

Artificial Intelligence for Composition–Structure–Property Optimization of Ferroelectric Ceramics

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Abstract

Ferroelectric ceramics occupy a critical position in modern electronics, sensing, actuation, energy storage, and electromechanical transduction, yet their development remains constrained by complex coupling among chemical composition, crystallographic structure, microstructure, processing history, and functional property response. Artificial intelligence offers a powerful means to navigate this high-dimensional design space, but its effective use requires more than isolated predictive models. It demands integrated computational, experimental, data, and governance architectures that can support reproducible discovery, deployment, and lifecycle management. This paper examines artificial intelligence for composition–structure–property optimization of ferroelectric ceramics from a system-level perspective. It argues that progress depends on aligning machine learning architectures with physical priors, multi-fidelity characterization, automated experimentation, and robust data infrastructure. The discussion considers structural trade-offs among accuracy, interpretability, throughput, cost, and sustainability, as well as the institutional arrangements needed to ensure fairness, reproducibility, and policy coherence. Case illustrations include perovskite ferroelectrics, barium titanate-based dielectrics, lead-free piezoelectric systems, and multilayer ceramic capacitor manufacturing. The paper concludes that artificial intelligence can accelerate ferroelectric ceramic design only when treated as a socio-technical capability embedded in material science infrastructure rather than as a standalone algorithmic substitute for domain expertise. Such an approach can improve discovery outcomes while preserving scientific accountability and enabling responsible deployment.

Keywords

ferroelectric ceramics; materials informatics; composition–structure–property relationships; Bayesian optimization; autonomous experimentation; governance; sustainability.

1. Introduction

Ferroelectric ceramics are foundational materials for capacitors, actuators, sensors, transducers, memories, energy harvesters, and electrocaloric devices. Their functional behavior arises from a delicate interplay among composition, crystal symmetry, domain configuration, grain structure, defect chemistry, and processing conditions. Small changes in dopant concentration, sintering atmosphere, particle size, or cooling rate can shift phase stability, polarization switching, dielectric loss, and breakdown strength in ways that are difficult to predict from first principles alone. This sensitivity has made ferroelectric ceramic development a highly empirical enterprise, often relying on expert intuition, historical recipes, and iterative laboratory experimentation. The scale and complexity of the design space exceed the capacity of conventional trial-and-error methods, especially when multiple properties must be optimized simultaneously under manufacturing and environmental constraints.

Artificial intelligence has therefore emerged as a promising approach for accelerating composition–structure–property optimization in ferroelectric systems [1], [2], [3].

The opportunity is not merely to replace human intuition with statistical prediction. Rather, artificial intelligence can coordinate heterogeneous knowledge across simulation, synthesis, characterization, and application requirements. Machine learning models can approximate expensive first-principles calculations, infer property trends from sparse experimental data, generate candidate compositions, and guide sequential experiments under uncertainty [4], [5]. Generative models can propose novel chemistries or processing pathways that lie outside known exemplars, while Bayesian optimization and active learning can allocate scarce experimental resources toward the most informative or promising regions of the design space [6]. These capabilities are particularly relevant for ferroelectric ceramics, where each sample may require powder preparation, calcination, shaping, sintering, electrode application, poling, and multiple electrical measurements. The cost of exhaustive search is therefore prohibitive, and intelligent sampling becomes a practical necessity.

However, the deployment of artificial intelligence in this domain cannot be evaluated solely by predictive accuracy. Ferroelectric ceramic optimization is a system-level problem involving instrumentation, data provenance, materials supply, manufacturing tolerance, environmental impact, and regulatory expectations. A model that predicts dielectric permittivity with high accuracy may still fail in deployment if its training data are biased toward a narrow processing window, if its uncertainty estimates are unreliable, or if its recommendations cannot be manufactured at scale. Similarly, a closed-loop autonomous laboratory may accelerate discovery but introduce new dependencies on proprietary software, fragile hardware integrations, and opaque data pipelines. These concerns connect materials informatics to broader debates about robustness, fairness, sustainability, and governance in artificial intelligence-enabled science [1], [4].

This paper argues that artificial intelligence for ferroelectric ceramics should be understood as an infrastructure problem as much as a modeling problem. The central challenge is to design architectures that integrate physical knowledge, experimental feedback, data standards, uncertainty quantification, and institutional controls. Such architectures must support trade-offs among exploration and exploitation, model complexity and interpretability, automation and human oversight, and local optimization and global sustainability. The discussion proceeds by reviewing the physical and manufacturing foundations of ferroelectric ceramics, examining artificial intelligence architectures for composition–structure–property mapping, analyzing closed-loop experimental infrastructure, and assessing governance and policy implications. The aim is to provide a system-level account of how artificial intelligence can be responsibly embedded in ferroelectric ceramic research and deployment.

2. Ferroelectric Ceramics as Coupled Material and Manufacturing Systems

Ferroelectric ceramics are typically crystalline oxides with perovskite, tungsten bronze, Aurivillius, or related structures. In perovskites such as barium titanate and lead zirconate titanate, the functional properties depend on cation substitution, oxygen vacancies, domain wall mobility, grain size, and phase coexistence near morphotropic boundaries. The composition–structure–property relationship is therefore multi-scale. At the atomic scale, bond covalency and tolerance factors influence polarization stability. At the mesoscale, grain boundaries and domains control switching, loss, and breakdown. At the device scale, electrode geometry, layer thickness, sintering density, and thermal history determine

capacitance, reliability, and lifetime. Artificial intelligence must contend with this hierarchy rather than treating material response as a single-variable function [7], [8].

The manufacturing dimension further complicates optimization. Ferroelectric ceramics are produced through routes such as solid-state reaction, sol–gel processing, hydrothermal synthesis, tape casting, and spark plasma sintering. Each route creates distinct impurity profiles, particle morphologies, and densification behavior. For multilayer ceramic capacitors, for example, thin dielectric layers require uniform particle packing, controlled binder burnout, compatible electrode co-firing, and minimal defect concentration. Aqueous tape casting has attracted attention because it can reduce organic solvent use and support thinner layers, but it also introduces sensitivity to slurry chemistry, drying, and lamination [13]. Artificial intelligence models trained only on laboratory pellet data may not transfer to tape-cast films because the processing variables and failure modes differ. This illustrates why composition–structure–property optimization must be coupled to process–structure–property modeling and device-level constraints.

Data scarcity is a persistent challenge. Unlike fields with massive standardized datasets, ferroelectric ceramics research often generates small, heterogeneous datasets collected under different protocols. Reported values for dielectric constant, piezoelectric coefficient, coercive field, and energy density may depend on measurement frequency, electric field amplitude, temperature, sample geometry, and poling history. Without careful metadata, pooling data across laboratories can introduce systematic bias. Machine learning strategies for small datasets therefore emphasize feature selection, physics-informed descriptors, transfer learning, and uncertainty-aware validation [14]. The physical interpretability of descriptors is also important because researchers need to understand why a composition is promising, not merely that a model ranks it highly.

Ferroelectric optimization also involves conflicting objectives. High permittivity may accompany high dielectric loss. Large piezoelectric response may come with temperature instability or lead content. High energy density may require high breakdown strength, which can conflict with dense, defect-free processing. Lead-free alternatives address environmental concerns but often lag in performance or manufacturability. Artificial intelligence can support multi-objective optimization by mapping Pareto fronts and identifying candidates that satisfy trade-offs among performance, cost, toxicity, and reliability. However, such optimization is only meaningful when objectives and constraints are defined through stakeholder engagement and regulatory context. A purely technical objective function may obscure social and environmental consequences, including energy-intensive sintering, hazardous precursor use, and end-of-life disposal. The next section examines architectures that can represent these coupled considerations without reducing them to a single scalar target.

3. Artificial Intelligence Architectures for Composition–Structure–Property Mapping

An effective artificial intelligence architecture for ferroelectric ceramics usually combines representation learning, surrogate modeling, uncertainty quantification, and optimization. Representation learning transforms composition, structure, processing, and characterization data into numerical descriptors that machine learning models can use. These descriptors may include elemental properties, ionic radii, electronegativity, tolerance factors, valence states, phase fractions, grain size distributions, and processing parameters. Physics-informed representations can improve extrapolation beyond the training set, while purely data-driven embeddings can discover latent relationships that experts may not have encoded [15], [16]. The choice of representation is a structural trade-off: highly engineered descriptors can

enhance interpretability and small-data performance, but they may also limit flexibility and reproduce existing biases.

Surrogate models approximate expensive simulations or experiments. For ferroelectric ceramics, density functional theory can provide polarization, phase stability, and defect energetics, but it is computationally costly for large compositional spaces. Machine learning potentials and surrogate models can accelerate screening by predicting properties such as formation energy, band gap, dielectric response, and piezoelectric coefficients [17], [18]. These models are most useful when their uncertainty is calibrated. If a model is confident in the wrong region of composition space, it may misdirect experiments. Ensemble methods, Gaussian processes, and Bayesian neural networks provide uncertainty estimates, but calibration remains difficult when data are sparse and non-identically distributed. Active learning addresses this by selecting experiments that reduce uncertainty or maximize expected improvement [11], [12]. In ferroelectric ceramics, active learning can prioritize compositions near phase boundaries, dopant combinations that may stabilize desired phases, or processing windows that improve density and breakdown strength.

Generative models add another architectural layer. Variational autoencoders, generative adversarial networks, and diffusion models can propose new compositions or microstructures by learning from known examples. In materials science, inverse design seeks to generate candidates with desired properties rather than merely predict properties of given candidates [3]. For ferroelectric ceramics, inverse design might specify targets such as high energy density, low loss, and lead-free composition, then generate candidate chemistries or processing routes. However, generative models can produce physically invalid or synthetically inaccessible candidates. Constraint satisfaction, physics-based filtering, and manufacturability assessment are therefore essential components of the architecture. The system must close the loop between generation, simulation, synthesis, characterization, and property validation.

Multi-fidelity modeling is particularly relevant because ferroelectric data come from sources with different cost and accuracy. First-principles calculations, phase-field simulations, laboratory measurements, and industrial qualification tests represent different fidelity levels. A multi-fidelity architecture can learn from abundant low-fidelity data and selectively query high-fidelity experiments. Transfer learning can adapt models trained on one ferroelectric family to another, such as from barium titanate to lead-free bismuth-based systems. Yet transfer can fail when the underlying physics changes. Therefore, system-level design must include domain shift detection, recalibration, and human review. The architecture should also support explainability, not because interpretability always improves accuracy, but because scientific acceptance and safety require understanding of model reasoning. Material scientists, process engineers, and policymakers need to assess whether a recommendation is physically plausible, economically feasible, and consistent with regulatory constraints. Artificial intelligence is most valuable when it augments expert judgment rather than displacing it.

4. Closed-Loop Experimental Infrastructure and Autonomous Optimization

The most ambitious vision for artificial intelligence in ferroelectric ceramics is the closed-loop laboratory, where models propose experiments, robotic systems synthesize and measure samples, and results feed back into model refinement. Such infrastructure can increase throughput, reduce human error, and capture negative results that are often lost in conventional publication. However, autonomous experimentation is a socio-technical system, not merely a collection of instruments. It requires sample tracking, data schemas, equipment

interfaces, scheduling, safety controls, and maintenance protocols. Technical debt can accumulate quickly when data pipelines are ad hoc, models are tightly coupled to specific instruments, or software dependencies are undocumented [19]. For ferroelectric ceramics, the physical complexity of powder processing, sintering, and electrical testing makes full automation difficult. Partial automation may be more realistic, with humans handling critical steps such as precursor preparation or interpretation of anomalous results.

Data infrastructure is the foundation of closed-loop optimization. The FAIR principles, which emphasize findable, accessible, interoperable, and reusable data, provide a useful framework for materials informatics [22]. For ferroelectric ceramics, interoperability requires standardized metadata for composition, synthesis route, sintering profile, measurement conditions, and uncertainty. Datasheets for datasets and model cards can document provenance, intended use, limitations, and ethical considerations [20], [21]. Without such documentation, models may be reused in inappropriate contexts, leading to unreliable predictions or safety concerns. A ceramic capacitor intended for consumer electronics, for example, may have different reliability requirements than one used in automotive or aerospace systems. Model cards can clarify whether a model was trained on laboratory-scale pellets or production-scale tape-cast films, and whether it accounts for temperature, voltage, and frequency dependence.

The integration of process data is especially important. In multilayer ceramic capacitor manufacturing, dielectric layer thickness, electrode composition, lamination pressure, binder burnout, co-firing profile, and termination processes all influence final properties. Aqueous tape casting is one route that can reduce solvent emissions and enable thin layers, but it requires careful control of slurry rheology, drying, and shrinkage [13]. Artificial intelligence can optimize these parameters if sufficient process data are available. Yet the data are often proprietary and fragmented across suppliers, manufacturers, and research laboratories. Governance arrangements such as data trusts, consortium agreements, and precompetitive research platforms may be needed to enable sharing while protecting intellectual property. Such arrangements must also address fairness: smaller institutions and developing economies may lack the infrastructure to contribute to or benefit from advanced autonomous laboratories.

Sustainability is another dimension of infrastructure design. Ferroelectric ceramics often require high-temperature sintering, hazardous precursors, and rare or critical elements. Artificial intelligence can help identify lower-temperature processing routes, reduce lead content, improve yield, and extend device lifetime. But these benefits are not automatic. Optimization objectives must explicitly include energy consumption, greenhouse gas emissions, water use, and material criticality. If models optimize only for dielectric constant or piezoelectric coefficient, they may recommend compositions that are environmentally harmful or supply-chain fragile. A sustainable architecture therefore links property prediction to lifecycle assessment and circular economy considerations. It also requires policy support for open data, responsible sourcing, and recycling infrastructure. Closed-loop experimentation should be evaluated not only by discovery speed but also by its contribution to long-term environmental and social resilience.

5. Robustness, Fairness, Governance, and Policy Implications

Robustness in artificial intelligence for ferroelectric ceramics has multiple meanings. Statistical robustness concerns performance under distribution shift, noisy measurements, and outliers. Physical robustness concerns the validity of predictions outside the training domain. Operational robustness concerns whether models and automated systems continue to function

when instruments fail, data drift, or supply conditions change. For ferroelectric materials, distribution shift can occur when a model trained on one synthesis route is applied to another, when measurement protocols change, or when raw materials vary in purity. Robustness testing should therefore include stress tests across processing conditions, temperature ranges, electric fields, and device geometries. Uncertainty quantification should inform decision-making, and human operators should be able to override model recommendations when physical intuition or safety concerns warrant it.

Fairness is less commonly discussed in materials science, but it has important implications. Access to high-quality data, computational resources, and automated laboratories is unevenly distributed across institutions and countries. If artificial intelligence accelerates discovery primarily in well-funded settings, it may widen gaps in scientific capacity and technological sovereignty. Fairness also concerns the representation of applications. Research may prioritize high-value consumer electronics or military systems while neglecting energy access, medical devices for underserved populations, or sustainable construction materials. Governance frameworks should encourage inclusive agenda-setting and benefit-sharing. Open datasets, shared benchmarks, and collaborative model development can reduce barriers, but they require funding, training, and infrastructure. Policy interventions may include support for national materials data repositories, standardized reporting requirements, and international cooperation on critical materials.

Governance must also address the risks of automation in scientific research. Autonomous systems can generate large volumes of experimental data and candidate designs, raising questions about authorship, accountability, and environmental impact. If a model recommends a hazardous synthesis route, who is responsible? If an automated laboratory produces misleading results due to calibration drift, how are errors detected and corrected? These questions require clear protocols for validation, auditing, and incident reporting. Model cards and datasheets offer documentation tools, but they must be embedded in institutional review processes and regulatory frameworks [20], [21]. In industrial settings, qualification standards for ferroelectric components already exist, but they may not anticipate machine learning-driven design. Policymakers should work with engineers, material scientists, and ethicists to update standards without stifling innovation.

From a policy perspective, artificial intelligence for ferroelectric ceramics intersects with semiconductor policy, energy policy, environmental regulation, and research funding. Ferroelectric components are critical for capacitors, sensors, and actuators, which are essential to electrification, renewable energy, and advanced manufacturing. Governments may therefore view artificial intelligence-enabled materials discovery as a strategic capability. However, policy should avoid narrow techno-nationalism that fragments data and duplicates effort. International collaboration on data standards, benchmark datasets, and sustainability metrics can accelerate progress while promoting equitable participation. Funding agencies should support not only model development but also the maintenance of data infrastructure, experimental facilities, and interdisciplinary training. The most significant breakthroughs may come from teams that combine materials science, computer science, process engineering, and social science.

Finally, governance must remain adaptive. Ferroelectric ceramics and artificial intelligence are both rapidly evolving fields. Regulations written for current capabilities may become obsolete as new generative models, autonomous laboratories, and lead-free compositions emerge. Adaptive governance uses iterative review, stakeholder engagement, and continuous

monitoring to adjust rules as evidence accumulates. It also recognizes that different applications require different levels of oversight. A laboratory-scale screening model may need modest documentation, while an artificial intelligence system controlling production of automotive capacitors may require rigorous validation, traceability, and fail-safe design. A tiered approach can balance innovation and precaution. The system-level challenge is to create an ecosystem in which artificial intelligence accelerates composition–structure–property optimization while remaining transparent, robust, fair, and aligned with sustainability goals.

6. Conclusion

Artificial intelligence for composition–structure–property optimization of ferroelectric ceramics is a promising but demanding undertaking. The material class exhibits complex multi-scale physics, sensitive processing pathways, and conflicting property requirements. Machine learning can accelerate screening, guide experiments, and uncover non-intuitive design rules, but it cannot succeed as a disconnected predictive tool. It must be embedded in an architecture that integrates physical descriptors, uncertainty-aware models, multi-fidelity data, automated experimentation, and lifecycle assessment. The most valuable systems will combine human expertise with algorithmic search, allowing researchers to interrogate model reasoning and adapt to unforeseen physical behavior.

Infrastructure and governance are not peripheral concerns. Data standards, metadata, model documentation, and interoperable laboratory interfaces determine whether artificial intelligence can be reproduced, audited, and scaled. Sustainability and fairness require deliberate choices about objectives, access, and benefit-sharing. Policy should support open but secure data ecosystems, interdisciplinary training, and international cooperation while maintaining appropriate safety and environmental safeguards. Case illustrations such as barium titanate-based dielectrics, lead-free piezoelectrics, and aqueous tape casting for multilayer ceramic capacitors show that optimization is always entangled with manufacturing reality and regulatory context [13]. The field should therefore measure success not only by discovery speed or predictive accuracy but also by robustness, reproducibility, environmental performance, and equitable impact. Treated as a socio-technical capability, artificial intelligence can help transform ferroelectric ceramic development into a more efficient, transparent, and responsible enterprise.

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