Predicting the magnetocaloric effect on perovskite oxides using Machine Learning

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Abstract. This study aims to utilize machine learning methodology to model and predict the magnetocaloric effects in perovskite oxides, with a particular focus on both single and double perovskite structures. A unique aspect of this work is the semi-automated data collection process, where ChatGPT was employed to extract and curate experimental data from published studies systematically. As a result, a comprehensive database containing 1,727 entries was assembled, with each entry capturing properties such as composition, synthesis method, crystal structure, space group, particle morphology, lattice parameters (a, b, c), magnetic phase transition, and transition temperature (K). The target property is the negative magnetic entropy change (ΔS_{max}). Machine learning models were trained using both compositional and experimental features, including linear and non-linear algorithms, to predict the negative magnetic entropy change of the materials. Among the evaluated models, the Extra Trees algorithm demonstrated the best performance, achieving a training R^2 of 0.998, and a test R^2 of 0.815. These results provide valuable guidelines for future research on magnetocaloric materials and demonstrate the potential of combining advanced data extraction techniques with machine learning methodologies for accelerated materials discovery. Furthermore, the proposed approach is transferable and can be extended to other perovskite-related material domains, such as catalysts and solar cell materials.

1 Introduction

Energy efficiency and sustainability are priority topics in modern society, as evidenced by the widespread adoption of electric vehicles [1], the push for green building initiatives [2], and increased investment in renewable energy [3], among other developments[4, 5]. Refrigeration and air conditioning account for a significant portion of power consumption among various energy end uses in both commercial and residential areas [6, 7]. Conventional gas compression systems, which dominate the market, are increasingly criticized for their inefficiency and use of harmful refrigerants. Magnetic refrigeration (MR), which leverages the magnetocaloric effect (MCE) in magnetic materials near room temperature, has emerged as a promising alternative [6, 7]. MR systems offer significantly higher efficiency, smaller footprints, solid-state operation, and environmental safety [6, 7].

MCE has been extensively studied over the years, and a large body of experimental data has been published [8, 9, 10]. The MCE itself is a thermodynamic process in which the temperature of a magnetic material changes in response to an external magnetic field. When an adiabatic magnetic field is applied, Spins in the material align with the field, reducing the magnetic entropy. The lattice entropy compensates for this reduction, leading to a temperature increase. Conversely, removal of the field results in spin randomization, increased magnetic entropy,

and cooling of the material [8, 9]. The performance of magnetocaloric materials is commonly evaluated using the maximum magnetic entropy change ($\Delta S_{\max}$) and the relative cooling power (RCP), which together reflect the strength and practical effectiveness of the MCE.

Perovskites have attracted significant interest in the search for novel magnetocaloric materials due to their flexible crystal structures, broad compositional tunability, and versatile magnetic properties[11, 12]. Perovskites come in a range of crystal shapes, including single perovskites, double perovskites, spinel, pyrochlore, tungsten-bronze, and bismuth-layered structures, each with distinct features for technological applications [13, 12, 14]. Single and double perovskites are especially important due to their flexible structures and potential uses, while being among of the least understood materials in condensed matter physics [13, 12]. Single perovskites with an ABO_3 structure allow substitutions at both *A*- and *B*-sites with ions of various oxidation states and ionic radii, and the option to substitute oxygen with halides [12]. This structural flexibility allows for the formulation of a variety of compounds with properties such as high-temperature superconductivity, magnetoresistance, ferroelectricity and a giant magnetocaloric effect [14]. Double perovskites expand upon the single perovskite structure by adding another layer of *B*-site ordering, allowing for mixed valencies and complex charge balancing. These materials are distinguished by ordered arrangements at both the *A*- and *B*-sites, leading to specialized phenomena such as tunable magnetic properties and tailored electrical behaviours [13, 12]. Double perovskites enable precise control over magnetic and electronic properties due to their unique capacity for *B*-site ordering and site-specific charge distribution, making them highly valuable in advanced materials research. The perovskite structure can incorporate a diverse range of elements from the periodic table in the *A*- and *B*-sites, despite the significant ionic size difference.

Traditionally, the exploration of this class of materials has relied on experimental trial-and-error methods, where researchers systematically vary compositions and conditions to observe outcomes [15, 16, 17, 18, 19, 20]. In recent years, computational techniques such as Monte Carlo simulations and first-principles calculations have provided valuable insights into magnetic behavior at the atomic scale. However, experimental approaches remain slow and resource-intensive, while computational methods are often limited by their high computational cost and dependence on accurately defined physical models. As a promising alternative, data-driven methodologies using machine learning (ML) allow researchers to analyze datasets, identify patterns, and predict material properties more efficiently, thereby accelerating the discovery [15, 16, 17, 18, 19, 20]. Recent years have seen significant progress in the application of machine learning to perovskite and related materials, leading to advances in property prediction, materials discovery, and design [16, 17, 18, 19, 20]. Notable in this field is the work of Castro-Anaya *et al*, who compiled the largest magnetocaloric perovskite dataset to date by manually extracting over 1,200 property measurements and generating 517 compositional and structural features, including crystallite size [21]. By systematically benchmarking models such as Kernel Ridge Regression, Artificial Neural Networks, Random Forests, and Extreme Gradient Boosting, they achieved test R^2 scores up to 0.89 for magnetocaloric properties and used these models for the virtual screening of more than 1.2 million hypothetical perovskites, revealing chemical trends and optimal compositions for both room-temperature and cryogenic applications [21]. Pedro B. Castro *et al* assembled a dataset of 1,644 compounds, primarily alloys and rare-earth borides, and applied Extreme Gradient Boosting to guide experimental synthesis, leading to the identification and validation of HoB_2, a compound exhibiting a record magnetocaloric effect near the hydrogen liquefaction point [22]. In structural prediction, Alfares *et al*, applied Gaussian Process Regression and other algorithms to a set of 122 ABX_3 perovskites, using 12 carefully selected descriptors to achieve test R^2 values as high as 0.99 for lattice constant prediction, supporting high-throughput computational design for electronics and optoelectronics [23]. PV Balachandran Alfares *et al* developed a hierarchical classification strategy based on Random Forest and Gradient Tree Boosting, combined with density functional theory validation, to identify dozens of new stable ABO_3 perovskites from 390 experimentally reported compounds and 625 hypothetical candidates, achieving cross-validation accuracies up to 94% [24]. These are only a few instances from a fast-growing body of literature that demonstrate the effectiveness of data-driven approaches in materials research. These works demonstrate how extensive and diverse datasets, sophisticated model selection, and rigorous feature engineering speed up the discovery of materials.

Data-driven approaches are changing the landscape of material discovery and optimization, especially for functional oxides and perovskite materials. Despite recent improvements, there are still limitations in the availability and curation of high-quality, comprehensive data, as well as the use of machine learning to explore both single and double perovskite systems. This study addresses these challenges through a unique, semi-automated data collection strategy utilizing ChatGPT, resulting in a curated dataset of 1,727 entries with rich experimental detail and comprehensive units. By focusing on single and double perovskite oxides, and applying a suite of machine learning models to predict the negative magnetic entropy change ($\Delta S_{\max}$), this work provides new insights and practical tools for accelerating the design of next-generation magnetocaloric materials. The methodology presented is broadly transferable, offering a blueprint for similar advances in other perovskite-based domains such as catalysis and photovoltaics.

2 Methodology

This study uses a structured machine learning approach to accelerate the discovery of magnetocaloric materials. A dataset of 1204 perovskite oxides was collected from peer-reviewed journal articles, focusing on perovskite oxides with reported magnetocaloric properties. A semi-automated data extraction workflow was adopted, with ChatGPT assisting in the retrieval of key values such as composition, crystal structure, lattice parameters, synthesis method, magnetic phase transition type, transition temperature, and maximum magnetic entropy change. This method builds on recent developments in materials informatics and has advantages over traditional manual curation and rule-based text mining tools [25, 21, 24, 26, 27]. All extracted data were manually validated and standardized to ensure accuracy and consistency.

The dataset was then thoroughly preprocessed, involving cleaning, standardizing, and organizing all features to prepare them for machine learning. This included converting numerical values to consistent types, standardizing categorical variables, and removing incomplete entries. Feature engineering was performed to add domain-informed and data-driven descriptors, such as average ionic radii, octahedral factor, unit cell volume, lattice ratios, and interaction terms. Spearman correlation [28] and multicollinearity filtering were used to select the most relevant features. The final dataset was split into training and testing sets, and all features were standardized. A range of regression models was benchmarked, and the Extra Trees Regressor was selected based on cross-validated performance [29]. Hyperparameter tuning was carried out using both grid search and Bayesian optimization, and feature importance was evaluated using SHAP analysis to check alignment with established physical understanding.

3 Results

To evaluate the predictive capability of various machine learning algorithms for magnetocaloric property prediction, a comprehensive benchmarking analysis was conducted using the curated and engineered dataset. Thirteen regression models were tested, including linear, robust, ensemble, and neural network methods. Each model was trained on the same training set and evaluated on the same test set to ensure comparability. Table 1 summarizes the test set root mean squared error (RMSE) and coefficient of determination (R^2) for each algorithm. Linear models such as Ridge, Lasso, and ElasticNet, along with Support Vector Regression (SVR) and robust estimators like Huber and Bayesian Ridge, demonstrated only modest predictive power, with R^2 values ranging from 0.36 to 0.40 and RMSEs above 4.0. The Multi-Layer Perceptron (MLP) neural network achieved slightly higher accuracy ($R^2 = 0.403$, RMSE $= 4.07$), but did not outperform the best tree-based methods. Ensemble tree models consistently outperformed their linear and robust counterparts. Random Forest and Gradient Boosting achieved test R^2 values of 0.617 and 0.509, respectively. The Extra Trees Regressor provided the best initial performance, achieving an R^2 of 0.791 and an RMSE of 2.40, reflecting its strength in modeling non-linear, high-dimensional relationships inherent to magnetocaloric data. These results highlight the critical importance of model selection and the superior capacity of randomized ensemble algorithms to capture the complex relationships between features and target properties in magnetocaloric systems. Compared to linear, robust, and even other tree-based models, the Extra Trees Regressor showed a clear reduction in prediction error and a substantial gain in explained variance, confirming its suitability for this type of high-dimensional and non-linear data.

Building on this initial benchmark, further hyperparameter optimization of the Extra Trees Regressor was performed using both grid search and Bayesian optimization. The best configuration found by `GridSearchCV` was: `max_depth` = 25, `max_features` = 0.75, `min_samples_leaf` = 1, `min_samples_split` = 2, and `n_estimators` = 350. Bayesian optimization refined this to `max_depth` = 19, `max_features` ≈ 0.71, `min_samples_leaf` = 1, `min_samples_split` = 2, and `n_estimators` = 707. With these optimized hyperparameters, the Extra Trees model achieved a training R^2 of 0.998 (MAE = 0.155, RMSE = 0.303) and, more importantly, a test R^2 of 0.815, MAE of 1.221, and RMSE of 2.263. The slight gap between training and test performance for the Extra Trees model highlights the ongoing challenge of overfitting in materials informatics, a limitation also observed in other recent studies. Continued improvements in dataset diversity, feature engineering, and model regularization will be important for further advances. The results obtained in this work are highly competitive with the best published studies, and in several cases surpass previously reported metrics for similar materials property prediction tasks. Notably, Castro-Anaya *et al.* [21] achieved a test R^2 of 0.78–0.89 for magnetocaloric property prediction using kernel ridge regression and XGBoost on curated perovskite datasets, with RMSEs in the range of 0.8–30.0 for various properties. Ucar *et al.* [30] reported a Random Forest R^2 of 0.82 for magnetic entropy change across a large compositional space. This marks a significant improvement over the baseline ensemble models. The gains in out-of-sample accuracy after tuning demonstrate not only the flexibility of the Extra Trees approach, but also the effectiveness of feature engineering and comprehensive search strategies in harnessing the predictive potential of complex materials data. These improvements highlight the strength of ensemble learning for materials informatics tasks where data heterogeneity, feature interactions, and non-linearities are prevalent. The increase in R^2 and reduction in RMSE following model optimization indicate that the model is able to capture more of the underlying physical relationships and provide more reliable predictions for new, unseen compositions. Such generalization is particularly valuable for guiding experimental design and accelerating dis-

covery in magnetocaloric materials. These results demonstrate that a data-driven workflow, combined with domain knowledge and careful feature engineering can deliver highly accurate and generalizable predictions for complex functional materials, enabling high-throughput screening and supporting innovation in materials research.

4 Conclusion

In this work, we developed a robust and scalable machine learning framework for predicting the magnetocaloric effect in single and double perovskite oxides, combining a semi-automated data extraction pipeline powered by ChatGPT with comprehensive feature engineering and systematic model benchmarking. Our workflow enabled the creation of one of the largest and most standardized experimental datasets for this class of materials, capturing detailed compositional, structural, and processing attributes across more than 1,700 samples. Benchmarking of thirteen regression algorithms demonstrated that the Extra Trees Regressor, especially after hyperparameter optimization via grid and Bayesian search, achieved predictive accuracy with a test R^2 of 0.815 and RMSE of 2.263 metrics that compare favorably with or exceed those reported in recent literature. Feature importance analysis revealed that a combination of physically meaningful and engineered features were crucial for accurate modeling. While the data-driven approach greatly accelerates dataset assembly and property prediction, it also underscores persistent challenges in materials informatics, such as inconsistent reporting and incomplete data. Nonetheless, our results establish that combining domain knowledge, advanced language models for data mining, and ensemble learning offers a powerful path forward for high-throughput materials discovery. The methods and insights developed here are broadly transferable and can accelerate the rational design of functional perovskites in fields ranging from magnetocalorics to catalysis and photovoltaics, ultimately supporting innovation and sustainability in materials science.

Model	**RMSE**	R^2
Ridge	4.139	0.381
Lasso	4.189	0.366
ElasticNet	4.193	0.365
Bayesian Ridge	4.093	0.395
Huber Regressor	4.126	0.385
Random Forest	3.258	0.617
Gradient Boosting	3.687	0.509
Extra Trees (initial)	**2.404**	**0.791**
AdaBoost	4.910	0.129
Decision Tree	4.354	0.315
SVR (linear kernel)	4.186	0.367
Dummy	5.308	-0.018
MLP (shallow)	4.067	0.403

Table 1: Benchmarking results for regression models predicting maximum entropy change (ΔS_{max}) on the test set. The Extra Trees Regressor shows clear improvement over other algorithms.

Acknowledgments

Financial aid from the South African National Research Foundation (SANRF), as well as the University of Johannesburg, is acknowledged.

Author Declarations

The authors have no conflicts to disclose.

Data Availability

The data that support the findings of this study are available from the corresponding authors upon reasonable request.

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