

A New Physics-Informed Artificial Intelligence Methodology for Lithium-Ion Battery State of Health Prognosis

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Abstract

Accurate estimation of the State of Health (SOH) of lithium-ion batteries is essential for the safe operation and lifecycle management of battery systems in electric vehicles and energy storage applications. Existing approaches face significant limitations: physics-based models are computationally expensive and require chemistry-specific parameterization; data-driven methods offer high accuracy but tend to be dataset-specific and lack physical consistency, leading to poor generalization across different operating conditions. This study develops an Enhanced Physics-Informed Neural Network (PINN) framework that integrates data-driven learning with multiple physical degradation constraints to achieve accurate, stable, and generalizable battery SOH estimation. Building upon a dual-network architecture comprising a Solution Network and a Dynamic Network, the proposed framework introduces a multi-physics enhancement strategy incorporating three physically meaningful degradation factors—temperature effects modeled via Arrhenius relationships, capacity degradation laws, and charging efficiency dynamics—through dedicated expert subnets. Experiments on the NASA PCoE battery aging dataset demonstrate that the Temperature-Enhanced PINN reduces MSE by 36.68% relative to the baseline PINN, while the Capacity-Enhanced PINN achieves a 42.13% MSE reduction. These results, validated through 30 independent training runs, demonstrate that embedding physically meaningful degradation mechanisms significantly improves both predictive accuracy and training stability. The optimized framework achieves RMSE of approximately 1.64% and MAE of approximately 1.32%, suitable for practical battery management system deployment.

Keywords

Physics-Informed Neural Network, Battery State of Health, Lithium-Ion Battery, Machine Learning and Degradation Prognosis.

1. Introduction

1.1 Importance and Applications of Lithium-Ion Batteries

In recent years, lithium-ion batteries have emerged as the primary energy storage devices across numerous critical applications, with the distinctive advantages of high energy density, low self-discharge rate, and long service life (Schmuck et al. 2018). Their widespread adoption spans multiple domains: in the automotive sector, these batteries serve as the cornerstone of electric vehicle (EV) technology (Harper et al. 2019); in the renewable energy sector, they play a vital role in solar home systems (Zubi et al. 2020); in grid-scale energy storage, they facilitate load balancing and grid stabilization (Shen and Gao 2020); and in aerospace applications, they power satellites requiring exceptional reliability (Zhao et al. 2022). Portable electronic devices constitute perhaps the most ubiquitous application, powering smartphones, laptops, and countless consumer electronics (Liang et al. 2019).

1.2 Significance of Battery SOH Estimation

The SOH of a battery is defined as the ratio of the current available capacity to the initial capacity, serving as a fundamental indicator of battery degradation (Zhang and Li 2022):

$$\text{SOH} = (\text{Current Capacity} / \text{Nominal Capacity}) \times 100\% \quad (1)$$

When the SOH drops to 80%, the battery typically reaches its first service life threshold. Accurate SOH estimation is essential for preventing catastrophic failures in safety-critical applications, enabling optimal battery utilization and maintenance scheduling, supporting second-life applications in stationary energy storage, and informing battery management system (BMS) operations including charging strategy optimization and cell balancing.

1.3 Challenges and Research Motivation

Despite substantial progress in battery health modeling, accurate SOH estimation remains challenging due to the coupled and nonlinear nature of degradation processes (Berecibar et al. 2016; Che et al. 2023). Physics-based models provide mechanistic interpretability but suffer from high computational cost and require chemistry-specific parameterization (Baghdadi et al. 2016; Xu et al. 2021). Data-driven methods achieve high accuracy but generalize poorly to new battery types or operating conditions (Attia et al. 2020; Richardson and Howey 2017; Luo et al. 2022). These limitations motivate the exploration of Physics-Informed Neural Networks (PINNs) that combine physical interpretability with data-driven flexibility (Raissi et al. 2019; Karniadakis et al. 2021).

This paper presents an Enhanced PINN framework with the following primary contributions: (1) a dual-network PINN architecture separating solution mapping from degradation dynamics; (2) a multi-physics expert subnet design integrating temperature, capacity, and efficiency degradation mechanisms; (3) a 21-dimensional physics-informed feature vector extracted from the CC-CV charging phase; and (4) a three-phase hyperparameter optimization strategy reducing search space by 83% compared to full grid search.

1.4 Research Objectives

Based on the challenges identified above, this research pursues four primary objectives: (1) develop a dual-network PINN architecture that separates SOH solution mapping from degradation dynamics modeling, enabling physics-consistent battery health estimation; (2) design a multi-physics expert subnet framework that integrates temperature, capacity, and efficiency degradation mechanisms through dedicated subnets; (3) construct a 21-dimensional physics-informed feature vector extracted from the CC-CV charging phase that captures universal degradation patterns across different batteries; and (4) establish a three-phase hyperparameter optimization strategy that systematically balances data fidelity and physics constraints while reducing search space by 83% compared to full grid search. These objectives are fulfilled and validated in Sections 3–6.

2. Literature Review

Battery State of Health estimation has been approached from three broad directions: physics-based modeling, data-driven machine learning, and hybrid methods that combine both. Physics-based approaches offer mechanistic interpretability but face computational and generalizability constraints, while data-driven methods achieve high accuracy but lack physical consistency and struggle with cross-battery generalization. Hybrid methods, particularly Physics-Informed Neural Networks (PINNs), have emerged as a promising direction to address these limitations. This section reviews the degradation mechanisms underlying SOH, the key methods developed across these three categories, and the specific PINN architectures that motivate the proposed framework.

2.1 Battery Aging Mechanisms and SOH Evaluation

Battery degradation involves complex physicochemical processes that progressively reduce performance (Birkel et al. 2017). The primary mechanisms include SEI growth on the anode, which continuously consumes lithium ions and increases internal resistance (Pinson and Bazant 2013); lithium plating during fast charging or low-temperature operation (Schindler et al. 2016); structural degradation from mechanical stress causing particle cracking (Liu et al. 2016); and electrolyte decomposition generating gaseous products (Vetter et al. 2005). These mechanisms are modulated by temperature (following Arrhenius behavior), depth of discharge, and charging rates, collectively manifesting as capacity fade and power fade. Their multi-physics nature directly motivates the expert subnet design, where dedicated subnets target thermal, capacity, and efficiency degradation pathways.

State of Health serves as a quantitative measure of battery condition relative to its initial state (Berecibar et al. 2016). Beyond capacity-based formulation, differential analysis techniques including incremental capacity analysis (ICA) and differential voltage analysis (DVA) reveal signature patterns associated with specific degradation mechanisms (Bloom et al. 2005), while electrochemical impedance spectroscopy (EIS) extracts characteristic time constants linked to specific degradation processes (Schmidt et al. 2011). These techniques confirm that SOH is a multi-faceted quantity influenced by interacting physical processes, justifying the multi-physics constraint approach adopted in this work.

2.2 Physics-Based Methods

Physics-based SOH estimation employs electrochemical models derived from first principles, including the Pseudo-Two-Dimensional (P2D) model (Fuller et al. 1994), single particle models (Ramadesigan et al. 2011), and aging-enhanced models incorporating SEI growth and lithium plating (Spotnitz 2003). Despite their theoretical foundation, these methods face significant challenges: extensive parameterization requirements (Tippmann et al. 2014), computational intensity precluding real-time deployment (Wang et al. 2020), and difficulty capturing simultaneous degradation mechanisms (Reniers et al. 2019).

2.3 Data-Driven Methods

Data-driven methods establish relationships between observable battery characteristics and health status. Severson et al. (2019) demonstrated that early-cycle voltage features can predict battery lifetime before significant capacity degradation. Subsequent work has employed LSTM and GRU networks for temporal dependencies (Luo et al. 2022), and feature engineering via differential voltage analysis ((Xia et al. 2023) and electrochemical impedance spectroscopy (Wang et al. 2023b). However, these methods generalize poorly to new battery types (Berecibar 2019) and lack physical interpretability (Wang et al. 2024).

2.4 Hybrid and Physics-Informed Methods

Hybrid approaches combine physical knowledge with data-driven flexibility. Sequential integration uses physics-based models to generate features refined by data-driven models (Thelen et al. 2022), while embedded integration incorporates physical knowledge through specialized loss functions (Aykol et al. 2021). PINNs, formalized by Raissi et al. (2019), incorporate physical knowledge through automatic differentiation and physics-informed loss terms (Karniadakis et al. 2021; Chen et al. 2021). Battery-specific PINN applications include: Wang et al. (2024) proposing a dual-network PINN with solution and dynamic networks; Hofmann et al. (2023) developing a temperature-aware PINN with Arrhenius relationships; Nascimento et al. (2023) combining physics-based models with Bayesian neural networks; and Wang et al. (2023a) developing an inherently interpretable PINN.

Formally, PINNs approximate the solution $u(x, t)$ of a physical system $F[u; \lambda] = 0$ using a neural network $\hat{u}_\theta$, trained to minimize:

$$\mathcal{A}(\theta) = \omega_{\text{data}} \mathcal{L}_{\text{data}}(\theta) + \omega_{\text{phys}} \mathcal{L}_{\text{physics}}(\theta) \quad (2)$$

where the physics loss evaluates residuals of governing equations at collocation points. For battery SOH estimation, this framework enables automatic differentiation to compute $\partial \text{SOH} / \partial t$ exactly, enforcing degradation dynamics as soft constraints embedded in the loss function during training (Raissi et al. 2019; Karniadakis et al. 2021). PINNs offer enhanced generalization beyond training distributions, effective learning from small datasets, and physical interpretability—all critical advantages for battery applications where data collection is expensive and cross-battery generalization is essential (Wang et al. 2023a; Nascimento et al. 2023).

Collectively, the literature reveals a clear gap: existing physics-based methods lack scalability, purely data-driven methods lack physical consistency and generalizability, and current PINN approaches typically incorporate only single-physics constraints. No existing work systematically integrates multiple physical degradation mechanisms—thermal, capacity, and efficiency—through dedicated expert subnets within a unified dual-network architecture. The proposed Enhanced PINN framework directly addresses this gap by embedding three complementary physics constraints through specialized subnets, supported by a 21-dimensional physics-informed feature vector and a systematic three-phase hyperparameter optimization strategy.

3. Methodology

3.1 PINN Architecture

The proposed framework employs a dual-network architecture, illustrated in Figure 1, that separates solution mapping from degradation dynamics modeling.

The Solution Network $F_{\theta}(\cdot)$ approximates the unknown mapping $u_i = f(t_i, x_i)$, where u_i denotes SOH at cycle i , t_i represents cycle index, and $x_i \in \mathbb{R}^{21}$ is the physics-informed feature vector:

$$\text{SOH} = \sigma(W_3 \cdot \text{ReLU}(W_2 \cdot \text{ReLU}(W_1[t, x] + b_1) + b_2) + b_3) \quad (3)$$

The network takes input $[t, x] \in \mathbb{R}^{22}$ through two hidden layers ($W_1 \in \mathbb{R}^{64 \times 22}$, $W_2 \in \mathbb{R}^{32 \times 64}$) with ReLU activations and dropout ($p = 0.3$), with sigmoid output ensuring $\text{SOH} \in [0, 1]$.

The Dynamic Network $G_{\varphi}(\cdot)$ models degradation dynamics $\partial u / \partial t = g(t, x, u)$:

$$d\text{SOH}/dt = V_3 \cdot \text{ReLU}(V_2 \cdot \text{ReLU}(V_1[t, x, \text{SOH}] + c_1) + c_2) + c_3 \quad (4)$$

with augmented input $[t, x, \text{SOH}] \in \mathbb{R}^{23}$ ($V_1 \in \mathbb{R}^{64 \times 23}$, $V_2 \in \mathbb{R}^{32 \times 64}$). Including current SOH as input enables state-dependent degradation acceleration modeling.

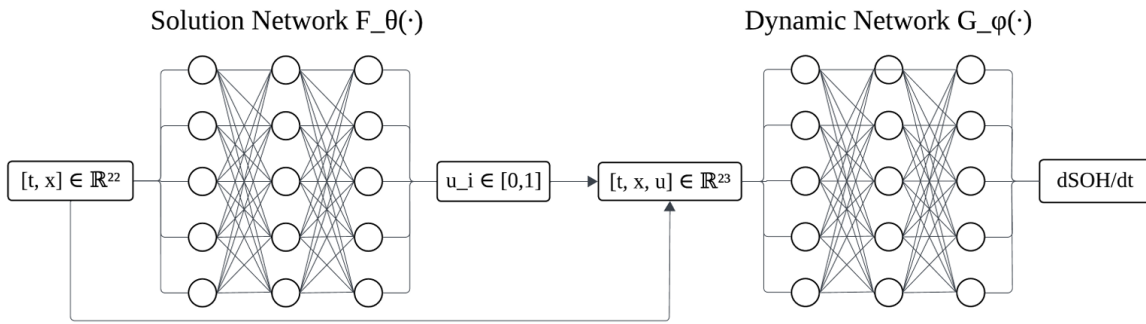


Figure 1. Proposed dual-network PINN architecture. The Solution Network maps charging features and cycle index to SOH predictions; the Dynamic Network models degradation rate. Enhanced variants incorporate specialized expert subnets.

3.2 Physics Constraints and Loss Function

The total loss integrates data fidelity, physics consistency, and monotonicity:

$$\mathcal{L}_{\text{total}} = \mathcal{L}_{\text{data}} + \lambda_{\text{phys}} \mathcal{L}_{\text{physics}} + \lambda_{\text{mono}} \mathcal{L}_{\text{mono}} \quad (5)$$

The data loss measures prediction accuracy:

$$\mathcal{L}_{\text{data}} = (1/N) \sum_i (\text{SOH}_{i_pred} - \text{SOH}_{i_true})^2 \quad (6)$$

The physics loss enforces consistency between solution and dynamic networks through the PINN residual $H(t, x) := \partial F_{\theta} / \partial t - G_{\varphi}(t, x, F_{\theta})$, computed via automatic differentiation:

$$\mathcal{L}_{\text{physics}} = (1/N) \sum_i | H(t_i, x_i) |^2 \quad (7)$$

The monotonicity loss penalizes SOH increases between consecutive cycles:

$$\mathcal{L}_{\text{mono}} = (1/M) \sum_j (1/(N_j - 1)) \sum_k \text{ReLU}(\text{SOH}_{j_pred}^{k+1} - \text{SOH}_{j_pred}^k) \quad (8)$$

Optimal weights $\lambda_{\text{phys}} \in [0.3, 0.7]$ and $\lambda_{\text{mono}} \in [0.05, 0.15]$ are determined through systematic parameter optimization.

3.3 Enhanced Expert Subnet Variants

Three enhanced PINN variants incorporate domain-specific physical constraints through specialized subnets whose outputs augment the mapping network input.

Temperature-Enhanced PINN processes five thermal features (T_{mean} , T_{std} , T_{max} , T_{min} , T_{slope}) to compute an Arrhenius degradation factor:

$$f_{\text{arr}} = \exp(-E_a / [R \cdot (T_{\text{mean}} + 273.15)]) \quad (9)$$

with constraint $\mathcal{L}_{\text{temp}}$ enforcing correlation between thermal features and degradation rate.

Capacity-Enhanced PINN processes accumulated charge features through a capacity subnet, computing:

$$f_{\text{cap}} = 0.7 \cdot Q_{\text{v,norm}} + 0.3 \cdot Q_{\text{i,norm}} \quad (10)$$

Efficiency-Enhanced PINN processes charging time and slope features, enforcing the inverse relationship between efficiency and degradation rate. TCE-Combined PINN integrates all three subnets in parallel:

$$d_{\text{final}} = d_{\text{dynamic}} \cdot f_{\text{arr}} \cdot (1 - f_{\text{cap}}) \cdot f_{\text{eff}} \quad (11)$$

3.4 Feature Engineering

A 21-dimensional physics-informed feature vector is extracted from the CC-CV charging phase within voltage range [4.0 V, 4.2 V] and current range [0.1 A, 0.5 A], capturing the constant-voltage phase where degradation effects are most pronounced. Features are organized into four physics-based groups (Table 1): the capacity group quantifies energy storage via accumulated charge ($\int V dt$, $\int I dt$); the efficiency group captures charge transfer kinetics via time and slope features (dV/dt , dI/dt); the stability group applies statistical descriptors (standard deviation, skewness, kurtosis, Shannon entropy) to voltage and current signals; and the temperature group extracts five thermal features capturing Arrhenius-type dynamics. All features undergo z-score normalization $x_{\text{norm}} = (x - \mu_{\text{train}}) / \sigma_{\text{train}}$, with parameters computed exclusively from training data to prevent data leakage.

Table 1. Physics-based feature grouping

Group	Physical Significance	Count	Subnet
Capacity	Energy storage ($\int V dt$, $\int I dt$)	2	Capacity
Efficiency	Charge transfer kinetics (time, slope)	4	Efficiency
Stability	Signal variability (std, skewness, kurtosis, entropy)	8	–
Temperature	Thermal dynamics (mean, std, max, min, slope)	5	Temperature

4. Data Collection

4.1 NASA PCoE Battery Dataset

This research uses the NASA Ames Prognostics Center of Excellence (PCoE) lithium-ion battery aging dataset, a standard benchmark in battery PHM research. It contains lifecycle data from four 18650 batteries (B0005, B0006, B0007, B0018) cycled under CC-CV protocol (1.5 A constant current to 4.2 V, then constant voltage to 20 mA cutoff) until 30% capacity fade. Dataset statistics are summarized in Table 2. SOH is computed as $\text{SOH}(n) = C_{\text{discharge}}(n) / C_{\text{initial}}$. Battery B0005 serves as the fixed test set; B0006, B0007, and B0018 are used for training and validation via leave-one-battery-out cross-validation.

Table 2. NASA PCoE battery dataset statistics

Battery	Total Cycles	Charge	Discharge	Init. Cap. (Ah)	Final Cap. (Ah)	SOH Range
B0005	616	170	168	1.856	1.287	0.693–1.000
B0006	616	170	168	2.035	1.154	0.567–1.000
B0007	616	170	168	1.891	1.401	0.741–1.000
B0018	319	134	132	1.855	1.341	0.723–1.000

4.2 Experimental Setup and Hyperparameter Optimization

Each model configuration undergoes 30 independent training runs with different random seeds. The three-phase hyperparameter optimization searches: Phase I over learning rates $\{0.0005, 0.001, 0.002\}$ and physics loss weights $\{0.3, 0.5, 0.7\}$ (9 configurations); Phase II over enhancement-specific loss weights and correlation thresholds (25 configurations); Phase III over monotonicity weights $\{0.05, 0.1, 0.15\}$ and early stopping patience $\{30, 50, 70, 100\}$ (12 configurations). This sequential strategy tests 46 total configurations versus 270 for full grid search—an 83% reduction in computational cost. Implementation uses PyTorch with Adam optimizer (weight decay = 10^{-4}), maximum 1000 epochs, and early stopping. Performance is evaluated using MSE, RMSE, and MAE, reported as mean $\pm$ standard deviation across 30 runs.

5. Results and Discussion

5.1 Basic PINN Performance

The baseline PINN achieves stable performance across 30 runs on Battery B0005: MSE = 0.000432 ± 0.000056 , RMSE = 0.020785 ± 0.001483 , MAE = 0.016709. Figure 2 illustrates the training dynamics, showing smooth data loss convergence with physics loss initially oscillating before converging, and monotonicity loss maintaining a persistent residual of approximately 0.015–0.025.

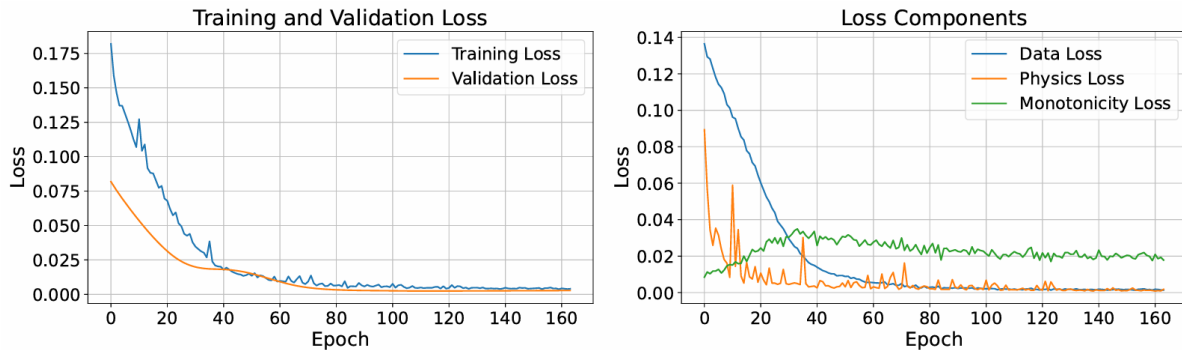


Figure 2. Training dynamics of the basic PINN. Left: training and validation loss convergence. Right: individual loss component evolution showing data, physics, and monotonicity losses. Early stopping activates around epoch 190.

Figure 3 illustrates the SOH prediction trajectory on the test set. The model captures the overall degradation trend, with increased oscillations beyond cycle 75 reflecting growing nonlinear degradation effects and a slight positive bias in mid-to-late lifecycle stages.



Figure 3. Basic PINN SOH prediction on Battery B0005. Predicted SOH closely follows the true degradation trend, with increased oscillations in later stages where nonlinear degradation effects become prominent.

5.2 Enhanced Model Comparison

Table 3 summarizes performance of all model variants. The Temperature-Enhanced PINN achieves 36.68% MSE reduction through Arrhenius-based thermal constraints. Figure 4 shows improved tracking during the nonlinear degradation phase after cycle 50. The Capacity-Enhanced PINN achieves the strongest individual performance (42.13% MSE reduction), with Figure 5 showing an additional 8.53% improvement over the temperature variant, confirming that accumulated charge features carry stronger long-term predictive signal. The Efficiency-Enhanced variant shows modest gains (2.18%), reflecting the indirect nature of efficiency–SOH coupling. The TCE-Combined model achieves 14.58% MSE reduction, demonstrating synergistic improvements from integrating multiple physics constraints.

Table 3. Enhanced PINN performance comparison on Battery B0005

Model	MSE	RMSE	MAE	MSE Improv.
Basic PINN	0.000432	0.020785	0.016709	—
Temperature-Enhanced	0.000273	0.016530	0.013671	36.68%
Capacity-Enhanced	0.000250	0.015810	0.012937	42.13%
Efficiency-Enhanced	0.000422	0.020547	0.016414	2.18%
TCE-Combined	0.000369	0.019219	0.015645	14.58%

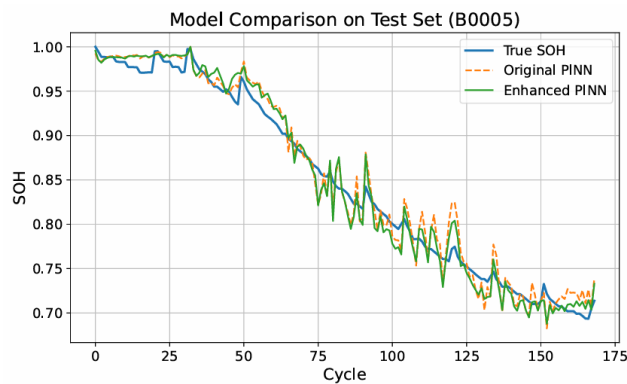


Figure 4. Temperature-Enhanced vs. Basic PINN on B0005. The temperature-enhanced model tracks true SOH more closely, particularly in the nonlinear degradation phase after cycle 50.

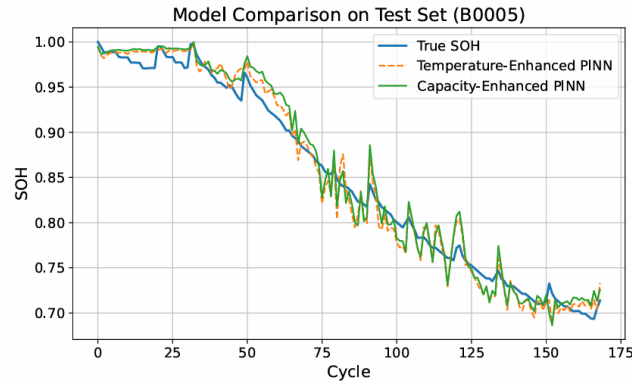


Figure 5. Capacity-Enhanced vs. Temperature-Enhanced PINN on B0005. The capacity-enhanced model achieves an additional 8.53% MSE reduction over the temperature-enhanced variant.

5.3 Feature Importance Analysis

Permutation importance analysis evaluates feature contributions by measuring MSE increase when each feature is randomly shuffled (repeated 5 times). Table 4 presents the results. Accumulated charge features dominate: current accumulated charge ranks first (0.0038) and voltage accumulated charge ranks third (0.0012), directly reflecting cumulative battery usage and degradation history. Temperature variability ranks second (temperature standard deviation, 0.0034), confirming that thermal variability—not only mean temperature—is a critical stress indicator consistent with Arrhenius kinetics. Higher-order descriptors (skewness, kurtosis, entropy) score near zero, suggesting they contribute little beyond accumulated charge and standard deviation. These rankings directly validate the expert subnet design: dedicated capacity and temperature subnets yield the largest individual performance gains.

Table 4. Top 10 most important features

Rank	Feature	Importance	Std Dev
1	Current Accumulated Charge	0.0038	0.0005
2	Temperature Std	0.0034	0.0002
3	Voltage Accumulated Charge	0.0012	0.0002
4	Temperature Max	0.0008	0.0001
5	Current Charging Time	0.0007	0.0001
6	Temperature Slope	0.0006	0.0001
7	Current Slope	0.0004	0.0001
8	Current Std	0.0004	0.0001
9	Voltage Std	0.0003	0.0001
10	Voltage Slope	0.0003	0.0001

5.4 Parameter Optimization Effects

The three-phase optimization yields an additional 20.88% MSE reduction over the default configuration. Table 5 presents the optimized hyperparameters alongside default vs. optimized performance. The reduced learning rate (0.0005) enables stable convergence balancing multiple loss terms. The physics loss weight reduction (0.5 to 0.3) prevents overly aggressive constraints from restricting data-driven learning, while the temperature loss weight increase (0.2 to 0.4) is consistent with feature importance rankings. Cross-battery validation (Table 6) confirms consistent generalization across all batteries.

Table 5. Hyperparameter optimization: configuration and performance gains

Parameter	Default	Optimized	Metric	Improvement
Learning Rate	0.001	0.0005	MSE	20.88%
Physics Loss Weight	0.5	0.3	RMSE	11.16%
Temperature Loss Weight	0.2	0.4	MAE	12.57%
Correlation Threshold	0.1	0.05		
Monotonicity Weight	0.1	0.05		
Early Stopping Patience	50	100		

Table 6. Cross-battery validation (optimized model)

Battery	MSE	RMSE	MAE	Cycles
B0006	0.000270	0.016391	0.013228	616
B0007	0.000295	0.017089	0.013624	616
B0018	0.000252	0.015825	0.012695	319
Avg	0.000273	0.016435	0.013182	—

6. Conclusion

This paper presents an Enhanced Physics-Informed Neural Network framework for lithium-ion battery SOH estimation integrating multi-physics domain knowledge through specialized expert subnets. The basic PINN dual-network architecture establishes a strong baseline, with physics constraints preventing physically implausible predictions and enabling cross-battery generalization without retraining. The Temperature-Enhanced PINN achieves 36.68% MSE reduction by capturing Arrhenius-type thermal acceleration of degradation. The Capacity-Enhanced PINN achieves 42.13% MSE reduction through explicit modeling of accumulated charge-based capacity fade. Systematic three-phase hyperparameter optimization yields an additional 20.88% MSE reduction. The optimized framework achieves $RMSE \approx 1.64\%$ and $MAE \approx 1.32\%$, suitable for practical BMS deployment.

This research makes several distinct contributions: a dual-network PINN architecture separating SOH mapping from degradation dynamics; a multi-physics expert subnet design enabling targeted integration of heterogeneous physical knowledge; a 21-dimensional physics-informed feature vector organized by physical phenomena; and a three-phase optimization strategy achieving 83% search space reduction with statistically significant performance gains. Feature importance analysis confirms that accumulated charge and temperature variability dominate predictions, validating the expert subnet choices, and consistent cross-battery performance across B0006, B0007, and B0018 confirms effective generalization. Future work includes combining all expert subnets in a unified TCE architecture with adaptive loss weighting, extending validation to LFP and NMC battery chemistries, incorporating probabilistic uncertainty estimation for safety-critical deployment, and investigating lightweight model compression for edge BMS deployment.

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Biography

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