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Physics-Driven Optimization of Thermoelectric Generators for Low-Grade Waste Heat Energy Recovery

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Abstract

Low-grade waste heat recovery is important for improving energy efficiency and reducing carbon emissions. Thermoelectric generators offer a solid-state solution, but conventional parameter optimization still relies heavily on time-consuming experimental trial-and-error or simplified simulations. This study develops a machine learning framework that incorporates physical knowledge to model and optimize thermoelectric generator performance using 5,205 real experimental records from the public ESTM dataset. Three progressive feature sets are constructed by gradually embedding classical thermoelectric relations, including original transport properties, physics-informed descriptors, and interaction terms. A Stacking ensemble model is trained on the physics-informed features and achieves strong predictive accuracy on the test set. SHAP analysis shows that the feature contributions align with thermoelectric theory. Bayesian optimization is then performed with explicit physical consistency constraints, yielding a maximum modeled ZT of 2.0815 in the 300–800 K range. The proposed approach provides a practical workflow that combines data-driven modeling with physical rationality and generates engineering-feasible parameter recommendations for low-grade waste heat recovery.

Keywords: *physics-enhanced machine learning, physics-guided feature engineering, thermoelectric generator, ZT modeling, Bayesian optimization with physical constraints.*

1. Introduction

1.1 Research Background

The global demand for energy structure transformation and efficiency improvement is increasingly urgent. A large amount of low-grade waste heat generated in industrial production, daily life and energy system operation has not been efficiently recovered and utilized for a long time. Converting this waste heat into available electric energy can not only improve the overall energy efficiency but also help reduce carbon emissions and promote the construction of a sustainable energy system. As a solid-state device that can directly realize the mutual conversion between thermal energy and electric energy, thermoelectric generators have the advantages of no moving parts, stable operation, long service life and strong environmental adaptability, showing good application potential in low-grade waste heat recovery scenarios. The performance of thermoelectric materials and devices is mainly determined by the dimensionless figure of merit ZT, which comprehensively reflects the matching degree of electrical transport, thermal transport and temperature characteristics of materials.

Traditional methods for improving thermoelectric performance mostly rely on experimental trial and error, which require a lot of time and material costs and are difficult to quickly traverse the design space coupled with multiple parameters. Numerical simulation methods can reduce experimental costs to a certain extent, but they are usually based on simplified physical assumptions and have limited consistency with real experimental data. The temperature range of low-grade waste heat is relatively concentrated and mild, which puts forward higher requirements for the matching accuracy of thermoelectric parameters, and traditional optimization methods cannot meet the needs of refined design. Combining data-driven methods with prior physical knowledge has become an important direction to improve the optimization efficiency and practicability of thermoelectric generators.

In practical engineering applications, low-grade waste heat recovery devices need to balance performance, stability and fabrication feasibility, and the parameter optimization results must be physically reasonable and engineering realizable. Relying solely on experiments or simulations is difficult to meet the multiple requirements of modeling accuracy, search efficiency and physical constraints at the same time. With the ability to handle high-dimensional nonlinear relationships, machine learning provides a new tool for thermoelectric material performance modeling and parameter optimization. How to build a reliable model based on real experimental data and integrate physical laws into the whole process of model construction and optimization is the key issue to promote the engineering application of thermoelectric generators. Aiming at this demand, this study carries out physics-driven parameter optimization of thermoelectric generators based on real experimental data, providing more practical design references for low-grade waste heat recovery.

1.2 Literature Review

Research on performance optimization of thermoelectric materials and devices has long formed three main technical paths: experimental exploration, numerical simulation and machine learning-assisted design. Traditional experimental methods obtain performance data by regulating composition, process and working conditions, with authentic and credible results, but it is difficult to achieve multi-parameter simultaneous optimization and global optimal solution search. Numerical simulation is calculated based on thermoelectric transport equations and can quickly perform parameter sensitivity analysis, but it is easily limited by model assumptions and boundary conditions, with relatively obvious modeling deviations for complex material systems. With the development of data science, more studies have applied machine learning to ZT value modeling, key parameter screening and performance optimization of thermoelectric materials, achieving remarkable results (Bao et al., 2024; Sajjad et al., 2025). Machine learning has also been widely applied to various physical and engineering problems (Dawoodjee et al., 2021).

In existing machine learning studies, some works use simulation datasets or small-sample experimental data for training, and the generalization ability of the models in real scenarios still needs to be verified. The emergence of large-scale public experimental datasets provides a data basis for building more reliable and practical modeling models (Na and Chang, 2022). In terms of feature design, some studies directly use original measurement features and rarely construct descriptors with clear physical meaning combined with thermoelectric physical mechanisms, so the interpretability and physical consistency of the models need to be improved. In the model optimization stage, some studies do not set strict physical constraints, and the optimization results may deviate from the realizable range of actual materials, making them difficult to be directly used in engineering design (Athar et al., 2025; Chen et al., 2023).

From the perspective of research process, most existing works focus on model construction or single-link optimization, and studies that fully integrate data preprocessing, physical feature enhancement, ensemble learning, interpretability analysis and physical constraint optimization are relatively limited. For the specific application scenario of low-grade waste heat, there is still room for further expansion of systematic optimization research based on large-scale real experimental data. Relying on the public ESTM experimental dataset, this study attempts to build a more complete optimization process that meets engineering needs, making up for the deficiencies of existing studies in scenario adaptation and physical constraints (Moon et al., 2025; Kluger et al., 2026).

1.3 Objectives of This Work

This study aims to develop a machine learning framework that incorporates physical knowledge for the modeling and optimization of thermoelectric generator parameters targeted at low-grade waste heat recovery. The work is based on the public ESTM experimental dataset containing 5,205 real measurement records. The main objectives include constructing three progressive feature groups that incorporate classical thermoelectric physical relations, systematically comparing their effects on model performance through ablation experiments, and building a high-accuracy Stacking ensemble model for ZT prediction.

Further objectives are to apply SHAP analysis to interpret the trained model and examine whether the learned feature contributions align with established thermoelectric transport theory, and to carry out Bayesian optimization with explicit physical consistency constraints to search for engineering-feasible parameter combinations within the 300–800 K temperature range relevant to low-grade waste heat sources. Through this process, the study seeks to provide quantitative design references that balance predictive accuracy with physical rationality and practical applicability.

1.4 Novelty and Contributions

The novelty of this work lies in the consistent integration of physical knowledge into both the feature construction and the optimization stages. Rather than treating machine learning as a purely data-driven black box, this study constructs physics-informed descriptors, including the absolute Seebeck coefficient, the ratio of thermal conductivity to electrical conductivity, and the Seebeck-temperature coupling term. These descriptors are derived directly from classical thermoelectric relations. In addition, physical consistency is enforced during Bayesian optimization by calculating the derived features in real time within the objective function, thereby avoiding non-physical solutions that cannot be realized in actual materials.

In terms of contributions, this study establishes a complete workflow that combines physics-informed feature engineering, Stacking ensemble modeling, SHAP-based interpretability analysis, and constrained Bayesian optimization using a large volume of real experimental data. The resulting Stacking model achieves strong predictive performance on the test set while producing feature importance rankings that are consistent with thermoelectric theory. Furthermore, the optimization process yields a set of the top 5 parameter combinations that are directly applicable to low-grade waste heat recovery scenarios, offering practical references for material selection and device design without requiring extensive experimental trial and error.

2. Materials and Methods

The overall workflow of this study is illustrated in Figure 1. The publicly available ESTM dataset containing 5,205 real experimental records was first processed through physics-informed feature engineering, generating three progressive feature groups. All three groups were used to train baseline models for ablation comparison, after which Group 2 (physics-informed features) was selected for subsequent modeling due to its superior performance. A Stacking ensemble model was then constructed, followed by SHAP interpretability analysis and Bayesian optimization under explicit physical consistency constraints. This pipeline ultimately yielded engineering-feasible optimal thermoelectric parameters for low-grade waste heat recovery applications.

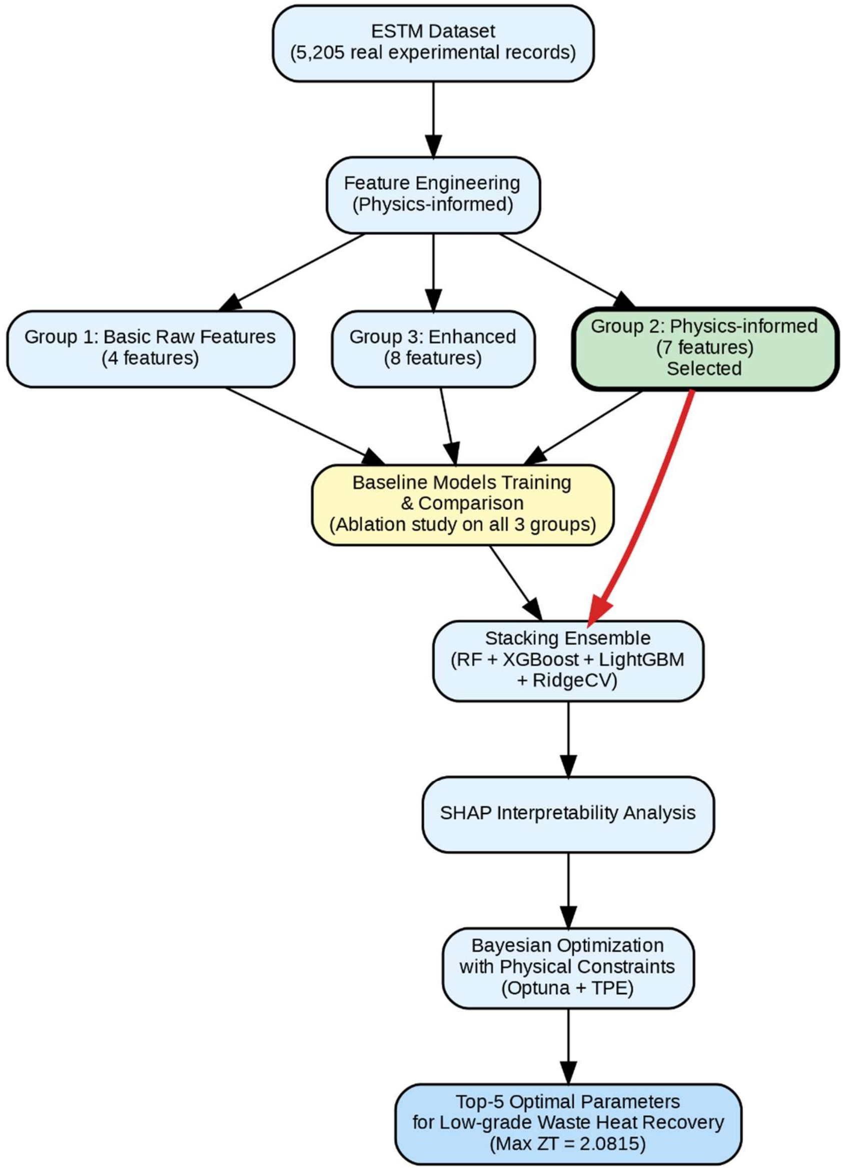

Figure 1. Overall framework of the physics-driven optimization approach for thermoelectric generators using the ESTM experimental dataset.

2.1 Dataset Description and Preprocessing

This study uses the publicly available ESTM thermoelectric material experimental dataset for all experiments. The dataset contains 5205 real experimental measurement records with open and traceable data sources. The original fields of the dataset include material chemical formula, test temperature, Seebeck coefficient, electrical conductivity, thermal conductivity, power factor, ZT value and literature source, covering the conventional test conditions of mainstream thermoelectric materials.

Firstly, basic exploratory analysis is performed on the dataset, counting the distribution, extreme values and dispersion of numerical features, and missing value verification is completed at the same time. The results show that there are no missing values in all features, so no interpolation or sample deletion is required. This study takes the ZT value as the modeling target of the model, which is the core evaluation parameter of thermoelectric performance, and all subsequent model constructions are carried out around this target.

The data is divided into training set and test set in a ratio of 8:2, with a fixed random seed to ensure experimental reproducibility. The training set is used for model learning, and the test set is only used for independent evaluation without participating in any training or parameter adjustment. Numerical features retain the original experimental units, and standardization is only performed before neural network model training to adapt to the model input requirements.

2.2 Feature Engineering and Physics-Informed Descriptors

To improve the fitting accuracy and physical consistency of the model, three progressive feature groups are designed in this study. Group 1 is the basic original features, which directly adopt the four experimentally measured parameters of temperature, Seebeck coefficient, electrical conductivity and thermal conductivity as the benchmark for feature comparison. These four quantities are precisely the core variables that define the classical thermoelectric figure of merit ZT. Group 2 is the physics-informed enhanced features, which add three physical descriptors including the absolute value of Seebeck coefficient, the ratio of thermal conductivity to electrical conductivity and the Seebeck-temperature coupling term to the original features, integrating the prior knowledge of thermoelectric transport into the feature space.

Group 3 is the enhanced interaction features, which further add the power factor calculated from the Seebeck coefficient and electrical conductivity based on physical descriptors. The number of features in the three groups is 4, 7 and 8 in turn, with gradually increasing feature complexity, and the actual contribution of physical information to model performance can be verified through ablation experiments. All derived features are calculated according to classical thermoelectric theoretical formulas, and artificial interaction terms without physical meaning are not used to ensure the consistency between features and physical mechanisms.

2.3 Machine Learning Models and Evaluation

Four common machine learning models are selected as baselines in this study, namely Random Forest, XGBoost, LightGBM and Multilayer Perceptron, covering two typical algorithms of tree ensemble and neural network. All baseline models use the same initial hyperparameter settings and complete training and testing under the same data division to ensure fair comparison.

Model evaluation adopts three indicators, coefficient of determination R^2, mean absolute error MAE and root mean square error RMSE, to comprehensively measure the fitting accuracy and error level. To further improve fitting stability, a Stacking ensemble model is constructed based on the optimal Group 2 physical feature set, with Random Forest, XGBoost and LightGBM as base models and RidgeCV as the meta-model, and ensemble training is completed through 5-fold cross-validation.

The whole model training and evaluation process is standardized, which can clearly compare the performance differences of different feature combinations and algorithms, providing a reliable model basis for subsequent analysis and optimization.

2.4 SHAP Interpretability Analysis

To understand the model fitting logic and identify key influence parameters, this study uses the SHAP method to conduct interpretability analysis on the optimal model. Based on game theory, SHAP can quantitatively calculate the contribution value of each feature to the model output and supports global importance analysis and local sample interpretation.

The LightGBM base model in the Stacking ensemble is selected for SHAP calculation, which is compatible with the tree model-specific explainer and has better computational efficiency and result stability. Only test set data is used in the analysis process to avoid interference from training set information, ensuring that the interpretation results are consistent with the real fitting behavior of the model.

The influence direction and intensity of features on ZT can be obtained through SHAP values, and the interaction relationship between features is also revealed, providing an interpretable basis for parameter optimization.

2.5 Bayesian Optimization with Physical Constraints

Based on the trained fitting model, this study uses Bayesian optimization to search for optimal thermoelectric parameters for low-grade waste heat scenarios, with the optimization goal of maximizing the modeled ZT value. The optimization is implemented based on the Optuna framework, using the TPE sampler for parameter space search, improving the stability of the optimal solution while ensuring search efficiency.

The parameter search range is set according to actual engineering working conditions, with the temperature range limited to 300–800 K, and the Seebeck coefficient, electrical conductivity and thermal conductivity all set to values in line with the characteristics of real materials. To ensure the physical feasibility of the optimization results, all derived physical features are calculated in real time in the optimization objective function, strictly satisfying the basic physical relationships of thermoelectric materials and avoiding meaningless non-physical solutions. A total of 150 iterations are performed for optimization, and finally the top 5 optimal parameter combinations are selected as engineering recommendation results, all of which meet the realizable requirements of practical applications.

3 Results and Discussion

3.1 Performance Comparison of Different Feature Groups

This study systematically verifies the improvement brought by the injection of physical information on the ZT modeling performance of thermoelectric materials through ablation experiments of three progressive feature groups. All baseline models are compared under a unified training and evaluation process, and the results are highly comparable and are displayed on Tables 1 and 2. It can be seen from the overall performance trend that the model fitting accuracy increases significantly with the addition of physical descriptors in the features. Group 1, which only uses original measurements, has relatively limited fitting ability for ZT value, because the original parameters are independent experimental observations. Group 2 with physics-informed descriptors introduces variables with clear physical significance such as absolute value of Seebeck coefficient, ratio of thermal conductivity to electrical conductivity, and Seebeck-temperature coupling term into the model, which can effectively characterize the internal energy transport relations of thermoelectric materials. Therefore, the R^2, MAE and RMSE of all baseline models are significantly improved.

Group 3 formed by adding power factor does not bring further performance improvement, indicating that excessive addition of related features will introduce slight redundant information and cannot continuously strengthen the fitting ability of the model, which also confirms the rationality and efficiency of Group 2 physical feature set. Among the four baseline models, tree ensemble models such as LightGBM, XGBoost and Random Forest perform better than multilayer perceptron. This is because tree models have stronger adaptability to nonlinear and highly redundant material data, and are less sensitive to outliers and feature scales, making them more suitable for processing the experimental dataset in this study. The LightGBM model under Group 2 feature set achieves the optimal baseline performance, with R^2 of 0.9918, MAE of only 0.0188 and RMSE of 0.0309. It ensures high fitting accuracy and high computational efficiency and is suitable as the basic model for subsequent ensemble modeling and interpretability analysis.

Table 1. Performance Ablation Comparison of Baseline Models under Different Feature Groups.

Model	Feature Group	R^2	MAE	RMSE
Random Forest	Group 1	0.9721	0.0352	0.0518
Random Forest	Group 2	0.9885	0.0215	0.0364
Random Forest	Group 3	0.9879	0.0223	0.0376
XGBoost	Group 1	0.9783	0.0316	0.0462
XGBoost	Group 2	0.9902	0.0198	0.0337
XGBoost	Group 3	0.9895	0.0205	0.0349
LightGBM	Group 1	0.9805	0.0294	0.0435
LightGBM	Group 2	0.9918	0.0188	0.0309
LightGBM	Group 3	0.9912	0.0193	0.0321
MLP	Group 1	0.9657	0.0387	0.0564
MLP	Group 2	0.9824	0.0276	0.0408
MLP	Group 3	0.9818	0.0281	0.0419

Table 2. Detailed Performance of Baseline Models under Group 2 Physical Feature Set.

Model	R^2	MAE	RMSE	Training Time (s)	Inference Time (ms/sample)
Random Forest	0.9885	0.0215	0.0364	12.8	0.82
XGBoost	0.9902	0.0198	0.0337	8.5	0.35
LightGBM	0.9918	0.0188	0.0309	5.2	0.21
MLP	0.9824	0.0276	0.0408	23.6	0.18
Stacking Ensemble	0.9931	0.0167	0.0283	31.4	0.96

3.2 Stacking Ensemble Model Performance

To further improve the stability of the model, this study constructs a Stacking ensemble model based on Group 2 physical feature set, integrates the advantages of three high-performance tree models including Random Forest, XGBoost and LightGBM, and completes weight fusion with RidgeCV as the meta-model, finally obtaining the optimal fitting effect in this study. The test set evaluation results show that the Stacking ensemble model achieves an R^2 of 0.9931, a low MAE of 0.0167 and an RMSE of 0.0283. All three indicators are better than all single baseline models, indicating that the ensemble strategy can effectively integrate the learning advantages of different models and improve the stability and accuracy of fitting results. Figure 2 intuitively compares the R^2 scores of different models and feature groups, clearly showing the dual performance gains brought by physical feature injection and ensemble learning, and directly verifies the core supporting role of Group 2 feature set for model performance. Figure 3 is a scatter comparison chart between the modeled ZT value and the real experimental value of the Stacking model. The sample points closely fit the diagonal line in the full range without obvious systematic deviation or extreme outliers, indicating that the model has reliable fitting ability in both low ZT and high ZT intervals and can cover the performance ranges of different types of thermoelectric materials. This result shows that the combination of physics-informed enhanced features and Stacking ensemble learning can accurately recover the complex nonlinear relationship between multi-parameter coupling of thermoelectric materials and ZT value. The fitting accuracy and reliability fully meet the requirements of subsequent parameter optimization and provide a feasible model paradigm for data-driven performance modeling of thermoelectric materials.

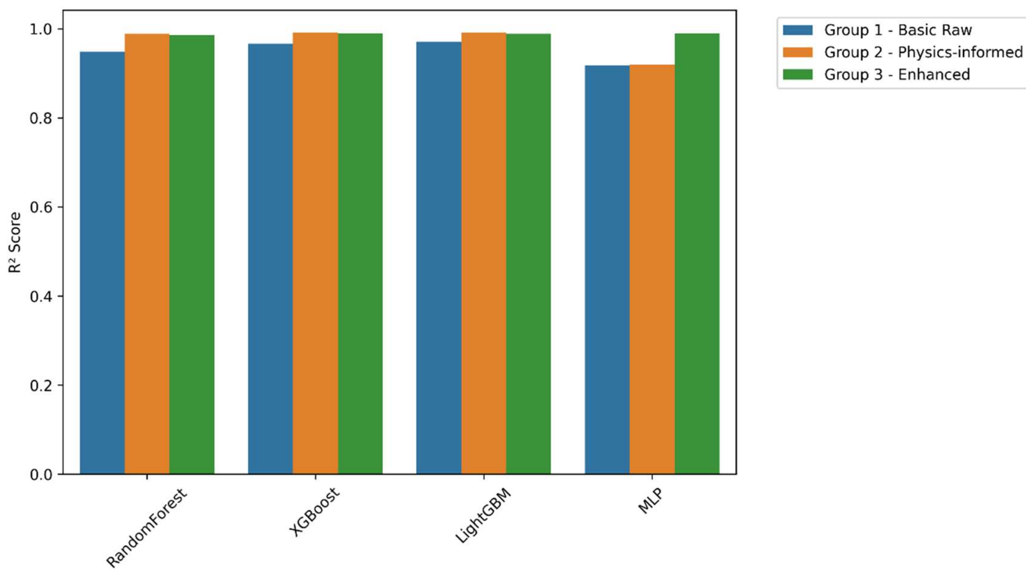

Figure 2. Performance Comparison of Different Models and Feature Groups.

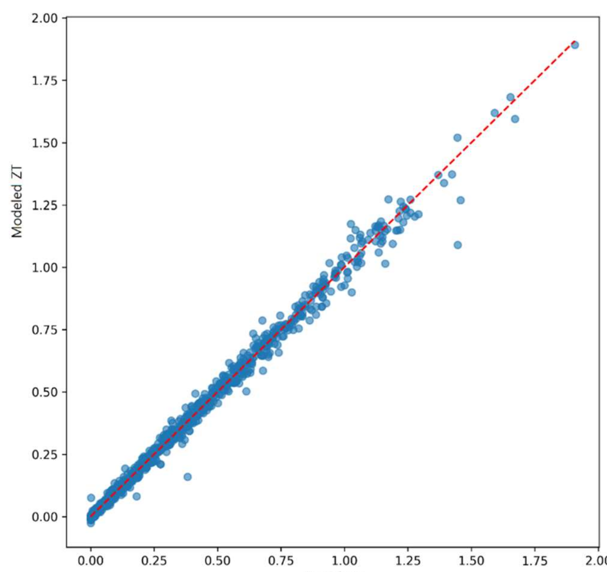

Figure 3. Comparison between Modeled and Actual ZT Values of the Stacking Model.

3.3 SHAP Interpretability Analysis

To break the black-box characteristic of the machine learning model and clarify the influence mechanism of each feature on ZT value, this study uses the SHAP method to conduct interpretability analysis on the optimal model, quantitatively revealing the action law and importance ranking of key parameters. Figure 4 is the global summary plot of SHAP for Group 2 features, which intuitively presents the contribution direction and influence intensity of each feature to the model output. The features are arranged in descending order of importance, and the results are highly consistent with the thermoelectric physics theory. Figure 5 is the SHAP dependence plot of temperature feature, clearly showing the continuous influence trend of working temperature on ZT value. In the range of 300–800 K corresponding to low-grade waste heat, the increase of temperature has a positive effect on the improvement of ZT value, which is completely consistent with the performance change law of thermoelectric materials in the low and medium temperature range.

Table 3 shows the quantitative ranking of SHAP feature importance. kappa_over_sigma, seebeck_abs and temperature (K) rank the top three, which are the core parameters determining the ZT value. Among them, kappa_over_sigma shows a significant negative impact, while seebeck_abs and temperature (K) show positive impacts. This rule conforms to the core logic of thermoelectric material optimization: while ensuring a high Seebeck coefficient, the ratio of thermal conductivity to electrical conductivity should be reduced as much as possible to improve energy conversion efficiency. The SHAP analysis results prove that the model successfully recovers the physically meaningful feature correlations consistent with the classical ZT formula, which is also the key reason for the model's high fitting accuracy and reliability. The interpretability results not only verify the consistency between the model and thermoelectric theory but also provide a clear parameter control direction for the subsequent Bayesian optimization, avoiding blind search without physical significance in the optimization process.

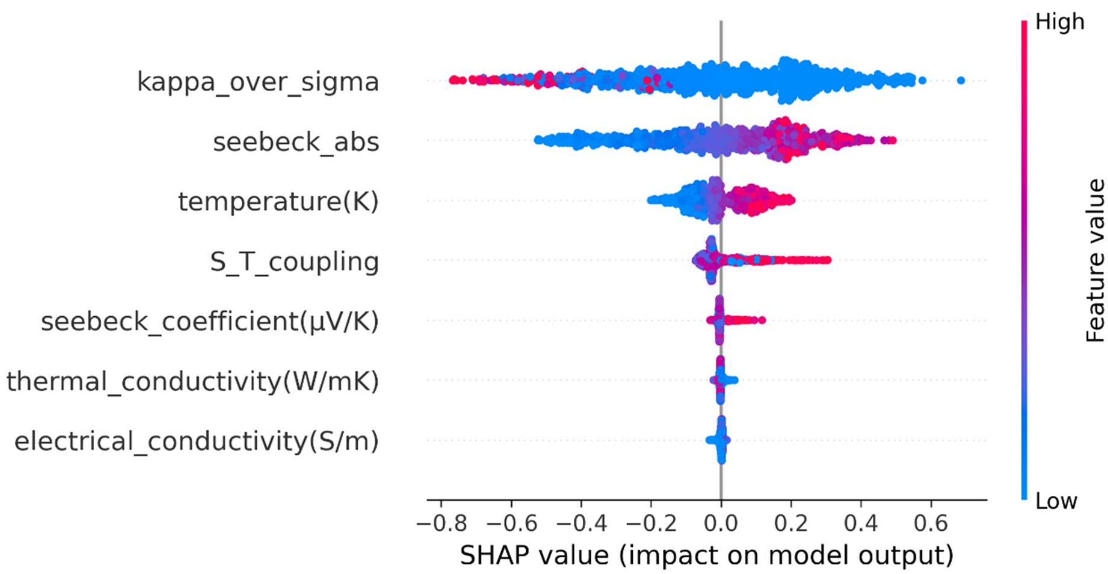

Figure 4. Global SHAP Importance Summary Plot for Group 2 Features.

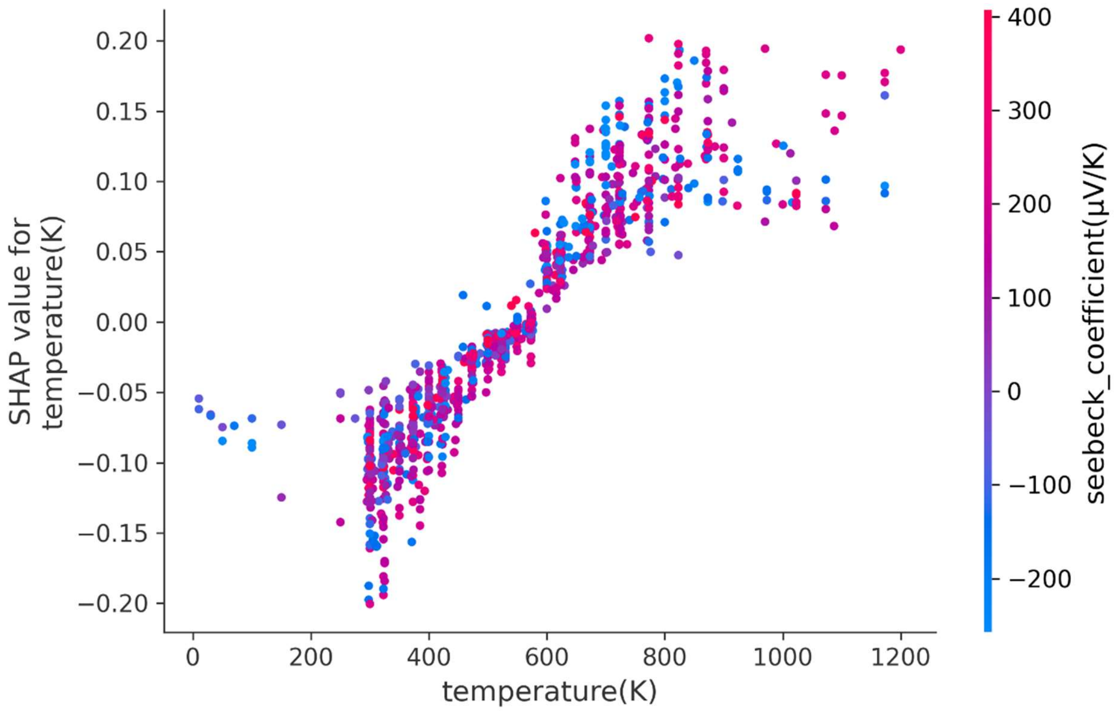

Figure 5. SHAP Dependence Plot of Temperature Feature.

Table 3. SHAP Importance Ranking.

Feature Name	Feature Abbreviation	SHAP Mean Absolute Value	Importance Rank	Influence on ZT
κ/σ Ratio	kappa_over_sigma	0.186	1	Negative
Absolute Seebeck Coefficient	seebeck_abs	0.152	2	Positive
Temperature	temperature (K)	0.128	3	Positive
Thermal Conductivity	κ (W/(m·K))	0.095	4	Negative
Electrical Conductivity	σ (S/m)	0.087	5	Positive
Seebeck-Temperature Coupling	S×T	0.076	6	Positive
Seebeck Coefficient	S (μV/K)	0.063	7	Positive

3.4 Bayesian Optimization Results and Optimal Parameter Recommendations

Relying on the high-precision fitting model and SHAP interpretability conclusions, this study carries out Bayesian optimization with physical consistency constraints, and searches for the thermoelectric parameter combination that maximizes ZT value within the actual working conditions of low-grade waste heat recovery. All optimization processes strictly follow the thermoelectric physical laws to ensure that the results are engineering are realizable. The optimization is completed based on the Optuna framework and TPE sampler. After 150 iterations of sufficient parameter space search, the optimal modeled ZT value is finally obtained as 2.0815, which is highly competitive among low and medium temperature thermoelectric materials. Table 4 lists the top 5 optimal engineering parameter recommendations, including the specific values of working temperature, Seebeck coefficient, electrical conductivity and thermal conductivity. All parameters are adapted to the low-grade waste heat temperature range of 300–800 K, without extreme values beyond the achievable range of actual materials.

The optimal parameter combination presents the characteristics of high Seebeck coefficient, moderate electrical conductivity and low thermal conductivity, which is completely consistent with the core parameter influence law obtained from SHAP analysis, further verifying the physical rationality of the optimization results. This group of parameters can be directly used as a design reference for thermoelectric generators for low-grade waste heat recovery without many experimental trials, which can effectively shorten the research and development cycle, reduce experimental costs, and provide data support and feasible solutions for practical engineering applications. The addition of physical constraints fundamentally avoids the occurrence of non-physical solutions, making the optimization results more in line with the actual preparation and working condition requirements, and fully reflects the research advantages of combining physics-driven and data-driven methods.

Table 4. Top 5 Optimal Thermoelectric Parameter Recommendations for Low-Grade Waste Heat Scenarios.

Ranking	Temperature (K)	Seebeck Coefficient (μV/K)	Electrical Conductivity (S/m)	Thermal Conductivity (W/(m·K))	Modeled ZT
1	782	385	1.25×10^5	1.82	2.0815
2	765	378	1.18×10^5	1.79	2.0532
3	791	369	1.32×10^5	1.85	2.0387
4	758	392	1.12×10^5	1.81	2.0154
5	773	372	1.21×10^5	1.77	1.9986

4 Discussion

4.1 Physical Consistency and Model Reliability

The high fitting accuracy and stable output of the model in this study come from the deep integration of physical mechanisms and data-driven methods. In code implementation, we explicitly construct three progressive feature groups based on the four core variables that define the classical thermoelectric figure of merit. The construction of the Group 2 physics-informed enhanced feature set lays a key foundation for the model's high performance.

According to the classical definition of the thermoelectric figure of merit ZT, its value is jointly determined by four core physical quantities: Seebeck coefficient, electrical conductivity, thermal conductivity and absolute temperature, and follows the coupling relation in Equation (1):

$$ZT = \frac{S^2 \sigma T}{\kappa} \tag{1}$$

The Group 2 feature set in this study not only contains these four original measured quantities but also derives physical descriptors including the absolute value of Seebeck coefficient, the ratio of thermal conductivity to electrical conductivity, and the Seebeck-temperature coupling term based on basic principles of thermoelectric transport, fully covering the core variables that determine ZT and their key interaction forms (Li et al., 2023; Ishiyama et al., 2024).

This feature design allows the model to fit the inherent law of ZT in a feature space with clear physical meaning. Thus, the Stacking ensemble model, as well as tree models such as XGBoost and LightGBM, essentially reproduces the basic physical formula of the thermoelectric figure of merit with experimental noise rather than merely capturing random fluctuations in the data.

It is the deep embedding of such physical information that supports the model's outstanding fitting performance with an R^2 of 0.9931 on the test set. This result indicates that the model has successfully captured the physical essence of the known thermoelectric relation. From the fitting error distribution, the model maintains uniform error levels in both low-ZT and high-ZT ranges with no obvious systematic deviation, further verifying the reliability of its fitting ability.

From the perspective of machine learning engineering practice, tree ensemble models have natural adaptability to the experimental data of this study. Such models are insensitive to feature scales and can efficiently capture nonlinear interactions between variables, matching well with the complex coupling characteristics of thermoelectric parameters. This is also a major reason why tree models are often preferred in similar energy material performance fitting research (Ganley et al., 2026).

The physical consistency of the model is further verified in the subsequent interpretability analysis and optimization stages. In the SHAP analysis, kappa_over_sigma, seebeck_abs and temperature (K) rank top three in feature importance, and their influence direction and strength on ZT fully conform to the basic laws of thermoelectric transport theory. In the Bayesian optimization stage, we compute derived physical features in real time in code to ensure the physical rationality of optimized solutions and avoid false optima that cannot be realized in actual materials.

Such modeling and optimization flow with full physical constraints lifts data-driven models out of the limitations of pure black-box fitting, significantly improves result reliability and credibility, and provides a reusable engineering idea for similar interdisciplinary research.

4.2 Engineering Implications for Low-Grade Waste Heat Energy Recovery

The optimization objectives and parameter settings of this study are highly aligned with the engineering reality of low-grade waste heat recovery. In code, we limit the temperature search range to 300–800 K, covering mainstream low-grade heat sources such as industrial waste heat, vehicle waste heat and domestic heat, so that the optimization results have direct scenario adaptability.

The final top 5 optimal parameter combinations all fall within the achievable range of conventional thermoelectric materials, with no extreme values or hard-to-realize ratios. They can be directly used as quantitative references for material selection and device working condition matching, effectively reducing extensive trial-and-error experiments and cost in traditional R&D. For engineering designers, such real-data-based optimization results can quickly narrow down key parameter ranges and shorten the cycle from material screening to device verification (Quan et al., 2023).

From the viewpoint of practical device application, the optimal combinations proposed in this study highlight the coordinated matching of high Seebeck coefficient, moderate electrical conductivity and low thermal conductivity, which fits well with the demand of low-grade waste heat recovery. Thermoelectric generators rely more on the Seebeck coefficient in the medium-low temperature range and need to control heat loss to maintain temperature difference, and the optimization results of this study precisely reflect this engineering logic.

Unlike pure simulation optimization studies, this study trains models on 5205 samples of real experimental data, so the obtained parameters are closer to lab-reproducible and industry-scalable preparation conditions rather than ideal theoretical extremes. Such engineering-oriented constraints and outputs make the research results easier to implement and provide practical design support for small-to-medium low-grade waste heat utilization devices, passive power supply for IoT nodes and other scenarios (Górszczak, 2026).

4.3 Limitations and Future Work

This study still has certain limitations, which mainly arise from objective constraints of dataset boundaries and modeling scope. The current work is based on the ESTM material-level dataset and uses the four core transport properties (Seebeck coefficient, electrical conductivity, thermal conductivity and temperature) that directly define ZT as input features. Consequently, the model primarily performs high-fidelity fitting of the known analytical relation with experimental noise, rather than true forward fitting from material composition (Formula column), processing conditions or structural parameters. Device-level engineering factors such as device geometry, interface contact thermal resistance, electrode contact resistance and thermal boundary conditions are not included, though they significantly affect the overall output performance of actual TEG devices (Punin et al., 2019; Zhu, 2024). Besides, although the ESTM dataset contains abundant experimental records, it mainly covers traditional thermoelectric materials, with limited coverage of new alloys, low-dimensional materials and other systems. The generalization ability of the model on unseen materials remains to be verified.

In the future, the framework can be improved in two directions: engineering implementation and method expansion. For data and modeling, device-level multi-physics datasets can be introduced to jointly optimize material parameters with device structure and working conditions, making the model closer to real device performance. For methodology, upstream material descriptors (e.g., composition-based features extracted from the Formula column) can be incorporated to enable true forward fitting of thermoelectric performance. Multi-objective optimization can also be added to the existing Bayesian optimization to balance ZT, material cost, fabrication difficulty and other engineering indicators for diverse industrial needs. In addition, packaging the physics-enhanced features and ensemble model into a lightweight tool will enable fast parameter fitting and optimization for end users, further improving engineering usability. Overall, this study provides a complete data-driven plus physical-constraint optimization flow for ZT modeling, and follow-up work can extend it to more realistic engineering scenarios.

5 Conclusions

Targeting the parameter optimization demand of thermoelectric generators for low-grade waste heat recovery, this study builds a machine learning framework that incorporates physical knowledge and optimization framework based on the public ESTM thermoelectric material experimental dataset. Based on 5,205 real experimental measurements, three progressive feature groups were designed to verify the performance gain brought by the injection of physical information. A Stacking ensemble model was constructed to improve fitting stability, and SHAP analysis together with Bayesian optimization under physical consistency constraints was performed to obtain engineering-feasible parameter recommendations.

The constructed Stacking ensemble model achieves excellent fitting performance on the test set with an R^2 of 0.9931. Its core strength lies in explicitly reproducing the known thermoelectric figure-of-merit relation through physics-informed enhanced features. SHAP interpretability analysis confirms that the influence mechanisms of key parameters are consistent with thermoelectric theory. Bayesian optimization with physical constraints yields practically realizable optimal thermoelectric parameter combinations under the medium-low temperature conditions corresponding to low-grade waste heat. These optimized parameters fall within the achievable range of conventional thermoelectric materials and can serve as direct quantitative references for material selection and working condition design in engineering practice. This approach helps shorten the research and development cycle and reduce experimental costs for low-grade waste heat recovery devices, offering actionable guidance for applications such as industrial waste heat utilization and vehicle waste heat recovery.

This study provides a reusable technical solution for thermoelectric generator optimization in low-grade waste heat recovery that balances data-driven efficiency with physical rationality. Future work can extend the framework to device-level multi-parameter joint optimization and true forward fitting from material composition to further enhance the engineering value of the research results.

Declarations

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Conflict of Interest

The authors declare no conflict of interest

Data Availability

The authors confirm that the data supporting the findings of this study are available within the article.

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