Supporting Information

Neural Network Driven by Electrochemical Performance Data for Predicting the Discharge Termination Time of Seawater Electrolyte-Based Metal-Air Batteries

Pengpeng Shen #, Yichi Pan #, Yurong Liu #, Ludan Zhang, Ning Niu, Guanjun Wang *, Dekun Yang *, Xinlong Tian *, Peng Rao *

State Key Laboratory of Tropic Ocean Engineering Materials and Materials Evaluation, School of Information and Communication Engineering, School of Electronic Science and Technology, Hainan University, Haikou 570228, China

# These authors contributed equally to this work

*Corresponding author: wangguanjun@hainanu.edu.cn (G. Wang), dekun.yang@hainanu.edu.cn (D. Yang), tianxl@hainanu.edu.cn (X. Tian), raopeng@hainanu.edu.cn (P. Rao)

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S1 Note S1: Dataset and Training Configuration Details

This section provides a comprehensive dataset description including the number of measurements per catalyst and the variability of experimental conditions. In addition, all relevant neural network training configurations are disclosed, including key hyperparameters such as window size, stride, prior kernel width, and Huber loss threshold. All raw electrochemical performance data are compiled in the attached table named Source Data.xlsx, which is available via the Supporting Information link at the end of this article. These measures ensure full transparency and reproducibility of our work.

The dataset contained nine catalyst-level records in total. Each record consisted of one CA time-series, one LSV curve, and one corresponding discharge termination time label. Among the three Pt/C-related records, two records were used as independent outer-test samples, denoted as Pt/C and Pt/C-Ref, while the third Pt/C record was used only for training/inner validation and was denoted as Pt/C-training.

Table S1. Dataset description.

Sample name	Data source
Cl-Fe-SA/NC	Our work
Fe-SA/NC	Our work
Fe-SAC/NC(py)	Our work
Fe-SAC/NC	Our work
FeCo-DSACS	Our work
NMC-Co9Se8	References
Pt/C	Our work
Pt/C-Ref	References
Pt/C-training	Our work

The CA time-series was segmented using a sliding window with a window size of 150 and a stride of 10. For the LSV prior construction, two Gaussian kernels were used to emphasize the half-wave potential and the limiting-current plateau region, with kernel widths of 0.025 V and 0.09 V, respectively. Model optimization was performed using the SmoothL1/Huber loss, where the threshold parameter was set to 1.0. Detailed key hyperparameters and training configurations are summarized in Table S2.

Table S2. Key hyperparameters and training configurations used in the proposed model.

Category	Hyperparameter	Value
Input preprocessing	CA window size	150
Input preprocessing	CA stride	10
Input preprocessing	LSV potential range	0.20-1.10 V

Input preprocessing	Number of LSV grid points	512
Training configuration	Maximum training epochs	15
Training configuration	Batch size	64
Training configuration	Optimizer	AdamW
Training configuration	Learning rate	1×10^{-3}
Training configuration	Weight decay	1×10^{-2}
Training configuration	Gradient clipping threshold	1.0
Training configuration	Loss function	SmoothL1Loss / Huber
Training configuration	Huber loss threshold	$\beta = 1.0$
Model setting	InceptionTime backbone	Frozen
Electrochemical prior	Prior strength	3.0
Electrochemical prior	E1/2 prior kernel width	0.025 V
Electrochemical prior	Plateau prior kernel width	0.09 V
Electrochemical prior	E1/2 prior gain	1.8
Electrochemical prior	Plateau prior gain	0.30
Electrochemical prior	Prior floor	0.03
Data augmentation	CA augmentation noise	0.002
Data augmentation	LSV augmentation noise	0.005
Prediction aggregation	Trim ratio	0.10

S2 Note S2: Ablation Comparison Studies

S2.1 Performance Comparison Between PBAP and Standard Attention Mechanism

The performance comparison results are shown in Fig. S1a-b, which quantifies the specific contribution of electrochemical priors. The results indicate that the standard attention mechanism cannot effectively extract and distinguish the critical information from the LSV curves of different catalyst samples. In contrast, the PBAP module can effectively establish the true correlation between the intrinsic LSV characteristics of catalysts and their discharge performance.

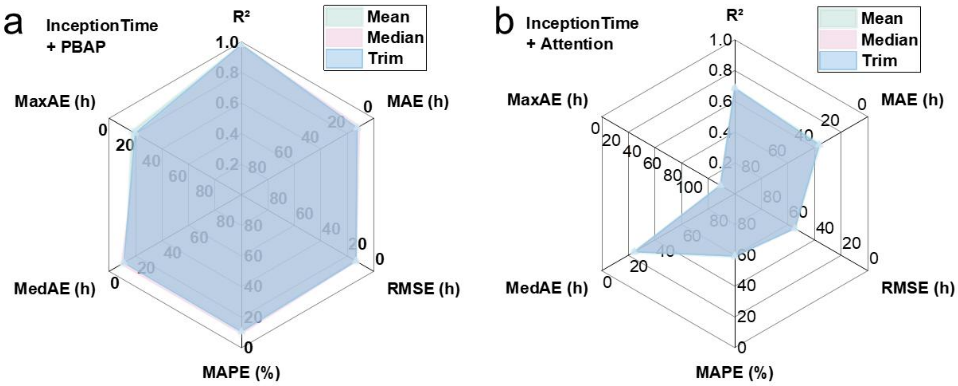

Figure S1. Performance comparison between InceptionTime + PBAP and InceptionTime with standard attention mechanism

S1.2 Systematic Validation of Backbone Freezing

As shown in Table S3, freezing the backbone network leads to a slight performance improvement and is a more reliable training option.

Table S3. Systematic validation results of backbone freezing strategy on model performance and generalization

InceptionTime + PBAP	mean	median	trim	No Freeze	mean	median	trim
R^2	0.981	0.983	0.981	R^2	0.947	0.965	0.954
MAE (h)	13.331	10.374	12.460	MAE (h)	21.318	15.488	19.091
RMSE (h)	13.574	12.883	13.419	RMSE (h)	22.498	18.198	21.016
MAPE (%)	11.435	8.824	10.610	MAPE (%)	20.431	14.194	18.476
MedAE (h)	12.937	9.024	11.177	MedAE (h)	19.159	13.832	16.900
MaxAE (h)	17.170	21.583	19.752	MaxAE (h)	30.070	29.817	30.179