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Machine Learning for Predicting Dielectric Energy-Storage Properties of Perovskite Oxides

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Abstract. Perovskite oxides with the ABO_3 structure are core candidates for dielectric energy-storage capacitors, whose recoverable energy density is governed by the dielectric constant, the breakdown field strength, and the nonlinear polarization response. This review surveys recent machine-learning studies on predicting these properties of oxide perovskites, covering three representative quantities—the dielectric constant, the breakdown field strength, and the ferroelectric Curie temperature—together with direct performance indicators such as recoverable energy density and efficiency. The works are compared along the evolution of methods, from manual descriptors and ensemble learning to graph neural networks, small-sample strategies, and generative inverse design, with dataset size, verification level, and accuracy documented. Three insights emerge: physical descriptor models remain competitive and interpretable under small-sample conditions; equivariant graph neural networks offer advantages for tensorial and finite-temperature tasks at higher data and computational cost; and generative inverse design is emerging, with preliminary success at the ferroelectric mesoscopic scale, but remains limited by scarce multimodal data and incomplete experimental-validation loops, which constitute the main challenges ahead.

Keywords: machine learning, perovskite oxides, dielectric energy storage, breakdown field strength, inverse design

1. Introduction

Perovskite oxides with the ABO_3 structure are compositionally flexible and have long been used in multilayer ceramic capacitors and energy-storage media. As devices miniaturize, the recoverable energy density has become the primary screening criterion, scaling with the dielectric constant and the square of the breakdown field for linear media and obtained from the polarization–electric field (P–E) loop for ferroelectrics and relaxors. Shen and Nan argued that, for ceramic and polymer dielectrics already close to their intrinsic limits, measured breakdown strengths leave limited room for further increases in E_b, making the improvement of εr and of relaxation behavior the more practical lever [1]. For bulk ceramics, however, measured E_b is often restricted by microstructural and defect conditions rather than an intrinsic ceiling [2]; here machine-learning-assisted optimization still has room to act.

Density functional theory (DFT) and density functional perturbation theory (DFPT) calculations provide dielectric tensors and soft-mode frequencies, a standard approach for analyzing the

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microscopic origin of dielectric response, but are computationally expensive. A- and B-site substitutions, multicomponent solid solutions, and varying composition ratios greatly expand the candidate space, making exhaustive computational and experimental screening challenging.

This paper organizes machine-learning work on oxide perovskite dielectric energy storage by method evolution: manual descriptors, graph neural networks, small-sample strategies, and generative inverse design. Section 2 defines the target properties, Section 3 follows this evolution, Section 4 discusses generative learning, and Section 6 concludes. Cross-dataset comparison remains difficult because data definitions and splitting protocols vary, while experimental validation is still limited for many predicted candidates.

2. Dielectric energy-storage properties and prediction challenges

This article focuses on dielectric energy-storage properties at two levels. At the level of direct performance indicators, the recoverable energy density W_{rec} and the efficiency η describe the overall storage capability, and the polarization parameters—maximum polarization P_{max}, remanent polarization P_r, and coercive field E_c—characterize the polarization–electric field (P–E) loop from which they are derived. At the level of key influencing quantities, three properties are most relevant. The static dielectric constant ε_r consists of an electronic contribution ε_∞ and an ionic contribution ε_{ion}; it sets the polarization level in the linear approximation but is hard to predict because the two contributions arise from different mechanisms. E_b determines the maximum working field and directly limits the recoverable energy density, but depends on the band gap and phonons and is modulated by grain boundaries and pores, with DFT values usually overestimating the experimental E_b severalfold. The ferroelectric Curie temperature T_c marks the ferroelectric–paraelectric phase transition; it sets the working temperature range but is highly sensitive to compositional perturbations and cation ordering. Actual energy-storage performance is set jointly by these quantities and the nonlinear P–E behavior, so ε_r alone cannot rank materials. Depending on the research objective, these properties can be addressed through regression, classification, or inverse-design approaches. Dielectric loss and frequency stability also matter, but the machine-learning literature on them is thinner, so this article does not elaborate.

3. Evolution of machine learning methods

3.1. Manual descriptors and ensemble learning

Shimano et al. treated dielectric prediction on 2,150 dynamically stable oxide structures as separate tasks. For the ionic contribution, the random forest reached $R^2 = 0.887$ on log(εion) under fourfold cross-validation, and $R^2 = 0.921$ on the electronic contribution ε∞; a SchNet graph convolutional network trained on the same log(εion) target reached $R^2 = 0.852$ under fivefold cross-validation, so the two models are compared on the same output. A three-class classifier based on the lowest optical phonon mode used three categories—$\omega opt^2 \leq 0$ (dynamically unstable), $0 < \omega opt \leq 2$ THz, and $\omega opt > 2$ THz—and achieved an accuracy of 0.885 [3]. Kim et al. predicted ε∞ and εion of ABO_3-type perovskites with LightGBM on 7,113 Materials Project structures plus 216 ABO_3 compounds, reaching combined R^2 of 0.79 and 0.67 [4].

In breakdown prediction, continuous regression and category screening differ. Li et al. used two-step XGBoost: first predicting the phonon cutoff frequency from features such as the band gap and lattice parameters ($R^2 = 0.854$), then using it as an intermediate descriptor to predict E_b ($R^2 = 0.872$). Trained on 209 DFT-verified perovskites, it screened 760 ABO_3 oxides from Materials Project and

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the Open Quantum Materials Database (OQMD), selecting $LaBO_3$, $AlBO_3$, and $LuBO_3$ [5]; the two-step design decouples stability from the breakdown upper limit. Sreedev et al. compiled 86 ABO_3 experimental samples and divided them into low, medium, and high classes according to $E_b < 250$, 250–1000, and >1000 MV/m; the 60 training samples had a distribution of 26:26:8, with the high-breakdown class underrepresented. The synthetic minority oversampling technique (SMOTE) balanced the minority class to 26:26:26 in feature space; applied only within the training folds of grid-search cross-validation, validation and test subsets never touched resampled data. The support vector machine (SVM) classifier reached macro precision/recall/F1 of 0.91, overall accuracy of 88%, and recall of 1.00 for the high-breakdown class [6].

Curie-temperature prediction emphasizes interpretability. Wang et al. collected over 280 experimental data points on lead-based piezoelectric ceramics, ranked and exhaustively screened feature combinations, and selected five features; after Bayesian tuning, the optimal gradient boosting regression (GBR) model reached $R^2 = 0.982$ on the test set, with Shapley additive explanations (SHAP) and partial-dependence plots revealing feature–T_c relationships [7]. Because the dataset comes from literature compilations with varying conditions, random splitting by composition tends to put formulations from the same family on both sides, overestimating extrapolation; the original authors also performed leave-one-system-out validation, with slightly increased error but still good predictive ability. The R^2 of 0.982 thus reflects in-distribution fitting, and predictions for entirely new formulation families still need verification. Another descriptor-to-experiment loop is Balachandran et al., who screened a new perovskite with $T_c = 898$ K in $BiBO_3$–$PbTiO_3$ and verified it experimentally [8]. A recent $BaTiO_3$-based high-entropy ceramic work closed the loop more completely: Pearson correlation screening reduced 12 physicochemical descriptors to four key features (configurational entropy ΔS, tolerance factor t, Pauling electronegativity (PEG), and B-site valence electron concentration); random forest was selected by leave-one-out cross-validation among six regression algorithms, and bootstrap resampling (1,000 times) built ensemble uncertainty. An expected-improvement (EI) acquisition function guided the screening of 110,000 candidate compositions, and the composition labeled 4A was identified after four iterative rounds, achieving $W_{rec} = 8.91$ J/cm³ and $\eta = 92.98\%$ at 600 kV/cm [9].

3.2. Graph neural networks and equivariant deep learning

Manual descriptors cannot fully capture tensorial properties or local-environment-sensitive defect behavior. Crystal graph neural networks (GNNs) treat atoms as nodes and neighboring bonds as edges, performing end-to-end regression and learning representations from the neighborhood structure; equivariant architectures further require outputs to transform with coordinate rotation, matching crystal space-group constraints. Kutana et al. trained two equivariant models from scratch, MACE for interatomic potentials and forces and Equivar for Born effective charges, on DFT molecular dynamics (MD) snapshots (178 $CaTiO_3$, 502 $BaTiO_3$, 191 $CaZrO_3$; PBEsol with Hubbard U). Five-fold cross-validation on $CaTiO_3$ gave a force R^2 of 0.9999 and a mean absolute error (MAE) of 0.0057 eV/Å. The dielectric tensor is not directly output: finite-field MD uses MACE for forces and Equivar for Born charges, computing the polarization and dielectric tensor and qualitatively reproducing the temperature dependence and phase transition of the $CaTiO_3$ tensor [10]. Compared with descriptor models, it delegates the structure-to-tensor link to the network at higher data and computational cost.

GNNs enhanced with persistent-homology features cut the MAE by 55% versus the original GNN in predicting defect formation energies of multi-substituted $BaTiO_3$ [11], and symmetry-aware

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equivariant convolutions distinguish the energies of different cation arrangements in the same material [12].

3.3. Small-sample handling strategies

Descriptor models train on hundreds of samples, whereas GNNs usually require thousands of structures, conflicting with scarce dielectric data. The scarcity has two sources: DFT tensor calculations and experimental characterization are slow, and public databases remain sparse in dielectric tensors and breakdown strengths. Three strategies address this: equivariant potentials trained from scratch and compared with foundation models pre-trained on Materials Project trajectory data [10]; persistent-homology features compressing local structural information [11]; and SMOTE synthesizing minority-class samples [6]. These paths start from knowledge transfer, representation compression, and distribution balancing, but no unified benchmark exists; different works choose their own splits and metrics, which is why the accuracies in Table 1 cannot be compared directly. Literature-compiled datasets often overlap in formulation; stratifying by data source, as Sreedev et al. did, alleviates leakage.

4. Generative learning and inverse design

Forward models answer "given a composition, predict a property," whereas inverse design requires "given a target property, generate a composition or microstructure." Park and Walsh fine-tuned a latent diffusion model with reinforcement learning, using creativity, thermodynamic stability, and diversity as multi-objective rewards to guide it beyond the training distribution toward new crystals [13]; joint inverse design of ε_r, E_b, and P–E loops for perovskite dielectrics has not yet been achieved, but the framework demonstrates feasibility. This study is therefore used here as a methodological reference rather than as direct validation of dielectric energy-storage performance.

For ferroelectrics, Liu et al.'s DeepMeso pushed generative modeling to the mesoscopic scale. High-throughput phase-field simulations generated 6,243 "3D microstructure–P–E loop" training pairs, the microstructure being a 32×32×32 voxelized polarization field and the loop a polarization curve over 400 electric-field steps. A three-dimensional convolutional neural network (CNN) trained as a surrogate for the phase-field simulation outputs the entire loop directly from the microstructure, with a mean R^2 of 0.973 on the 400-step polarization profiles (4,994 training, 1,249 test samples) and single-parameter accuracy above 99.6% for P_{max}, P_r, and E_c. For inverse design, a latent-space diffusion model based on a 3D U-Net with classifier-free guidance generates a 3D polycrystalline microstructure from the target loop or parameters; the frozen CNN surrogate predicts the loop in seconds for comparison, reaching a mean squared error (MSE) of 0.0497 and an R^2 of 0.9544 against the phase-field benchmark, with transferability verified on 63 ferroelectric systems [14]. The diffusion model always generates mesoscopic microstructures, not loops; the phase-field simulation appears only once, in the data-generation stage. The architecture separates the performance target from the microstructure, staying simulation-consistent until experimental validation; it turns experience-based regulation into a searchable generation problem. The remaining bottlenecks are scarce multimodal data, incomplete experimental-validation loops, and an unassessed gap between the surrogate model and real device performance.

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5. Comparative summary of representative works

This section summarizes the reviewed works along four dimensions—material system, predicted property, dataset size, and verification level. The purpose is overview rather than ranking: the studies differ in task type, data source, splitting scheme, and evaluation metric, so the accuracies in Table 1 cannot be compared directly.

Dataset scale and validation depth vary markedly across the reviewed studies. Descriptor and ensemble models often use tens to hundreds of experimental samples, whereas graph and surrogate models rely on thousands of calculated structures, molecular-dynamics snapshots, or simulated microstructures. Their reported metrics therefore answer different questions: random or repeated cross-validation mainly measures interpolation within a dataset, leave-one-system-out and cross-system tests provide a stronger test of transfer, and experimental synthesis offers the most direct confirmation but is available for only a few studies. High R^2 or low error on one split does not by itself establish extrapolation to new compositions, processing conditions, or device-scale behavior. References [12] and [13] demonstrate useful methods for crystal ordering and generation, but they do not directly validate dielectric energy-storage performance. Future comparisons should report data provenance, split strategy, uncertainty, and an external or experimental test wherever possible. Accordingly, external validation should be prioritized when assessing whether a model can support practical materials screening.

Table 1. Comparison of representative works

Material/system	Prediction target	Dataset size	Model	Key result	Validation
Stable oxides	ε_{ion} / ε_{∞}	2,150 DFT/DFPT	RF / SchNet	RF R^2 = 0.887/0.921; SchNet R^2 = 0.852	Cross-validation; DFT data [3]
Inorganic materials + ABO_3	ε_{∞} / ε_{ion}	7,113 MP + 216 ABO_3	LightGBM	Combined R^2 = 0.79/0.67	Repeated CV; DFT data [4]
ABX_3 perovskites	E_b	209 training + 760 candidates	Two-step XGBoost	ω: R^2 = 0.854; E_b: R^2 = 0.872	Held-out tests; computational screening [5]
ABO_3 perovskites	E_b class	86 experiments	SVM + SMOTE	Macro P/R/F1 = 0.91; high-class recall = 1.00	Stratified test; experimental data [6]
		>280 experiments	GBR + SHAP	Test R^2 = 0.982	Test set and leave-one-system-out [7]

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Table 1. (continued)

$BiBO_3$–$PbTiO_3$	T_c + stability	Tens of thousands of candidates	Classification + regression	T_c = 898 K	Active learning and synthesis [8]
$BaTiO_3$ high-entropy ceramics	W_{rec} + η	65 initial; 110,000 candidates	RF + EI	W_{rec} = 8.91 J/cm³; η = 92.98%	LOOCV, active learning, synthesis [9]
$CaTiO_3$/$BaTiO_3$/$CaZrO_3$	Finite-temperature dielectric tensor	178/502/191 MD snapshots	MACE + Equivar	Force prediction: R^2 = 0.9999, MAE = 0.0057 eV/Å; dielectric-tensor temperature dependence qualitatively reproduced	Five-fold CV; DFT/MD benchmark [10]
Multi-substituted $BaTiO_3$	Defect formation energy	~7,700 O vacancies	GNN + persistent homology	MAE reduced by 55%	Random split; DFT benchmark [11]
Multicomponent crystals	Cation-ordering energy	High-throughput DFT	Equivariant GCNN	Distinguishes inequivalent orderings	Methodological reference; not direct energy-storage validation [12]
General crystals	Inverse crystal design	DiffCSP benchmark	RL + latent diffusion	Multi-objective rewards	Methodological reference; not direct energy-storage validation [13]
Ferroelectric mesostructures	P–E loop / microstructure	6,243 pairs; 63 systems	3D CNN + diffusion	Surrogate R^2 = 0.973; generation MSE = 0.0497, R^2 = 0.9544	Cross-system phase-field benchmark [14]

Note: RF, random forest; CV, cross-validation; LOOCV, leave-one-out cross-validation; MD, molecular dynamics; MSE, mean squared error; MP, Materials Project; RL, reinforcement learning; GCNN, graph convolutional neural network; DFT, density functional theory; DFPT, density functional perturbation theory; SVM, support vector machine; SMOTE, synthetic minority oversampling technique; GBR, gradient boosting regression; SHAP, Shapley additive explanations; EI, expected improvement; GNN,

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graph neural network; CNN, convolutional neural network; MAE, mean absolute error; P/R/F1, precision/recall/F1-score. R^2, accuracy, F1, and MAE describe different tasks and data sources and cannot be compared directly.

6. Conclusion

This paper presents three main findings on machine-learning prediction of dielectric energy-storage properties of oxide perovskites. First, under small-sample conditions, physical descriptor models remain practical and competitive: they encode prior chemical and structural knowledge into low-dimensional features, train on a few hundred samples, and, with interpretation tools such as SHAP, their predictions can be understood and audited. Second, for tasks that involve tensorial responses, finite-temperature behavior, or defect-sensitive local environments, equivariant graph neural networks offer advantages over manual descriptors, because they learn structure–property relations end to end and respect crystal symmetry; these advantages, however, come at higher cost in data, computation, and interpretability, so descriptor models remain a reasonable starting point when datasets are scarce. Third, generative inverse design remains in an early stage: latent diffusion and reinforcement-learning frameworks have shown feasibility for crystals and mesoscopic microstructures, yet scarce multimodal data, incomplete experimental-validation loops, and the absence of a unified benchmark still constrain the field. The reviewed works differ substantially in data sources, splitting schemes, and evaluation indicators, so their reported accuracies cannot be ranked directly; Table 1 documents these differences rather than asserting a performance order. Future work should move toward shared benchmarks and standardized metrics, curated open datasets covering dielectric tensors and breakdown data, closed-loop designs in which generative models propose candidates and experiments verify them, and systematic assessment of surrogate-model fidelity before deployment across distinct material systems. Only with such foundations in place can machine learning translate into a dependable tool for accelerated discovery of energy-storage dielectrics.

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