10486-3>
- [108] Verma, Praveen Kumar, and Hitesh Vasudev. "Artificial Intelligence, Machine Learning, and High-Throughput Material Discovery Tools." *Smart Sustainable Materials Advancing Remanufacturing and Technology: Sustainable Materials and Technology: Materials Science & Engineering to Ecology (Volume I)*. Cham: Springer Nature Switzerland, 2026. 429-457.
https://doi.org/10.1007/978-3-032-26150-2_23
- [109] Wu, Ke, *et al.* "The Applications of Machine Learning in Micro-Nano Materials Research: From High-Throughput Screening to Intelligent Design." *Small* (2026): e75132.
<https://doi.org/10.1002/sml.75132>
- [110] Kumar Yadav, Avadhesh. "Artificial intelligence in accelerating materials discovery: opportunities and challenges." *ChemistrySelect* 11.7 (2026): e07191.
<https://doi.org/10.1002/slct.202507191>
- [111] Pattebahadur, Kanchan L., and Snehal D. Desmukh. "AI and Machine Learning in Material Discovery." *Recent Advancements in Materials Science* (2026): 15.
- [112] Wakabayashi, Yuki K., and Takuma Otsuka. "Bayesian Optimization for Self-Driving Materials Laboratories: From Algorithms to Physics-Informed Workflows." *arXiv preprint arXiv: 2608. 26016* (2026).
- [113] Yu, Guoen, *et al.* "Closed-loop active-inverse learning for constrained discovery of high-resistivity Fe-based amorphous alloys." *Materials & Design* (2026): 116895.
<https://doi.org/10.1016/j.matdes.2026.116895>

<https://doi.org/10.31875/2410-4701.2026.13.08>

© 2026 Prakash Hota and Sekhar Hota.

This is an open-access article licensed under the terms of the Creative Commons Attribution License (<http://creativecommons.org/licenses/by/4.0/>), which permits unrestricted use, distribution, and reproduction in any medium, provided the work is properly cited.