Physics-Informed Feature Disentanglement for Autonomous Acceleration of Lithium-Ion Battery Design and Analysis

Codex, Cursor, Comet, GPT-5.2 Thinking, Gemini (Flash)*

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Abstract

The multi-dimensional design space of battery design presents a critical "dimensionality crisis": the design space is so wide that traditional machine learning models fail to capture complex, non-linear parameter interactions. This study proposes an AI-driven framework based on physics-informed feature disentanglement to overcome these limitations. By integrating a specialized feature extraction algorithm with a linear regression model trained on high-fidelity PyBaMM simulations, we successfully isolated entangled electrochemical signatures from raw voltage profiles into deterministic physical markers. Our results demonstrate that this framework achieves a high coefficient of determination (R^2) exceeding 0.9 for key parameters when physics-informed features are used. Crucially, the model's reliability is secured by correlating AI decision-making with internal physical phenomena, such as the evolution of lithium concentration. This mechanism-aware approach supports forward performance prediction and interpretability toward future autonomous inverse design of LFP architectures, effectively bridging the gap between theoretical modeling and rapid industrial application.

*As of 2026-01-30. Codex: OpenAI software engineering agent (codex-1). Cursor: AI-assisted IDE (cursor.com). Comet: Comet ML platform for experiment tracking and LLM evaluation (comet.com). GPT-5.2 Thinking: OpenAI reasoning model. Gemini (Flash): Google Gemini 2.5 Flash (fast variant).

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Preprint. Under review.

1 Introduction

The rapid proliferation of renewable energy infrastructure and the staggering surge in electricity demand—driven largely by the expansion of AI-centric data centers—have catalyzed a global transition in power management. In this landscape, the Energy Storage System (ESS) market has emerged as a primary growth engine for the battery industry [1], providing the critical buffer required for grid stability. To meet the stringent operational demands of ESS [2], including long-term reliability, inherent fire safety, and cost-effectiveness, Lithium Iron Phosphate (LFP) has been increasingly adopted as the global standard. [3]

Despite its widespread implementation, the performance of LFP-based cells is dictated by a multi-dimensional design space where electrode architectures—defined by porosity, particle size, and loading levels—interact in highly nonlinear ways [4, 5]. Navigating this complexity via traditional experimental studies remains fundamentally constrained; for instance, independently controlling specific variables like cathode loading while keeping other physical parameters constant is nearly impossible in a laboratory setting due to manufacturing tolerances. To overcome these physical limitations, this work proposes a methodology based on fully controlled simulation data and AI-driven feature disentanglement to accelerate the optimization of LFP cathode architectures.

Current methodologies for electrode design predominantly rely on physics-based simulations or empirical "trial- and-error" approaches. While electrochemical models like the pseudo-two-dimensional (P2D) framework [6] provide deep insights into lithium-ion transport, their main drawbacks are not computational cost but the difficulty of measuring or fitting all required parameters and the resulting inaccuracy of predictions. Conversely, while machine learning (ML) [7–10] models offer rapid prediction, they often struggle with the high-dimensional and non-linear interactions inherent in battery electrodes [11]. For instance, while simple linear regression may accurately predict performance under highly controlled, single-variable conditions (e.g., varying only loading levels), its predictive power, quantified by the coefficient of determination (R^2), degrades sharply as the number of input variables increases. This "dimensionality crisis" is particularly acute in LFP systems [12], where the characteristic two-phase reaction behavior and transport complexities introduce significant non-linearity between architectural parameters like porosity and electrode thickness.

In this work, we demonstrate an AI-driven framework for the autonomous acceleration of LFP cathode design, utilizing a physics-informed [13] feature disentanglement approach. Here we use "feature disentanglement" to mean the separation of entangled electrochemical signals into interpretable physical markers, achieved in practice by "feature extraction" (e.g., dQ/dV-based metrics). We generate a comprehensive dataset of 1,000 simulations using the Python Battery Mathematical Modeling (PyBaMM) framework, systematically controlling five key physical parameters—porosity, particle radius, and electrode thickness—to map the electrochemical parameter space. To overcome the performance degradation observed in traditional models, we introduce a specialized feature extraction algorithm integrated with a linear regression (OLS) prediction model [8, 19]. This approach allows for a "mechanism-aware" analysis that identifies the hidden interactions between architectural variables, maintaining high predictive accuracy even as the complexity of the design space expands.

We provide a comparative analysis of prediction difficulty and a feature importance matrix linking AI decisions to physical phenomena such as lithium concentration evolution. This mechanism-aware interpretability supports forward performance prediction; inverse design of LFP cathode architectures is left as future work.

2 Schema

The proposed schema represents a bidirectional design and diagnostic framework that integrates physics-informed feature disentanglement to bridge the gap between electrode architecture and electrochemical performance. It consists of a Forward Design mode, which functions as a virtual prototyping tool by instantaneously generating predicted discharge voltage curves and dQ/dV profiles from user-defined physical parameters—such as electrode thickness and porosity—thereby drastically accelerating the battery development cycle. Simultaneously, the schema incorporates an Inverse Diagnosis mode that derives internal material properties from empirical performance data, allowing

for the non-destructive estimation of key physical parameters to analyze manufacturing quality variance or diagnose degradation mechanisms like SEI growth without invasive cell disassembly.

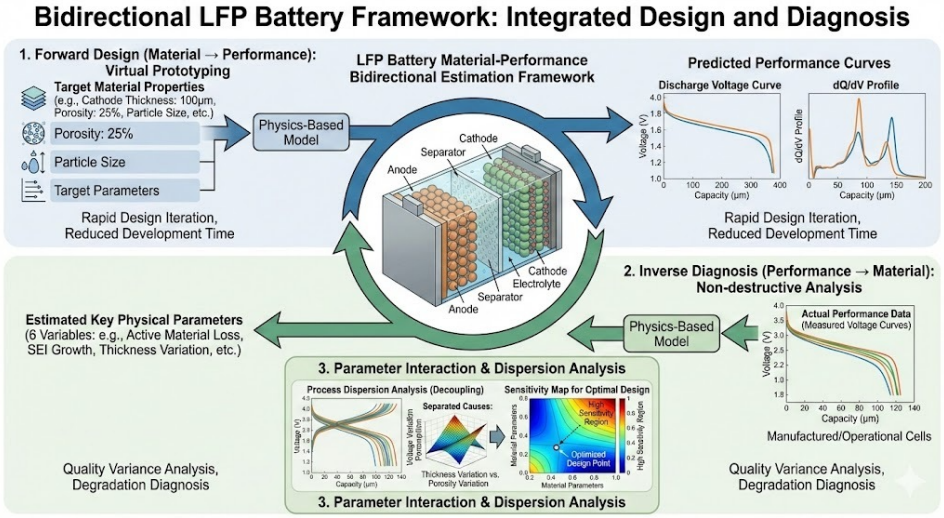


Figure 1: Bidirectional LFP framework: parameter estimation and performance prediction.

3 Methodology

3.1 Experimental Design

We conducted a systematic experimental study to evaluate the performance of linear regression models for identifying battery physical properties from discharge curves. The experimental design consists of four main stages: parameter combination generation, random sampling, battery simulation, and model training.

3.1.1 Parameter Combination Generation

We systematically generated parameter combinations to investigate the effect of varying the number of input parameters on prediction performance. Five physical properties of lithium iron phosphate (LFP) batteries were selected as targets: positive and negative electrode thickness, positive and negative electrode porosity, and positive particle radius (units as in Table 1). For each combination size $n \in \{1, 2, 3, 4, 5\}$ we generated all $\binom{5}{n}$ combinations, giving 5, 10, 10, 5, and 1 combinations respectively; within each combination, the selected parameters varied within predefined ranges and the rest were fixed. The parameter ranges are given in Table 1.

Table 1: Parameter ranges for LFP battery simulation

Parameter	Minimum	Maximum
Positive electrode thickness	5.0×10^{-5}	1.5×10^{-4}
Negative electrode thickness	4.0×10^{-5}	1.2×10^{-4}
Positive electrode porosity	0.15	0.40
Negative electrode porosity	0.25	0.50
Positive particle radius	5.5×10^{-8}	1.0×10^{-6}

3.1.2 Random Parameter Sampling

For each parameter combination we drew 200 parameter sets by Latin Hypercube Sampling (LHS) [18] with a fixed seed (42). LHS partitions each dimension into N equal-probability intervals and samples one point per interval, ensuring uniform coverage and reproducibility.

Algorithm 1 LFP Battery Property Identification Pipeline

Input: Parameter set $\mathcal{P} = \{p_1, \ldots, p_5\}$ (5 physical properties), combination sizes $n \in \{1, 2, 3, 4, 5\}$, number of samples $N = 200$, random seed $s = 42$
Output: Set of trained models $\mathcal{M}$, evaluation metrics $\mathcal{E}$, predictions $\mathcal{Y}$

1. Initialize $\mathcal{M} \leftarrow \emptyset$, $\mathcal{E} \leftarrow \emptyset$, $\mathcal{Y} \leftarrow \emptyset$.
2. For each combination size $n \in \{1, \ldots, 5\}$ and each combination c of n parameters from $\mathcal{P}$: (a) sample N parameter sets via LHS with seed s; (b) run PyBaMM discharge simulations and validate (voltage 2.0–3.6 V); (c) extract features (mean, std, min, max, median, range, IQR, final value, slope per state variable); (d) for each target $t \in c$, merge features with t, split data 60/20/20 with seed s, standardize on train set, fit linear regression by OLS, compute R^2/MAE/RMSE/MAPE on test set, and append the model and metrics to $\mathcal{M}$, $\mathcal{E}$, $\mathcal{Y}$.
3. Return $\mathcal{M}$, $\mathcal{E}$, $\mathcal{Y}$.

3.1.3 Battery Simulation

For each of the 200 parameter sets we ran a discharge simulation in PyBaMM [14] with the Doyle–Fuller–Newman (DFN) [6] model and the Prada2013 LFP parameter set; outputs include voltage, current, and internal states (e.g., electrode potentials, particle surface concentrations). Simulations were validated to satisfy a 2.0–3.6 V voltage range and physical consistency.

3.1.4 Feature Extraction

From each simulation we extracted, per state variable, the mean, standard deviation, min and max, median, range, interquartile range, final value, and linear slope. This produced one feature vector per sample (200 per combination).

3.2 Machine Learning Pipeline

3.2.1 Data Preprocessing and Splitting

Features were merged with parameter values by sample ID and split 60/20/20 into train/validation/test with a fixed seed. Inputs were standardized to zero mean and unit variance using the training set: $z_i = (x_i - \mu_i)/\sigma_i$, with μ_i, σ_i computed from the training set and the same transform applied to validation and test sets.

3.2.2 Model Training

We used linear regression $y = \beta_0 + \sum_{i=1}^{p} \beta_i x_i + \epsilon$ fitted by ordinary least squares on the standardized training set, implemented with scikit-learn [19].

3.2.3 Model Evaluation

Performance was evaluated on the test set. We report the coefficient of determination

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2} \tag{1}$$

where $\hat{y}_i$ is the predicted value and $\bar{y}$ is the mean of the true values, along with MAE, RMSE, and MAPE (MAPE computed only over samples with $y_i \neq 0$). These metrics were also computed on the training and validation sets to assess overfitting.

3.3 Complete Experimental Pipeline

The pipeline is summarized in Algorithm 1. It yields 80 experiments in total (5+20+30+20+5 over the five combination sizes), each producing a trained model and test metrics.

4 Results

4.1 Single-Variable Linear Regression Baseline

To establish a definitive predictive baseline for autonomous battery design, we first evaluated the fidelity of linear surrogate models [8, 19] under strictly controlled, single-variable conditions using a library of 1,000 synthetic datasets generated via the Python Battery Mathematical Modeling (PyBaMM) [14] framework. This in silico validation methodology effectively isolates the deterministic impact of individual electrode parameters on $LiFePO_4$ (LFP) cell performance [15], successfully bypassing the high sampling variability and time-intensive feedback loops that typically bottleneck experimental materials discovery [16, 17].

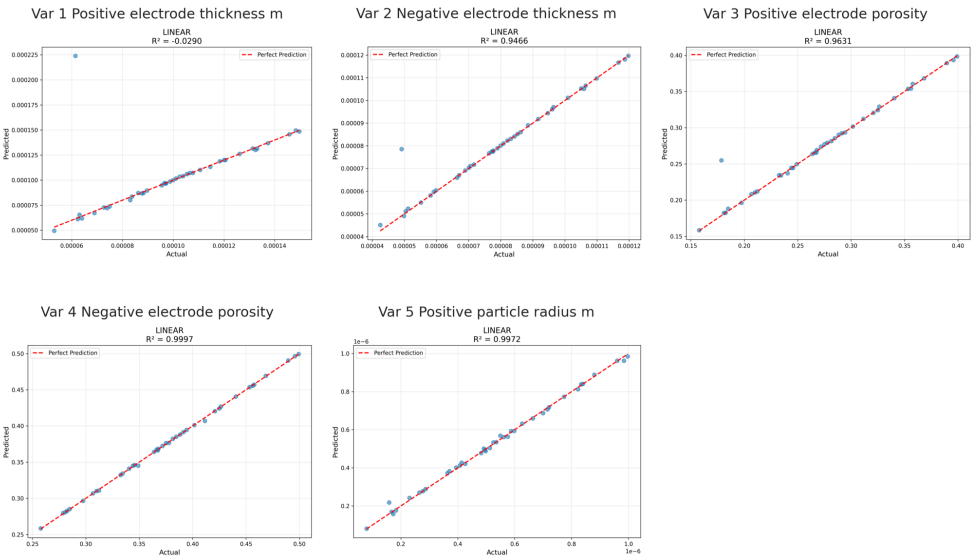


Figure 2: Single-variable linear regression (R^2 per target).

As illustrated in our regression analysis (Figure 2), the framework demonstrates exceptional predictive accuracy across the majority of the primary physical parameters. Notably, near-perfect correlations were achieved for negative electrode porosity ($R^2 = 0.9997$) and positive particle radius ($R^2 = 0.9972$), while negative electrode thickness ($R^2 = 0.9466$) and positive electrode porosity ($R^2 = 0.9631$) also exhibited robust predictive power. These results confirm that within a mechanism-defined simulation environment [6, 14], the fundamental relationships governing electrochemical response remain largely linear when architectural variables are modified independently, providing a rigorous "ground truth" for subsequent multi-dimensional modeling.

The mechanistic interpretation of these findings [12, 15] suggests that the AI model is not merely fitting numerical noise but is capturing physically meaningful electrochemical signatures inherent to the LFP chemistry. The superior predictability of the positive particle radius ($R^2 = 0.9972$) is particularly telling; it underscores that in LFP systems, characterized by one-dimensional lithium-ion diffusion paths and low ionic conductivity, the solid-state diffusion within the cathode serves as the primary rate-determining step. Consequently, the particle radius provides a dominant and linear signal for the model to capture. Conversely, the comparatively lower predictive fidelity for negative electrode thickness and the negligible correlation observed for positive electrode thickness ($R^2 = -0.0290$) reveal a critical sensitivity threshold. In the "positive-limited" design typical of commercial LFP/Graphite cells, variations in the thickness of the positive electrode can yield non-monotonic or effectively "silent" performance changes within specific electrochemical bounds.

4.2 Pairwise Parameter Combinations

Figure 3 shows the pairwise accuracy heatmap. The main finding is a critical conflict zone: the combination of positive and negative electrode thicknesses (Pair 1-2) exhibits $R^2 = -2.00$, while most other pairs maintain high fidelity ($R^2 > 0.98$). This suggests a severe signal redundancy; since

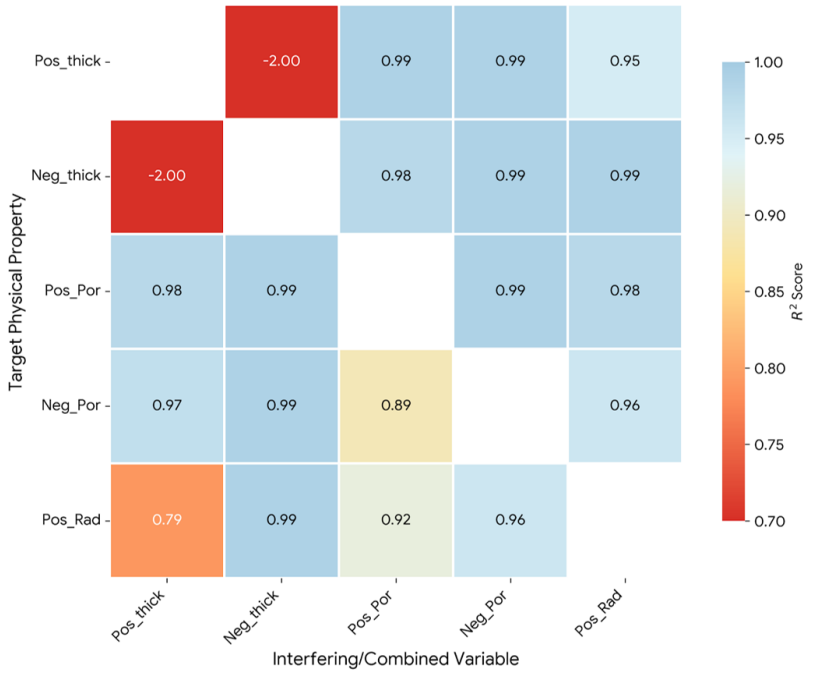


Figure 3: Pairwise R^2 heatmap; thickness pair shows conflict zone ($R^2 = -2.00$).

both parameters primarily dictate the total loading and ohmic response of the cell, their individual impacts on the terminal voltage overlap extensively. This "strong coupling" effect renders the simple linear model incapable of distinguishing the deterministic contribution of each electrode's thickness. These results demonstrate that while linear regression is robust for independent variables, certain physical pairings create an "identification bottleneck" due to mechanistic entanglement. Identifying these interference patterns is crucial for defining the limits of AI-driven design and highlights the necessity of the dQ/dV feature extraction introduced in subsequent sections to resolve such physical overlaps.

4.3 Effect of Feature Number on Model Performance

To systematically investigate how model performance scales with the number of input features, we evaluated the predictive accuracy across all possible parameter combinations ranging from single-variable (1-set) to full five-variable (5-set) configurations. This analysis provides crucial insights into the "dimensionality crisis" [12] by quantifying the performance degradation that occurs as the complexity of the design space increases.

Figure 4 presents the heatmap of test R^2 as a function of the number of features. The single-feature condition confirms the baseline established in Figure 2, with most variables near unity.

However, the progressive introduction of additional features exposes the fundamental limitations of simple linear models in multi-dimensional spaces. For negative electrode porosity, the R^2 score decreases monotonically from 1.000 (1 feature) to 0.804 (5 features), representing a 19.6% relative degradation. Similarly, negative electrode thickness shows a gradual decline from 1.000 to 0.865, while positive electrode porosity exhibits a more modest reduction to 0.891. These patterns suggest that as more variables are simultaneously varied, their electrochemical signatures become increasingly entangled, creating interference that the linear model cannot fully decouple.

Interestingly, positive particle radius and positive electrode thickness demonstrate non-monotonic behavior, with R^2 scores fluctuating based on specific feature combinations. For instance, positive particle radius achieves $R^2 = 0.997$ with a single feature, drops to 0.922 with two features, but recovers to 0.994 with three features before stabilizing around 0.977-0.990. This suggests that certain feature combinations can actually improve predictive performance by providing complementary

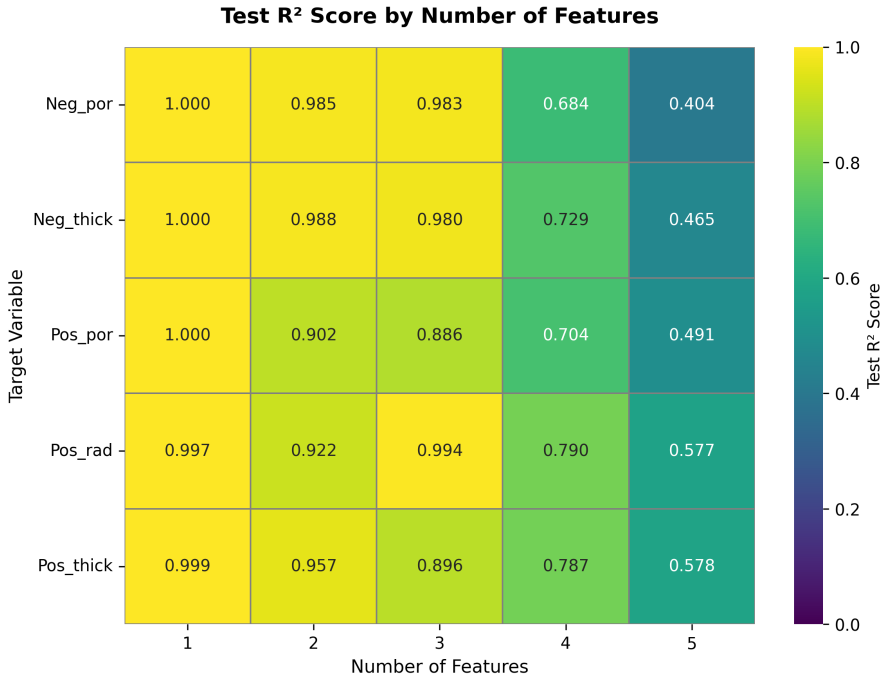


Figure 4: Test R^2 vs. number of features (1–5).

information, while others introduce conflicting signals. These observations highlight the complex, non-linear interactions between architectural parameters and underscore the necessity of advanced feature extraction methods, as demonstrated in the following section.

4.4 Overcoming Dimensionality Limits via Physics-Informed Feature Extraction

To overcome the limitations of simple data augmentation and resolve the dimensionality crisis [12], we implemented a physics- informed feature extraction strategy utilizing differential capacity (dQ/dV) analysis [20, 21]. The fundamental rationale for this approach lies in the inherent nature of raw voltage-time ($V - t$) data, where electrochemical signals are deeply "entangled" in multi-variable environments. Particularly in Lithium Iron Phosphate (LFP) systems, the characteristic flat voltage plateaus make it exceptionally difficult for a linear model to distinguish subtle shifts caused by structural parameters, such as electrode thickness or porosity, from raw voltage values alone. In contrast, feature extraction via dQ/dV [20–24] transforms these subtle slope changes into distinct peaks that represent specific phase transition mechanisms. These peaks serve as unique "physical signatures," providing the model with clear, deterministic markers of the battery's internal state.

Figure 5 illustrates the transformative impact of this feature extraction on the model's predictive fidelity. For the identification of Positive Electrode Thickness (POS THICK), the baseline linear regression model (left) struggled to overcome multi-variable interference, resulting in high dispersion and a low R^2 of 0.5783. However, by providing physically meaningful dQ/dV markers as inputs (Super FE Model, right), the model successfully filtered out the "crosstalk" between variables, allowing predictions to align almost perfectly with the identity line, achieving an R^2 of 0.9946. The quantitative success and the observed limitations of this feature extraction are summarized in Table 2. While the Super FE model achieved a near-perfect improvement for POS THICK ($R^2 = 0.9946$) and a substantial gain for NEG THICK ($R^2 = 0.8581$), it is important to note that this specific method is not universally applicable to all parameters. As evidenced by the steady performance observed in POS POROS, NEG POROS, and POS RADIUS, the results remained nearly identical to the baseline linear regression.

This suggests that while dQ/dV peaks are excellent at capturing structural information related to phase transitions, they may dilute diffusion-related kinetic signatures or introduce non-linearities that a linear model cannot easily map. Therefore, future research must consider a wider array of feature

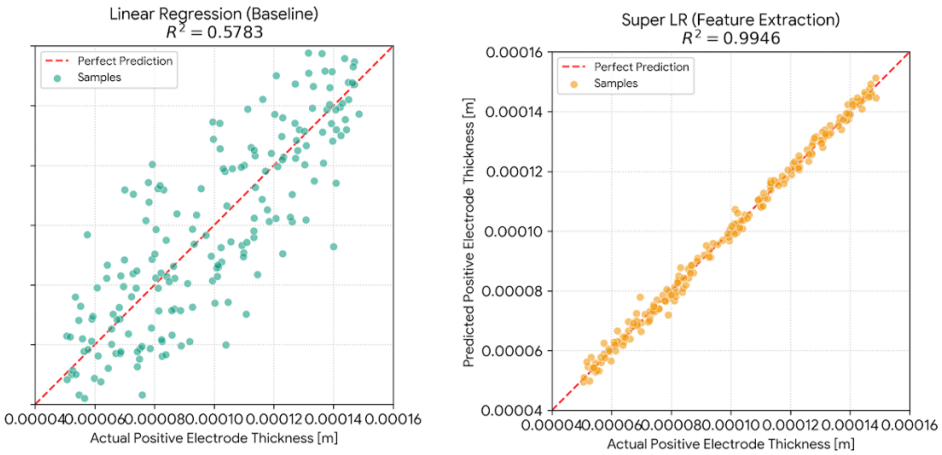


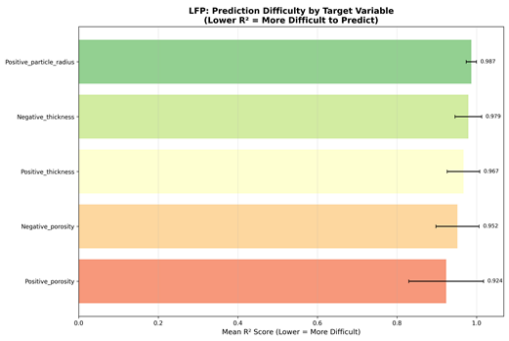
Figure 5: POS THICK: baseline vs. feature extraction (R^2 0.58 vs. 0.99).

extraction techniques—such as voltage relaxation analysis, dV/dQ, or frequency-domain features—to develop an optimized, hybrid feature set tailored to the unique physical sensitivities of each target parameter.

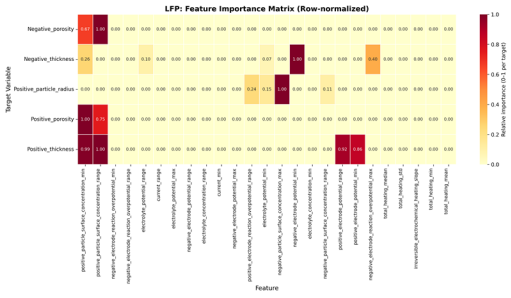
Table 2: Baseline LR vs. super FE model R^2.

Target Parameter (Abbr.)	Baseline LR	Super FE Model	Performance Summary
POS THICK	0.5783	0.9946	Near-perfect improvement (↑)
NEG THICK	0.6668	0.8581	Substantial improvement (↑)
POS POROS	0.6274	0.6043	Steady performance
NEG POROS	0.3389	0.3402	Steady performance
POS RADIUS	0.7404	0.7430	Steady performance

4.5 Prediction Difficulty and Feature Importance Analysis



(a) Analysis of prediction difficulty using R^2 scores and error bars.



(b) Feature importance matrix for physical property identification.

Figure 6: Robustness: (a) prediction difficulty; (b) feature importance matrix.

To evaluate the robustness of the proposed framework, we conducted a comprehensive analysis of prediction difficulty and feature-target correlations (Figure 6). Figure 6(a) shows prediction difficulty; positive porosity is hardest ($R^2 = 0.924$), positive particle radius easiest ($R^2 = 0.987$). Figure 6(b) shows that thickness and porosity correlate strongly with

positive_particle_surface_concentration_* features, consistent with lithium concentration evolution. This "mechanism-aware" learning ensures that the framework provides physically consistent predictions, serving as a transparent tool for autonomous battery design.

5 Discussion

The results confirm that physics-informed feature extraction [13, 20, 21] is critical for overcoming the dimensionality crisis. The pairwise thickness combination (Pair 1–2) that exhibited $R^2 = -2.00$ (Figure 3) illustrates this crisis: raw voltage-based linear regression cannot disentangle strongly coupled parameters. By contrast, dQ/dV-based feature extraction resolves this entanglement for key targets such as POS THICK (Figure 5), turning slope changes into distinct physical markers. The dramatic POS THICK improvement and the need for hybrid strategies are discussed in Section 4.1.

The feature importance analysis (Figure 6) supports mechanism-aware interpretability.

5.1 Limitations

While our framework demonstrates strong predictive performance across most physical parameters, several limitations should be acknowledged. First, the dQ/dV feature extraction method is not universally applicable to all parameters. As shown in Table 2, while POS THICK and NEG THICK show substantial improvements, other parameters such as POS RADIUS and porosity levels show results that are nearly identical to the baseline. This suggests that dQ/dV peaks, while excellent for capturing structural information related to phase transitions, may dilute diffusion-related kinetic signatures that are critical for identifying certain parameters like particle radius.

Second, our study is based entirely on PyBaMM simulation data [14], which, while providing controlled experimental conditions, may not fully capture the variability and noise present in real-world experimental data [10, 30]. The transition from simulation to experimental validation remains a critical next step.

Third, the linear regression model, while effective for many parameters, has inherent limitations in capturing highly non-linear relationships. As demonstrated in Figure 4, certain parameter combinations exhibit non-monotonic behavior, suggesting that more sophisticated non-linear models [25] may be necessary for comprehensive coverage of the design space.

Finally, our framework has been validated on a specific LFP chemistry and may require adaptation for other battery chemistries with different electrochemical behaviors. The generalizability to other cathode materials (e.g., NCM, NCA) [11, 16] would need to be established through additional studies. Electrode architecture innovations such as 3D conductive scaffolds [26] and magnetically ordered microstructures [27] could be integrated with our inverse design pipeline in future work.

6 Conclusion

This study overcomes the "dimensionality crisis" through physics-informed feature disentanglement and dQ/dV-based feature extraction, achieving high predictive fidelity ($R^2 > 0.9$) across key physical parameters when physics-informed features are used. The feature importance analysis (Figure 6) confirms that the model captures physically meaningful mechanisms rather than merely fitting numerical noise, supporting its use for forward prediction; autonomous inverse design remains future work. Future work will focus on integrating Reinforcement Learning (RL) to further optimize the inverse design process [28] and on bridging high-fidelity simulations with real-world experimental data. Data-driven approaches have similarly accelerated discovery in related materials domains [28, 29, 10, 30].

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A Appendix / supplemental material

Optionally include supplemental material (complete proofs, additional experiments and plots) in appendix. All such materials **SHOULD be included in the main submission.**

AI Co-Scientist Challenge Korea Paper Checklist

The checklist is designed to encourage best practices for responsible machine learning research, addressing issues of reproducibility, transparency, research ethics, and societal impact. Do not remove the checklist: **The papers not including the checklist will be desk rejected.** The checklist should follow the references and follow the (optional) supplemental material. The checklist does NOT count towards the page limit.

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