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Role of Computational Material Science in Improving the Properties of Piezoelectric Smart Materials: A Review †

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Abstract: Piezoelectric smart materials have gained significant attention in various technological applications due to their ability to convert mechanical energy into electrical energy and vice versa. These materials have diverse energy harvesting, sensing, actuation, and biomedical engineering applications. Research investigations on piezoelectric smart materials encompass many areas, including material development, characterization, modeling, device design, and manufacturing techniques. Computational material science is crucial in advancing these materials' understanding, design, and optimization. This research paper aims to provide an overview of the computational approaches employed in piezoelectric smart materials. The state-of-the-art computational techniques used for modeling piezoelectric materials are reviewed, and their applications in device design are explored along with performance optimization. This comprehensive review highlights the potential of computational material science in shaping the future of piezoelectric smart materials. It is observed that density functional theory and molecular dynamics are commonly used techniques. At the same time, finite element and phase field methods are employed for specific applications requiring continuum modeling or phase evolution simulations. Further exploration reveals that computational material science optimizes existing smart materials' structural and compositional parameters through modeling and simulation. This improves properties such as enhanced performance, increased durability, and greater functionality. In addition, computational material science is employed to design and predict the properties of new piezoelectric materials by utilizing advanced modeling techniques, enabling the discovery and development of materials with tailored piezoelectric properties for specific applications. Recent research advancements in piezoelectric smart materials have contributed to developing materials with improved properties, advanced fabrication techniques, and expanded application possibilities. These advancements have paved the way for the realization of innovative devices and systems that harness the unique capabilities of piezoelectric materials.

Keywords: piezoelectric; smart material; computational material science; properties; density functional theory; molecular dynamics

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1. Introduction

In recent years, material science has experienced noteworthy advancements, primarily influenced by integrating computational methods and experimental approaches. Computational material science (CMS) has emerged as a potent instrument, effectively employing computer simulations and theoretical models to interpret the complex relationships between material structure and properties. By providing valuable insights into the fundamental behavior of materials at the atomic and molecular scales, CMS has paved the way for designing and optimizing novel materials with customized properties [1]. An exemplary class of materials that has greatly benefitted from this collaboration is smart materials, particularly piezoelectric smart materials.

Smart materials represent a class capable of reacting to external stimuli by undergoing controlled and reversible changes in their properties [2]. These materials possess unique characteristics, like shape-memory effect, magnetoresistance, and piezoelectricity, which render them applicable in various domains, from electronics and sensors to biomedical devices and aerospace engineering. Piezoelectric smart materials have garnered significant attention because they convert mechanical stress into electrical charges and vice versa. This piezoelectric effect enables vital functions such as energy harvesting, actuation, and sensing, making them pivotal contributors to the progress of cutting-edge technologies. Although piezoelectric smart materials hold significant promise, numerous factors, such as material composition, crystal structure, and processing techniques, still restrict their performance. Conventional trial-and-error experimental methods for material optimization are time consuming and costly, prompting researchers to seek more efficient alternatives. CMS is a potent ally in this context, offering valuable insights and precise predictions that aid in designing and optimizing piezoelectric smart materials. This review's primary purpose is to investigate and emphasize the crucial role played by CMS in enhancing these materials' properties. By leveraging computational tools, like density functional theory (DFT), molecular dynamics (MD) simulations, and finite element analysis (FEA), researchers can acquire a deeper comprehension of the fundamental mechanisms governing the piezoelectric response in these materials.

This research endeavors to narrow the gap between empirical observations and theoretical forecasts, facilitating a more organized and focused material design and optimization strategy. This review attempts to offer a comprehensive and accurate understanding of the behavior of piezoelectric smart materials at the electronic and atomic scales. This is where the significance of this study lies. Researchers can enhance and improve materials with improved performance and productivity by disclosing the inherent properties that affect the piezoelectric effect, effectively generating opportunities for cutting-edge applications and addressing the current limitations. Employing the computational method accelerates the material discovery process, allowing researchers to investigate various designs and pinpoint potential candidates for experimentation. This makes the development of advanced piezoelectric smart materials more efficient and cost effective, resulting in reduced time and resources required for trial-and-error synthesis. Recent research advancements have culminated in piezoelectric smart materials exhibiting enhanced properties, exemplified by the development of lead-free piezoelectric ceramics with comparable performance to traditional lead-based counterparts; advanced fabrication techniques, such as additive manufacturing, enabling intricate and customized device geometries; and new application possibilities, demonstrated through the integration of piezoelectric materials in self-powered wearable sensors for healthcare monitoring, showcasing their potential in the emerging field of personalized healthcare technologies. Most of the research in CMS for piezoelectric smart materials revolves around specific areas like implementing computational techniques to investigate fundamental mechanisms of the piezoelectric effect in varied materials to formulate studies focused on exploring crystal structure, polarization, and strain coupling to interpret the origin of piezoelectricity in various materials; utilizing simulations to predict and understand how specific chemical compositions and crystal structures can influence the piezoelectric response, enabling the targeted synthesis of high-performance materials, using computational studies to understand the impact of defects, grain boundaries, and interfaces on piezoelectric properties to develop strategies to mitigate their adverse effects; and employing multiscale modeling by combining techniques like FEA, MD simulation, and DFT to bridge the gap between atomistic-level phenomena and macroscopic material properties [3]. A lot of research of the highest quality has been undertaken in the area of piezoelectric smart materials since the 1880s, especially on the piezoelectric effect, piezoelectric coefficients that have primarily contributed to the present state of demand for developing new piezo materials using CMS, as presented in Figure 1 [4–11].

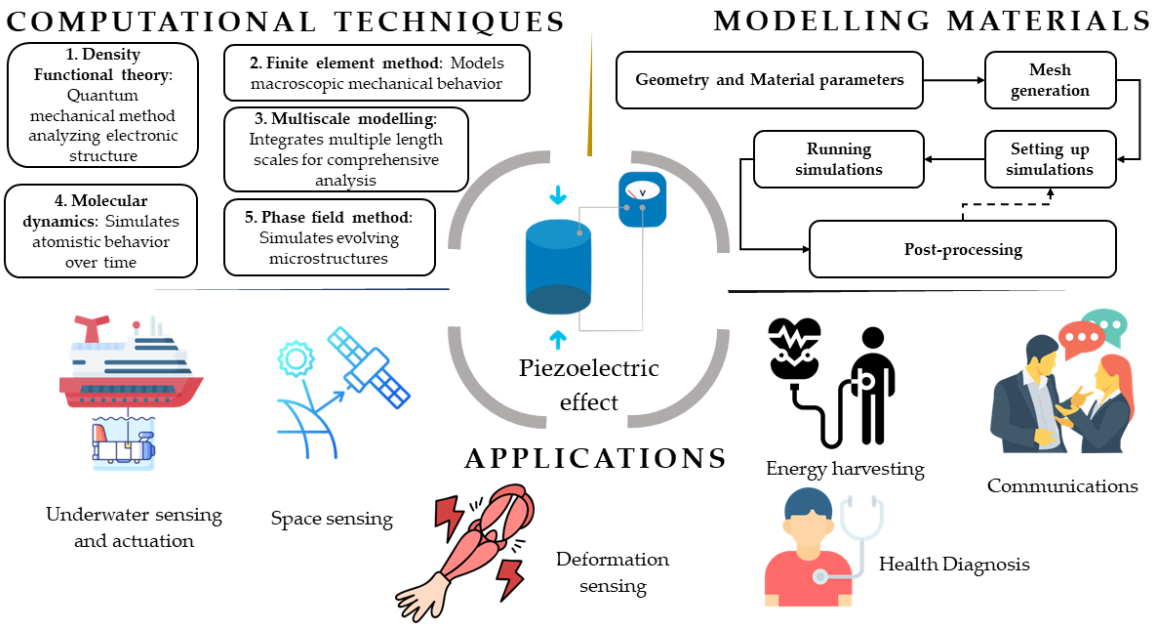

Figure 1. Role of computational material science in improving the properties of piezoelectric smart materials.

2. Literature Review

2.1. Computational Modeling Techniques

Numerical methods used to simulate and analyze complex phenomena and systems via computer-based simulations are termed computational modeling techniques. These techniques help researchers and engineers to study the intricate processes, predict the outcomes, and gain insights that are not attainable via conventional experiments. Computational modeling approaches include DFT, FEA, and MD simulations, and others. These techniques are widely applicable in numerous fields, including physics, biology, chemistry, material science, engineering, and climate science.

2.1.1. Density Functional Theory (DFT)

DFT is employed in computational material science to interpret materials' electronic structure and properties. It is a powerful quantum mechanical model that systematically investigates the behavior of electrons within the material's crystal lattice. It also provides valuable insights into the relationship between the electronic structure and the material properties. It has become the foundation in the study and design of piezoelectric materials because of its high accuracy and efficiency in predicting material properties at atomic and electronic levels [12].

S. Yuan et al. utilized DFT and experimental data to explore the electronic properties and interactions within a van der Waals heterostructure. DFT calculations optimized the molecular and crystal structures of In_2Se_3 and MoS_2 nanosheets, identifying their most stable configuration. They also quantified charge transfer between them, elucidating their mutual electronic influence. Electronic band structures and density of states were calculated, revealing essential insights into energy levels, bandgaps, and electronic behavior. Additionally, DFT predictions aided in determining the piezoelectric coefficients of the individual nanosheets [13].

Similarly, Y. Chen et al. studied the electronic and piezoelectric properties of the In_2Se_3/transition metal dichalcogenide (TMDC) heterostructures. The authors used DFT for calculating electronic band structures and density of states (DOS) of the In_2Se_3/TMDC heterostructures and for calculating piezoelectric tensors, which described the coupling between electronic polarization and mechanical strain [14].

P. Hermet et al. investigated the potential of trigonal bismuth phosphate ($BiPO_4$) as a low-temperature piezoelectric material. They analyzed its crystal structure electronic properties and calculated piezoelectric coefficients using DFT. The findings highlighted $BiPO_4$'s suitability for cryogenic applications, as it exhibited robust piezoelectric responses at low temperatures. DFT was also applied to assess its thermodynamic stability in such conditions using phonon dispersion calculations. The results confirmed its sustained stability at low temperatures, affirming its viability for specialized applications in cold environments [15].

2.1.2. Finite Element Analysis (FEA)

A numerical method widely used by engineers and researchers in material science and engineering for the simulation and analysis of the behavior of complex structures and materials. This technique divides the complex structure or material into minute, finite-sized elements, such as triangles. The mathematical equations are then applied to these finite-sized elements to model their response to various loads, including thermal, mechanical, and electric. For piezoelectric smart materials, FEA is used primarily for understanding, improving, and optimizing their performance and properties.

Nguyen-Vinh et al. utilized FEA to create numerical models for piezoelectric actuators. They input piezoelectric coefficients, dielectric constants, and elastic properties into the simulations, enabling assessment of the actuator's response to electrical and mechanical loads. These simulations facilitated design optimization, sparing the need for costly and time-consuming experimental tests. The study accurately predicted the piezoelectric actuator's responses, encompassing displacement, strain, and stress reactions under diverse loading conditions [16].

Nguyen-Vinh et al. employed the extended finite element method (XFEM) to simulate dynamic fracture in piezoelectric materials, surpassing conventional methods by eliminating the need for re-meshing during complex crack propagation. This study used XFEM to analyze dynamic fracture behavior under various loading conditions, investigating crack propagation's interaction with electrical and mechanical loads. XFEM provided a solid foundation for examining crack propagation in piezoelectric materials, including analyzing crack growth direction, rate, and the influence of piezoelectric properties on the process [17].

S.T. Gu et al. employed FEA to implement imperfect interface models for piezoelectric composites. In their study, FEA was combined with weak formulations to overcome the challenges posed by the highly heterogeneous nature of piezoelectric composites. FEA was also applied to benchmark problems in order to validate the proposed models and numerical approaches so that researchers could compare the results with known solutions to ensure reliability and accuracy [18].

2.1.3. Molecular Dynamics (MD) Simulations

A robust computational technique that is primarily used to simulate the behavior of atoms and molecules over time in material science. It offers valuable insights into the dynamic evolution of materials at the atomic and molecular levels. It also provides valuable insights into the material's mechanical, electrical, and thermal properties. For piezoelectric smart materials, MD helps immensely in understanding, optimizing, and enhancing their properties and performance.

H. Hong et al. employed MD simulations to gain atomic-level insights into PVDF/TiO_2 nanocomposite film phase transformation. This method modeled individual atoms, revealing valuable information about their interactions. The simulations elucidated PVDF phase changes induced by TiO_2 nanoparticles and tracked atomic-scale rearrangements. The molecular arrangement of PVDF in response to the presence of TiO_2 nanoparticles at the atomic scale and the changes in the crystalline phase were monitored with the help of MD simulations [19].

Tang et al. used MD at various stages to gain an atomic-level understanding of stretchable polymer composites, combining a piezoelectric filler material with a flexible polymer matrix. Simulations informed composite design, revealing molecular structure, filler particle distribution, and interface interactions. Results showed stable structures and component interactions, guiding experimental synthesis. Modeling atomic interactions under deformation provided crucial insights into induced polarization and electric potential, determining piezoelectric response. Additionally, simulations aided microstructure analysis, shedding light on mechanisms contributing to ultrahigh piezoelectric performance. This provided molecular-level insights into filler–polymer matrix interaction and piezoelectric filler dispersion [20].

A. Chakrabarty et al. used MD simulations to analyze atomic-scale interactions between carbon nanotubes (CNTs) and the polyimide matrix. This approach provided detailed insights into the composite's microstructure, including the spatial arrangement of CNTs within the polyimide matrix, confirming successful dispersion. The simulations predicted crucial thermo-mechanical properties like the thermal expansion coefficient, Young's modulus, and piezoelectric coefficients. Modeling atomic interactions under various loading conditions obtained valuable data on the composite's response to temperature and mechanical deformation [21].

2.1.4. Phase Field Method (PFM)

The PFM for piezoelectric smart materials employs mathematical frameworks to simulate the behavior of materials with piezoelectric properties. It accounts for domain evolution, stress, and electric fields, enabling accurate predictions of material response under various conditions. This approach aids in designing efficient devices like sensors, actuators, and energy harvesters.

Yan et al. utilized the PFM to scrutinize grain-oriented modified $PbTiO_3$ material. This approach focused on domain formation and orientation within the microstructure. The study revealed the evolution of domain structure during synthesis, culminating in a grain-oriented microstructure. It also investigated domain switching in response to applied mechanical stress, a pivotal aspect in piezoelectric materials. The simulations demonstrated the generation of electrical voltage during mechanical deformation. Additionally, they examined the influence of defects, like grain boundaries and vacancies, on the domain structure and material behavior. The results provided a comprehensive understanding of how defects impacted the overall performance of grain-oriented modified $PbTiO_3$ material, offering insights into its response to mechanical and thermal stimuli in their presence [22].

Yan et al. utilized the PFM to model the domain structure of textured piezoelectric ceramics, which exhibit varying polarization directions. This analysis allowed for the assessment of ceramics' efficiency in converting electrical energy to mechanical motion and vice versa. The results aligned with experimental observations, confirming near-ideal electromechanical coupling in textured piezoelectric ceramics. Controlled crystallographic orientation, achieved through texture engineering, enhanced domain switching behavior, contributing to the near-ideal coupling coefficient. The phase field simulations offered valuable insights into the microstructure–property relationship. Theoretical modeling predicted the optimal texture and crystallographic orientation for achieving near-ideal electromechanical coupling [23].

Leng et al. utilized the PFM to investigate microstructure evolution and domain-switching behavior in water-quenched and acceptor-doped textured piezoelectric ceramics. The simulations also modeled the microstructure evolution during the water-quenching process, revealing textured microstructures and the impact of quenching rates. Additionally, the method was employed to simulate the texture engineering process, enabling control of crystallographic orientation for optimized microstructures. The PFM facilitated the simulation of domain-switching behavior in these ceramics, highlighting its influence on their piezoelectric performance and electromechanical properties [24].

2.1.5. Multiscale Modelling Approaches

Multiscale modeling for piezoelectric smart materials integrates micro- and macro-scale analyses to capture their complex behavior. It combines atomic-level interactions with continuum mechanics, providing a comprehensive view of material response. This approach is crucial for designing high-performance devices with enhanced piezoelectric properties for electronics and energy harvesting applications.

Maruccio C. et al. employed diverse multiscale modeling methods, such as atomistic simulations, MD, FEA, and continuum mechanics, to examine piezoelectric material behavior across various length scales. Atomistic and molecular simulations delved into atomic-level responses, tracking individual atoms or ions under mechanical and electrical influences. These simulations yielded crucial insights into the materials' mechanical and electrical behavior. The multiscale models facilitated the transition from the atomic/molecular to the macroscopic level, allowing predictions and analyses of overall material behavior in practical engineering applications [25].

Wang L. et al. applied a multiscale prediction approach to model the piezoelectric behavior of 2D Janus ZnBrI. This involved integrating methods like DFT for electronic structure and MD for mechanical response. Results reported piezoelectric coefficients, indicating anisotropy—differing coefficients along crystallographic axes. This insight is crucial for device design [26].

Lv et al. proposed a novel multiscale computational method for analyzing electromechanically coupled behavior in heterogeneous piezoelectric composites. This approach combines various numerical techniques to address phenomena across different scales. This method accurately and effectively predicts the composite's electromechanical behavior based on constituent properties. The results provide effective electromechanical properties, representing the composite's behavior [27].

3. Summary

Upon reviewing the studies, it can be interpreted that DFT can significantly improve the understanding and prediction of the properties of piezoelectric smart materials by accurately describing the electronic structure of materials with insights into energy band structure, charge distribution, band gaps, predicting the piezoelectric constants of varied materials, enabling the design and optimization of materials, and providing insights into the mechanisms that drive the piezoelectric response in materials. FEA aids in the optimization of piezoelectric smart material designs. By analyzing various configurations and geometries, researchers can identify the most efficient designs that maximize piezoelectric responses or specific properties. It is also used for performing stress analysis on piezoelectric materials to ensure that they can withstand mechanical loads without failure since this is important for designing durable and robust piezoelectric devices and structures. Piezoelectric smart materials exhibit coupled behavior between mechanical, electrical, and thermal fields. FEA can effectively handle these multiphysics problems, enabling researchers to study the interactions between these fields and optimize material performance under various conditions. MD simulations provided valuable insights into the mechanical responses, including elastic constants, stiffness, and deformation mechanisms of piezoelectric materials under external loads. Understanding thermal behavior is essential for designing piezoelectric devices that may experience temperature variations. MD helps study the thermal conductivity and thermal expansion of materials, guiding the development of materials with optimized thermal properties. The PFM enabled the study of domain morphology and microstructure evolution of piezoelectric materials. This included investigating the formation and growth of domains, domain switching, and the effect of microstructural features on material properties. Understanding domain wall motion is crucial for optimizing piezoelectric performance. PFM simulations provide information about the movement of domain walls under different conditions, guiding the design of materials with enhanced piezoelectric responses. The PFM is particularly valuable for multiscale modeling, where the piezoelectric response is influenced by microstructural

features at different length scales. Piezoelectric smart materials exhibit coupled behavior between mechanical, electrical, and thermal fields. The PFM can handle these multiphysics problems, providing a holistic understanding of the interactions between different fields and their impact on material properties. Multiscale modeling provides atomistic insights into piezoelectric materials' crystal structure, polarization, and interactions. Using techniques such as molecular dynamics and density functional theory, researchers can study the fundamental processes contributing to the piezoelectric response. It allows the investigation of defects, grain boundaries, and interfaces in piezoelectric materials. Understanding the impact of these features on the piezoelectric properties helps optimize the material's performance. By combining atomistic simulations with continuum methods, accurate prediction of piezoelectric coefficients is enabled. This information is crucial for selecting suitable materials for specific applications and designing high-performance devices. Piezoelectric smart materials exhibit coupled behavior between mechanical, electrical, and thermal fields. Multiscale modeling enables the study of these coupled phenomena, providing a comprehensive understanding of material behavior under different conditions. It also facilitates high-throughput screening of potential piezoelectric materials. A comparison of different computational techniques for piezoelectric modeling is shown in Table 1. By predicting material properties without extensive experimental efforts, identifying promising candidates for further investigation is possible.

Table 1. Comparison of computational techniques for piezoelectric material modeling.

Technique	Advantages	Limitations	Applications
Density Functional Theory	Accurate electronic properties can handle complex materials.	Computationally intensive; limited to small systems.	Design of novel piezoelectric materials; investigation of electronic properties.
Molecular Dynamics	Captures dynamic behavior applicable to large systems.	Limited to short time scales; relies on force field accuracy.	Study of piezoelectric polarization switching; investigation of defect effects.
Finite Element Analysis	Handles complex geometries can model various boundary conditions.	Requires mesh generation may lack atomic-level accuracy.	Design of piezoelectric sensors, actuators, and transducers.
Phase Field Method	Captures complex microstructural changes; suitable for multiphase systems.	Captures complex microstructural changes; suitable for multiphase systems.	Study of domain switching; ferroelectric domain structures in piezoelectric materials.
Multiscale Modelling	Captures interactions from atomistic to macroscopic scales.	Complex setup and calibration; computational costs can be high.	Investigating piezoelectric material behavior across different length scales; linking molecular and macroscopic behavior.

Computational design of piezoelectric materials is an efficient and robust approach for the optimization and discovery of materials with desired properties. Several techniques like first principle calculations, computational prediction of piezoelectric properties, machine learning, data-driven approaches, and topological optimization of piezoelectric structures are being used.

First principle calculations are similar to DFT and are crucial for piezoelectric materials' computational design. They can provide accurate predictions of the behavior of the materials by enabling researchers to model the electronic structure and properties of the material from quantum mechanical principles. Computational prediction of the piezoelectric properties can be predicted by employing FEA and MD simulations.

Machine learning techniques have transformed the study of materials by expediting the processes of material discovery and optimization. Large databases of material data are mined for patterns, correlations, and structure–property interactions using data-driven methodologies, including supervised and unsupervised learning. Thus, new materials' piezoelectric properties can be predicted using these models, offering helpful direction for experimental synthesis and characterization efforts. Additionally, researchers can

use machine learning to identify materials with improved piezoelectric performance and investigate high-dimensional property spaces [28].

The design and optimization of the geometry of the piezoelectric materials can be fulfilled using the technique known as topological optimization. Specific piezoelectric response or target material properties can be achieved by tailoring the topology of the piezoelectric materials with the help of adequately defined design objectives and constraints and utilizing numerical optimization algorithms. This approach allows the design of innovative and complex structures that minimize material usage and maintain mechanical integrity while maximizing the piezoelectric performance [29].

Multiphysics simulations and FEA are crucial in transducer and sensor design, optimizing response time, sensitivity, and frequency range. This ensures high-resolution ultrasound imaging and improves structural health monitoring. In energy harvesting, these techniques maximize efficiency for self-powered networks and wearables. For piezoelectric actuators used in precision positioning and adaptive optics, computational optimization designs high-displacement, force and response speed devices, ensuring stability and reliability. In biomimetic applications, it also emulates biological muscle behavior, benefiting prosthetics and robotics. Computational optimization fine-tunes parameters for seamless integration and reliable performance in real-world conditions, addressing stress distribution, thermal effects, and electrical connections.

In the case of existing smart materials, computational material science employs intricate modeling and simulation techniques to systematically fine-tune existing smart materials' structural and compositional aspects. This process enabled precise adjustments that improved properties, including enhanced performance, augmented durability, and expanded functionality. For instance, through simulations, researchers can explore the effects of altering crystal structures or introducing specific dopants, predicting how these changes will influence the material's behavior and performance in real-world applications. This targeted optimization approach is pivotal in pushing the boundaries of material science, enabling the development of smart materials with superior capabilities and broader application potential.

Challenges and Future Directions

The field of CMS has made significant strides in improving the properties of piezoelectric smart materials. However, several challenges still exist, and future research directions are essential to continue advancing this area of study. Piezoelectric smart materials exhibit complex behaviors and nonlinear responses under varying conditions. Capturing these phenomena accurately in simulations remains a challenge. Further development is required for the existing advanced computational techniques, like higher-order FEA, multiscale modeling, and PFM, to be efficiently used for modeling and understanding the complex behavior of piezoelectric materials. These challenges need to be addressed to obtain accurate predictions of the device's performance and the properties of the materials. The reliability and accuracy of computational models depend on the gap between theory and experiment. To enhance these two, bridging the gap is essential. Collaborating between researchers and experimentalists is essential for validating and refining the simulation results to ensure that computational predictions align with real-world behavior. As computational resources continue to improve, novel techniques and technologies must be explored to push the boundaries of computational material science. Machine learning, artificial intelligence, and high-performance computing offer exciting prospects for accelerating materials discovery and optimization processes. Integrating these emerging technologies with traditional computational approaches will enhance efficiency and unlock new opportunities for designing superior piezoelectric smart materials.

4. Conclusions

The utilization of various computational techniques for modeling and optimizing the behavior of piezoelectric materials like DFT, FEA, MD, and PFM have been discussed.

CMS has paved the way for designing and optimizing piezoelectric transducers and sensors with enhanced sensitivity and performance. It has facilitated the development of energy harvesting systems capable of efficiently converting mechanical vibrations into electrical energy, opening possibilities for self-powered and sustainable electronic devices. Also, utilizing computational methods in piezoelectric actuators and artificial muscles has resulted in the development of highly responsive and lifelike motion devices, which have significant applications in fields like prosthetics and robotics. Combining bio-inspired design principles in piezoelectric devices has created advancements in the creation of biomimetic sensors and medical designs, which leads to developments in healthcare and haptic feedback systems. The prospects of computational material science in this field are promising. Modeling complex phenomena and nonlinearities remains a challenge. Still, developing advanced techniques, like higher-order finite element and phase-field methods, can overcome these hurdles and yield more accurate predictions. Bridging the gap between theory and experiment through closer collaboration between computational researchers and experimentalists will ensure the reliability and applicability of computational models. Integrating emerging computational technologies, like machine learning and artificial intelligence, with traditional computational approaches can unlock new opportunities for designing superior piezoelectric smart materials with tailored properties. As this field continues to progress, it holds immense potential for shaping the future of technology across multiple industries. The advancements made through computational approaches will undoubtedly continue to drive innovation, leading to the development of highly efficient, sustainable, and versatile piezoelectric smart materials that benefit society in diverse ways.

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