Computational optimisation of PSS molecular weight to maximise PEDOT: PSS film conductivity under processing constraints

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***Abstract*—The electrical conductivity of PEDOT:PSS films is highly sensitive to the molecular weight of PSS and the processing conditions involved during fabrication. Optimizing these parameters experimentally is often labor-intensive and resource-demanding, motivating the need for computational approaches to guide materials design. In this study, a Multi-Fidelity Bayesian Optimization (MF-BO) framework is employed to identify the optimal PSS molecular weight and processing parameters that maximize film conductivity. High-fidelity experimental data from literature were combined with synthetically generated low-fidelity datasets to balance accuracy and computational efficiency. In parallel, a Random Forest regression model was developed to predict film conductivity from processing variables, offering an interpretable and robust machine-learning baseline. The integration of MF-BO for process optimization and Random Forest for predictive modeling establishes a scalable, data-driven workflow for enhancing PEDOT:PSS film performance, demonstrating the potential of hybrid optimization and learning strategies in accelerating materials discovery and process engineering.**

***Index Terms*—PEDOT:PSS, conductivity prediction, Bayesion Optimisation, Predictive modelling, Optimisation techniques**

I. INTRODUCTION

Poly(3,4-ethylenedioxythiophene):poly(styrene sulfonate) (PEDOT:PSS) has become one of the most versatile and widely utilized conducting polymers in modern electronic material systems due to its exceptional combination of high electrical conductivity, solution processability, transparency, and mechanical flexibility.[1] These properties make it a material of choice for diverse applications ranging from transparent electrodes and thermoelectric generators to bioelectronic devices and flexible sensors. Despite its broad adoption, enhancing the conductivity of PEDOT:PSS films remains a central research challenge, as film performance is intricately influenced by multiple interdependent factors such as PSS molecular weight (Mn), solvent composition, annealing temperature, and post-treatment conditions.[2]

Traditional research approaches have primarily relied on empirical and trial-and-error methods, which, while yielding important qualitative insights, often fall short in capturing the complex, multivariate relationships that dictate film conductivity.[3] Classical studies have demonstrated that polar solvent or acid treatments (e.g., DMSO, EG, sulfuric acid) can improve conductivity by several orders of magnitude through mechanisms such as phase separation, enhanced PEDOT crystallinity, and improved chain alignment.[4] However, the effect of PSS molecular weight has often been explored in isolation, with limited attention to its interaction with other process variables. Recent works indicate that conductivity exhibits a non-monotonic dependence on PSS molecular weight, where an optimal Mn balances phase separation and charge carrier mobility, while deviations in either direction lead to performance degradation.[5][6]

The advanced characterization like grazing-incidence wide-angle X-ray scattering (GIWAXS) and atomic force microscopy (AFM) described the morphological and structural development of PEDOT:PSS films, emphasizing the nanoscale domain structure and polymer chain ordering. Nonetheless, a thorough mapping of these parameters is still scarce. As a result, it has an impact on the possible prediction capability of the conventional mechanistic models. Different approaches adopted to overcome these limitations have been the development of computational optimization and machine learning frameworks where possible. Multi-fidelity Bayesian optimization (MF-BO) is a general technique that has been proven to be effective in large parameter space exploration through a combination of high-fidelity experimental data and low-fidelity computational/synthetic data.[7][8] This increases the efficiency of the samples and hastens the search for optimal configurations of materials satisfying the relevant processing constraints.

Recent developments in autonomous experimentation platforms, such as Polybot, further illustrate the integration of closed-loop optimization and real-time conductivity evaluation, uncovering hidden process–structure–property relationships that traditional experimentation often overlooks.[9] While maximizing electrical conductivity remains the primary optimization objective, practical device deployment requires balancing it with constraints such as substrate compatibility, adhesion, toxicity, and cost. The inclusion of such constraint-aware optimization frameworks represents an emerging direction in data-driven materials design.

Within this context, the present work focuses on the computational optimization of PSS molecular weight using multi-fidelity Bayesian optimization to maximize PEDOT:PSS film conductivity, complemented by a Random Forest predictive model to estimate conductivity from key processing parameters.[10] By combining data-driven optimization, synthetic data generation, and machine learning-based prediction, this study aims to develop a scalable and efficient workflow for guiding PEDOT:PSS processing, reducing reliance on extensive experimental trials, and accelerating the design of high-performance conducting polymer systems.

II. Motivation

PEDOT:PSS stands as a versatile and sustainable conducting polymer with immense applications in flexible electronics,energy devices, and bio-integrated technologies. Even though it is widely used, achieving consistent high conductivity remains challenging, as it is highly sensitive to several interdependent factors, such as solvent composition and other conditions, such as PSS molecular weight. Experimental optimization of these parameters can be tedious and time-consuming. The major motivation of this project is to develop a computational framework that efficiently optimizes processing parameters to maximise conductivity and to improve predictive analysis of process-property relationships.

III. Literature Review

Early studies demonstrated that post-treatment with organic solvents significantly enhances film conductivity by modifying the PEDOT to PSS ratio and promoting phase segregation. For instance, Lee reported that organic solvent surface treatment could increase conductivity by several orders of magnitude through morphological rearrangement. Similarly, [13] demonstrated that treatment with phosphoric acid effectively enhanced charge transport by reducing the insulating PSS content, thereby enabling its application in flexible solar cells. Later studies in [14] further demonstrated that the inclusion of solid chloroplatinic acid (HPtCl) could act as an effective secondary dopant, enhancing conductivity through protonic and electronic pathways .

A more recent line of research explores molecular weight optimization of the PSS component as a determinant of charge carrier transport properties. In [6] they investigated how the PSS molecular weight and its size distribution impact the mixed ionic–electronic transport process within PEDOT:PSS, concluding that lower molecular weight fractions lead to improved mobility and film uniformity . In [5], Fan et al. systematically further established the mechanism by which the molecular weight optimization influences conductivity, showing that controlled adjustment leads to efficient percolation networks within the polymer matrix . This structural tuning offers a promising approach for designing high-conductivity materials without solvent-based post-treatments.

Beyond molecular engineering, doping strategies remain a strong area of investigation.In [15], Ouyang et al. introduced secondary doping approaches such as high-boiling solvent additives and ionic liquids, which substantially enhanced conductivity by modifying the film morphology and improving interchain coupling. Earlier, in [3], Nardes et al. had shown that using sorbitol as a dopant yielded a simultaneous boost in work function and environmental stability. More environmentally friendly methods, such as solvent vapor treatment [4], further corroborate the role of solvent polarity and interaction energy in modulating PEDOT:PSS structures to achieve high conductivity.

The multifunctionality of PEDOT:PSS allows it to be applied in a broad range of electronic devices, including flexible displays, thermoelectrics, and bioelectronic interfaces . Reviews by Gunel Huseynova et al. [1] and Rivnay et al. [2] emphasized its growing utility as a transparent electrode material and its integration into organic electrochemical transistors for biointerfaces. These works highlight how structural and interfacial optimization directly enhances charge injection and extraction efficiency in device configurations.

While experimental optimization dominated earlier research, recent work has shifted toward autonomous and AI-driven materials design. The integration of Bayesian optimization provides a data-

efficient way to navigate large parameter spaces in thin-film processing. Foundational work by Shahriari et al. introduced Bayesian optimization as a framework for minimizing expensive function evaluations.[7] Extensions into materials research were developed through "Best Practices for Multi-Fidelity Bayesian Optimization in Materials" and "Automation of Thin Film Process Development", showing that combining high- and low-fidelity simulations reduces development time and cost. Wang et al. [9] extended this into an autonomous platform for electronic polymer solution processing, demonstrating real-time learning-based enhancement of PEDOT:PSS thin films.

Parallel advances in machine learning (ML) enable predictive modeling of materials' conductivity. Lundberg and Lee introduced model interpretation frameworks like SHAP, crucial for physically interpretable predictions in materials informatics. Rosa et al. and Wang Rajendran [10] demonstrated ML-based conductivity prediction, while Batra and Sankaranarayanan [12] emphasized multi-fidelity learning for materials simulations. These computational methodologies enable systematic exploration of the structure–property relationship, complementing empirical techniques.

IV. Methodology

1. Data collection

High-fidelity data used for this work has been collected from a research paper that experimentally showed the optimal PSS molecular weight for maximum conductivity.[5] To construct the low-fidelity dataset, a structured grid-based synthetic data generation method was employed.This approach systematically defines a parameter space using discrete, physically meaningful values for key processing parameters—PSS molecular weight (Mn), DMSO additive concentration, and annealing temperature (T)—and computes corresponding synthetic output values for viscosity, Raman quinoid fraction, π–π stacking distance, and film conductivity.

The method used here is a factorial grid sampling technique, where all combinations of selected parameter levels are enumerated to form a complete dataset. For this study, seven levels of Mn (10–70 kg/mol), three levels of DMSO (0, 5, 10 wt), and three levels of annealing temperature (60, 80, 100 °C) were combined, producing 63 unique parameter combinations. For each combination, dependent physical properties such as viscosity, Raman fraction, and π–π stacking distance were generated using linear trend functions inferred from experimental relationships reported in the literature.[11]

The synthetic conductivity values were calculated using a simple empirical analytical model that captures the monotonic trend between conductivity and the governing process variables,[12] defined as:

$$\sigma = \sigma_0 + a_1(\mathrm{Mn}) + a_2(\mathrm{DMSO}) + a_3(T) \qquad (1)$$

where σ_0 represents the base conductivity (50 S/cm), and a_1 are coefficients adjusted to reflect experimental trends reported in prior studies. A small Gaussian noise term $N(0, 0.5)$ was added to each synthetic conductivity value to introduce realistic experimental variability, ensuring that the dataset mimics practical measurement noise.

2. Data Visualisation

Once the dataset was prepared, the descriptive statistics were examined to understand the mean, median, variance, and standard deviation.This gave an overall view of the main characteristics of the data set. After that, several visualisation plots were created to better understand the distribution of data and how the features are related to each other.

The dataset contains both low- and high fidelity data.No missing values were found, and all column values are in the expected physical range.The conductivities vary significantly over a large range,showing non-linearity there by making it suitable for model training.

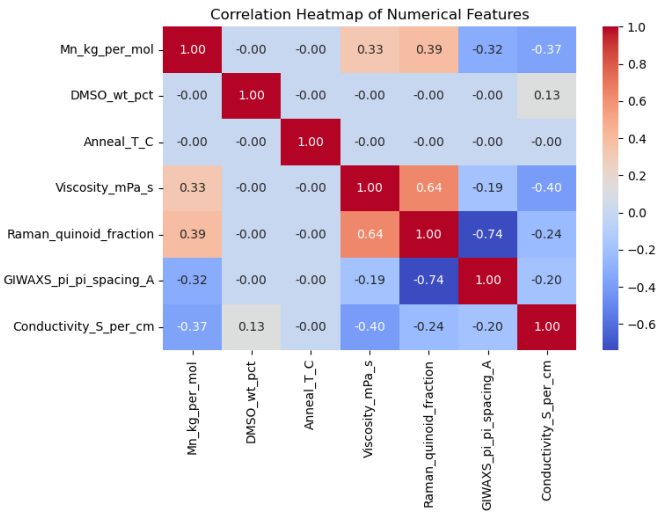

Fig. 1: Correlation Heatmap

The correlation heatmap between numerical features is useful for understanding relationships or

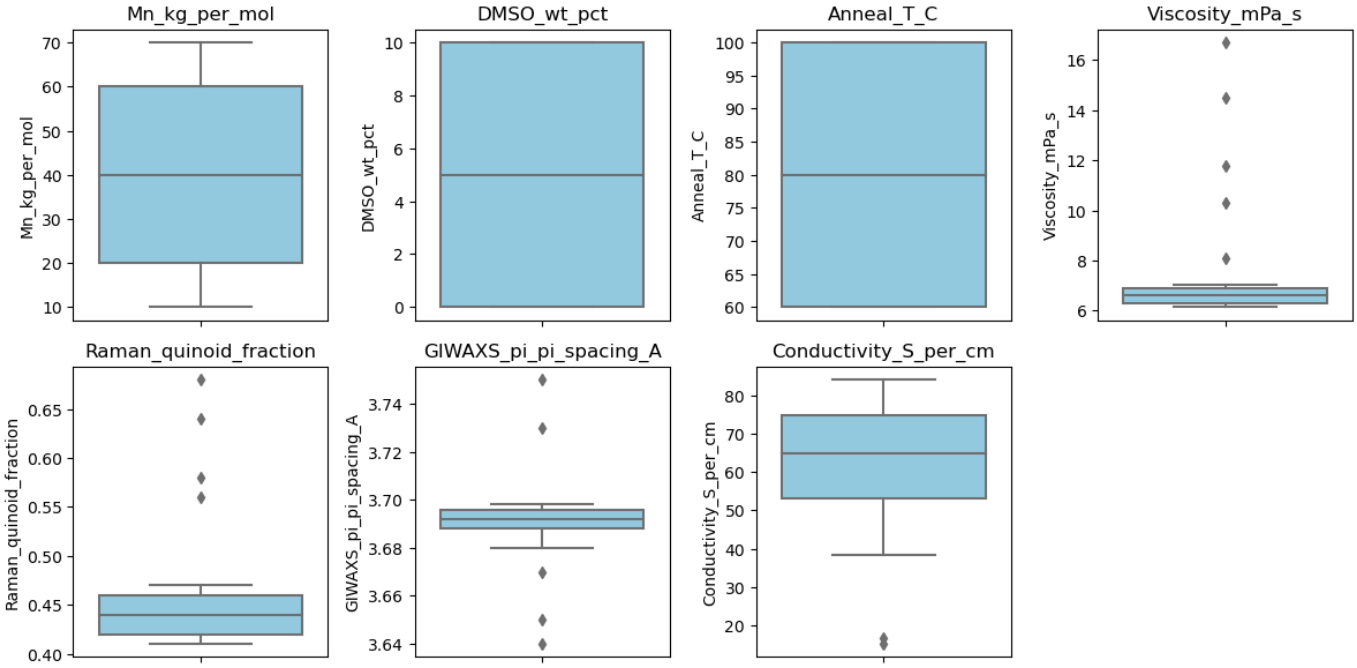

Fig. 2: Box plot of features

multicollinearity. Some of the features show positive correlation while others show negative correlation.

Most of the features are distributed evenly in a certain range. Features like viscosity, Raman_quinoid_fraction and GIWAXS_π–π stacking distance contains experimental outliers.There is no severe skewness present in any of the feature showing stable and bounded distribution.

Fig 3 illustrates the pairwise relationships between features. Certain features display clear positive or negative linear trends. The scatter plot does not reveal nonlinear discontinuities or abrupt changes, suggesting that the generated synthetic data is both consistent and realistic.

3. Development and Evaluation of Predictive Model

To predict the electrical conductivity of PEDOT:PSS thin films from their processing and structural parameters, both Random Forest and Gradient Boosting regression modeling were employed on a combined dataset consisting of high-fidelity measurements from the experiments and low-fidelity data that were synthetically generated. Prior to developing the models, all numerical features were z-score standardized to ensure that parameters with different magnitudes, such as molecular weight, viscosity, or π–π stacking distance, did not bias the learning algorithm. Since the conductivity values spread over multiple orders of magnitude, therefore, a logarithmic ($\log_{10}$) transformation was performed on the target variable to stabilize its variance, improve symmetry of the distribution, and enhance numerical performance of the learning algorithms. The bursty named data was then split into training and testing datasets for model evaluation in the 80:20 ratio.

In the configuration, Random Forest Regressor enabled capturing complex nonlinear interactions between processing conditions and resulting conductivity via 300 estimators, maximum depth of 8, and minimum of three samples per leaf node with high robustness. In parallel, a Gradient Boosting Regressor was implemented with 300 sequential boosting rounds, learning rate set at 0.05, and maximum tree depth of 5. Unlike Random Forest, the Gradient Boosting model achieves improvements in predictive accuracy by iteratively fitting new trees to the residual errors of the previous trees thereby building a strong ensemble through additive error correction. Both of these models have been evaluated on the test set using common regression metrics, namely the coefficient of determination (R^2), Root Mean Square Error (RMSE), and Mean Absolute Error (MAE) back-transformed into units of conductivity on the logarithmic domain. To signify physical units (S/cm) and ensure interpretability for material characterization, reverse mapping (10^y) was applied on the predictions.

SHAP (SHapley Additive exPlanations) analysis

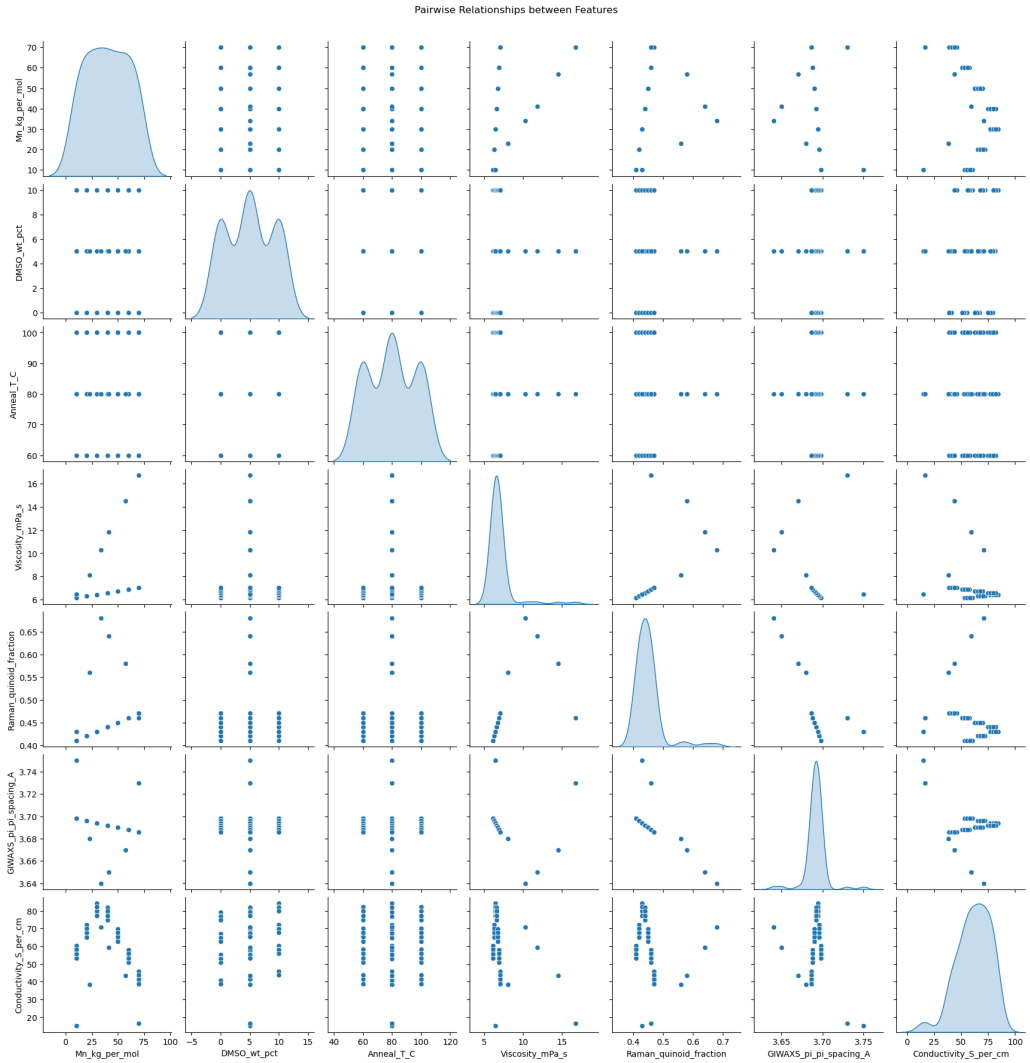

Fig. 3: Pairwise relation of features

was conducted for both the Random Forest and the Gradient Boosting model towards understanding the interpretability of the models. SHAP value describes the input feature contributions towards the predicted conductivity that shed light on how molecular weight, DMSO concentration, annealing conditions, viscosity, Raman quinoid-fraction, and GIWAXS π–π stacking distance affect film performance. The consistently significant drivers identified by both of the models were PSS molecular weight and microstructural descriptors in corroboration with established physical mechanisms. Eventually, both models were serialized via the `joblib` library for reproducible deployment into the multi-fidelity Bayesian optimization framework developed in this study. A comparative analysis was carried out between the two models in terms of their prediction capabilities and generalization abilities, as well as their appropriateness as surrogate functions for optimization tasks.

4. Optimization of Processing Parameters

To determine the optimal processing parameters that maximize the electrical conductivity of PEDOT:PSS thin films, a Multi-Fidelity Bayesian Optimization (MF-BO) framework was implemented. The optimization was carried out over a well-defined parameter space, which included both compositional variables—such as PSS molecular weight (Mn) and DMSO weight percentage—and processing variables such as spin-coating speed, annealing temperature, annealing duration, and morphological descriptors (viscosity, Raman quinoid fraction, and GIWAXS _π–π stacking distance. Each feature was assigned realistic bounds derived from experimental data and literature ranges. The trained Random Forest model acted as a surrogate model that estimated film conductivity based on these input parameters.

The Bayesian optimizer then iteratively queried this surrogate by proposing new candidate points within the search space, balancing exploration of uncertain regions and exploitation of high-performance areas through the Expected Improvement (EI) acquisition function.

This method, MF-BO, was selected for its efficiency in pinpointing global optima in a high-dimensional design space with few evaluations, which is critical for materials such as PEDOT:PSS, whose high-fidelity experimental data are scarce and costly to acquire. The optimizer incorporates various fidelity models (for example, low-fidelity synthetic simulations and high-fidelity experimental measurements) to gain a broader knowledge base while further tightening the predictions on more trustworthy data. This leads to greater sample efficiency and predictive reliability. MF-BO does not conduct an exhaustive search such as those performed by grid or random search; rather, it directs the search in an intelligent way toward the most promising areas of the parameter space, greatly alleviating computational and experimental burden.

V. Results and Discussion

Predictive analysis by Random forest and Gradient boosting models were successfully carried out.

1. Predictive analysis

(a) Random Forest Model

The Random forest model configured with 300 estimators and a maximum depth of 8 showed a considerable predictive capability in capturing nonlinear interactions between the processing parameters and conductivity values.The R^2 value of the model in $\log_{10}$ scale is found to be 0.729 which is pretty good predictive capability. Figure 4 illustrates the linear alignment of predicted vs actual conductivity values, confirming the model's capability in the prediction of film conductivity trends.

Figure 5 shows the residual distribution of the model exhibiting a roughly symmetric bell-shaped curve that is centered near zero, showing an unbiased and normal distribution of prediction errors. Furthermore, SHAP value analysis shown in Figure (6-7) revealed that PSS molecular weight, GIWAXS π–π stacking distance, and viscosity were the most influential factors determining the conductivity. This observation also aligns with the physical understanding as these features can directly affect the morphological order, chain packing, or charge transport pathways that in turn affect the conductivity.

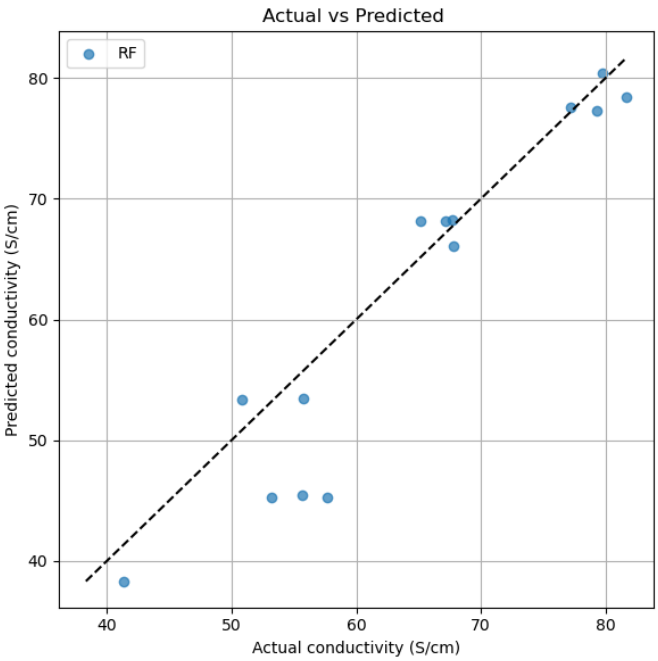

Fig. 4: Random Forest-Actual vs Predicted

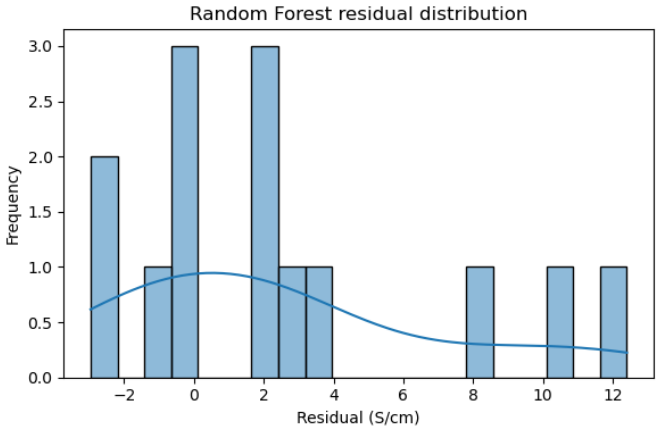

Fig. 5: Random Forest-Residual distribution plot

(b) Gradient Boosting Model

The Gradient Boosting Regressor, trained with 300 estimators, a learning rate of 0.05, and a maximum depth of 5, achieved good predictive capability with an R^2 value of 0.9931 having a close alignment of predicted and actual conductivity values.

Figure 8 shows the actual vs predicted plot that displays a linear alignment between both values. Figure 9 shows a zero-centered, symmetric, and normal curve showing unbiased prediction errors.

To check model's generalisation capability and check overfitting, 5-fold cross-validation was performed. The model achieved an average R^2 value of 0.64, an average RMSE of 0.07, and an average MAE of 0.03. This shows moderate predictive capa-

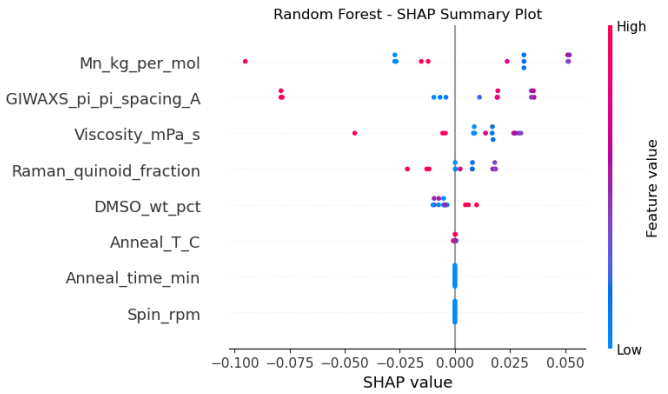

Fig. 6: Random Forest-SHAP summary

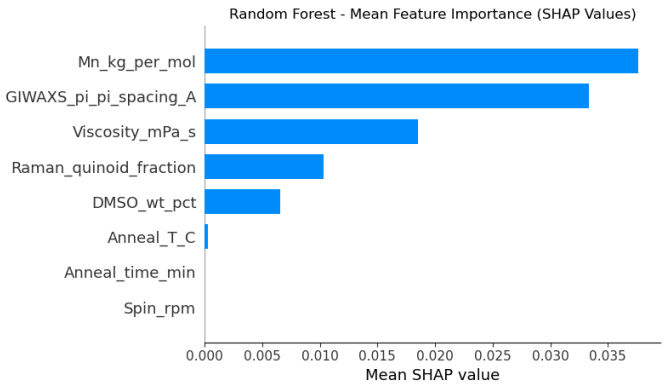

Fig. 7: Random Forest-SHAP Feature Importance

bility, showing that the model captures key property relationships, but performance fluctuates depending on data partition. This can be due to a small dataset. Nevertheless, less RMSE and MAE value suggests that the model provides meaningful predictions with better accuracy.

SHAP analysis shown in Figure (10-11) shows that PSS molecular weight, GIWAXS π–π stacking distance, and viscosity were the most influential factors governing the conductivity.

2. Optimisation Analysis

Following the predictive modelling, an optimisation framework was implemented to identify the optimal processing parameters that maximise PEDOT:PSS film conductivity. The framework utilised the trained Random Forest as a surrogate function to predict the conductivity, incorporating the different processing parameters. The MF-BO algorithm efficiently explored the parameter space by sampling uncertain regions and exploiting near high-conductivity zones using the Expected Improvement (EI) acquisition function. By combining both high-

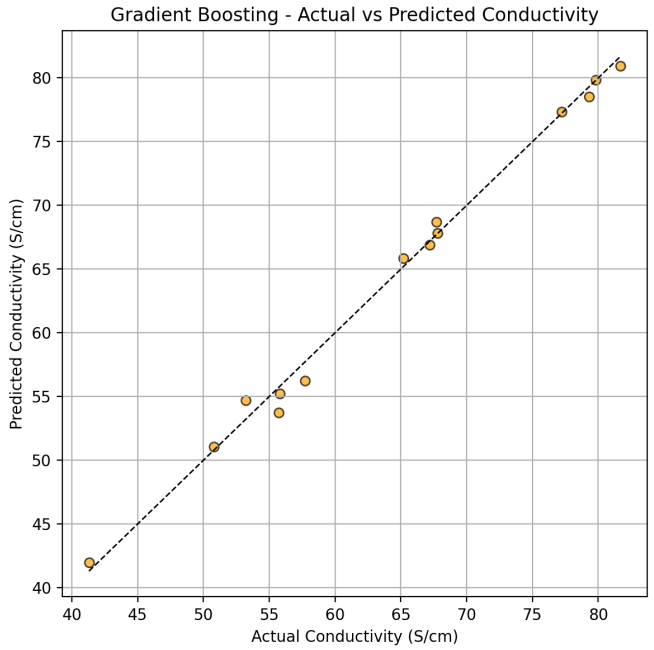

Fig. 8: Gradient Boosting-Actual Vs Predicted

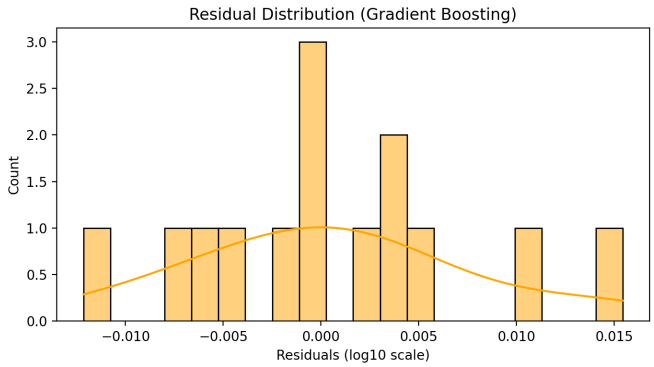

Fig. 9: Gradient Boosting- Residual distribution Plot

and low-fidelity data, the optimizer reduced the number of high-cost evaluations while maintaining prediction accuracy. Over 30 iterations, the optimization trajectory shown in Figure 12 displayed growing improvement in predicted conductivity, and then saturated towards an optimal region corresponding to moderate PSS molecular weight (30-40 kg/mol), DMSO 5 wt%, and annealing temperature 100-200°C.

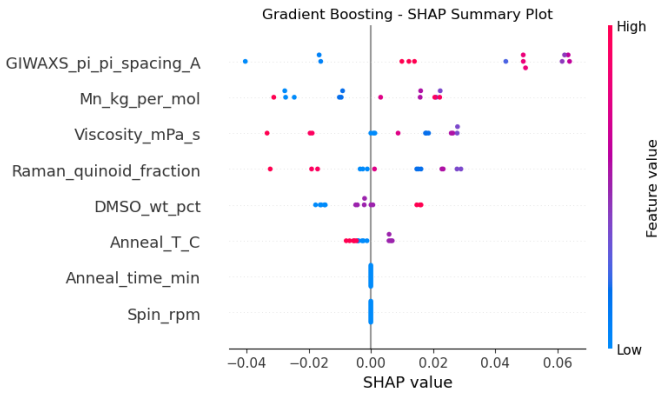

Fig. 10: Gradient Boosting-SHAP summary plot

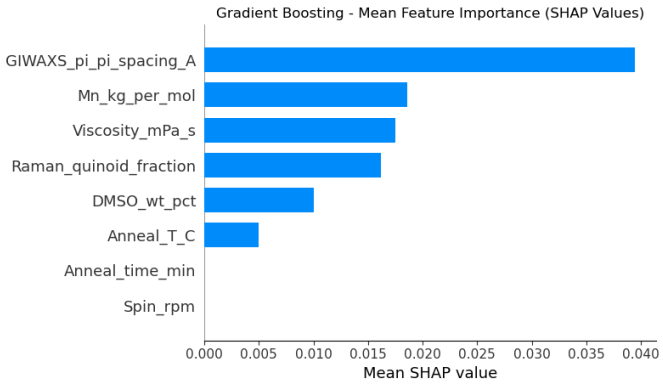

Fig. 11: Gradient Boosting-SHAP Feature importance

VI. Conclusion

This work shows that integration of machine learning techniques and optimization techniques enable researchers to improve the electrical conductivity of PEDOT:PSS thin films. The combined dataset containing high-fidelity experimental measurements and structured low-fidelity synthetic data trained predictive models that can capture the complex nonlinear interactions between PSS molecular weight, solvent concentration, and annealing conditions along with structural descriptors of the formed constructs such as viscosity, Raman quinoid fraction, and π–π stacking distance. Both Random Forest and Gradient Boosting regressor were evaluated, and both models showed fairly good predictive performance, consistent trends in importance of features, and were in accordance with already established physical mechanisms. Gradient Boosting showed higher accuracy with respect to in-sample but it does not generalize much, as per cross-validation-inherent difficulties in small materials datasets.

The capacity of the multi-fidelity Bayesian optimization framework was used to utilise the predictive model informatively as a surrogate for high efficient parametrical space exploration. The optimization path converged towards a region characterised by median molecular weights (30-40 kg/mol) of PSS with moderate DMSO concentrations and using rather high annealing temperatures; the same conditions correspond to known optimal processing windows from experimental literature values. This validates the potential of MF-BO to discover physically well-founded optima while keeping experimental demand to a minimum. The entire methodology developed in this work is scalable and computationally efficient for orienting conductive polymer processing and demonstrates how very machine learning and optimization have become much faster in materials design workflows.

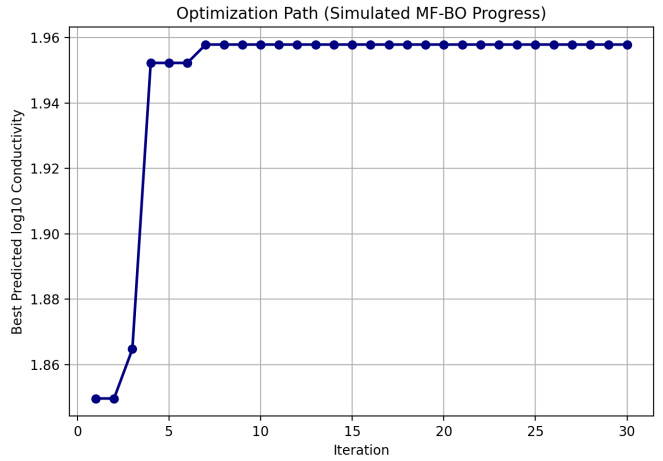

Fig. 12: Optimisation path

VII. Limitations

1. Dataset Size:

The dataset used in this work is also rather small in comparison to the datasets particularly required in ML since it has only synthetic low-fidelity values. It restricts the generalization capability of models and makes them vulnerable to overfitting, especially in Gradient Boosting.

2. Synthetic Data Approximation:

The trend-based approximations generated low fidelity data rather than physical simulation or detailed molecular modeling. Although they are adequate for optimization purposes, they will not capture all nonlinear physical behaviours as such.

3. Surrogate Model Constraints:

The Random Forest surrogate used in MF-BO lends very strong robustness, but does not offer the smoothness and uncertainty quantification features provided by Gaussian Processes, which might limit optimization performance.

4. Limited Feature Space:

Humidity, substrate type, coating thickness, oxygen exposure, and drying kinetics were not included due to lack of experimental availability.

VIII. FUTURE WORKS

This study illustrates how predictive modeling and multi-fidelity Bayesian optimization can work marvelously together to enhance the conductivity of PEDOT:PSS thin films; yet certain future promising avenues remain open for further exploration.

1. Experimental validation of optimized parameters:
The MF-BO framework predicted an optimum region located around moderate PSS molecular weights (30-40 kg/mol), 5 wt% DMSO addition and high annealing temperatures (100-200 °C). The future direction should be devoted to the fabrication of PEDOT:PSS films with the above optimal features followed by evaluation of the real conductivity and comparison of experimental results to compute predictions. This exercise will validate and refine the surrogate model as well as improve the robustness of the computational workflow further.

2. Append the dataset with some experimental and simulated data:
The current study has been limited because of the data size of high fidelity available. Increasing the experimental data points or adding more accurate physics-based simulations by molecular dynamics (MD), density functional theory (DFT), or phase-field modelling will alleviate overfitting and enhance prediction accuracy because these methods will deliver low fidelity data that more closely approximates reality than a simple trend-based approximation.

3. More structural and processing parameters:
Additional parameters such as film thickness, humidity during coating, spin-coating acceleration, substrate roughness, drying kinetics, and other GIWAXS/Raman descriptors could be captured in the future models to understand subtle micromorphological variations that strongly influence conductivity.

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