Optimizing Catalyst Layer Composition of PEMFC via Machine Learning: Insights from In-House Experimental Data

Speaker: Yuze Hou
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Fraunhofer ISE Fuel Cell Scientific Insights Webinar
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Our Mission in Our Department Fuel Cell

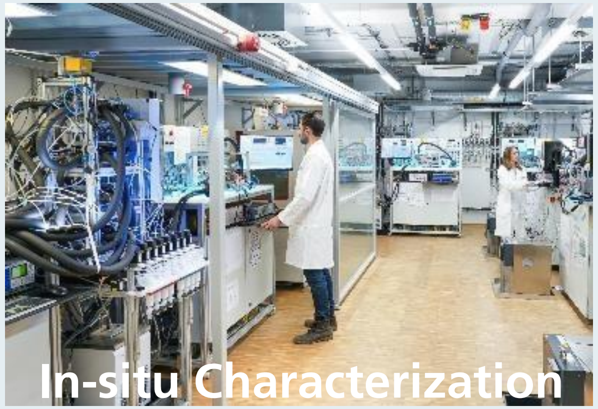
Assisting Global Industry with Scientifically Sound Services

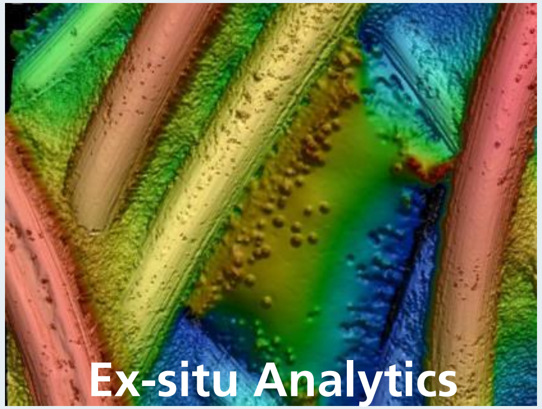
Understanding Fuel Cell Membrane Electrode Assemblies (MEAs)

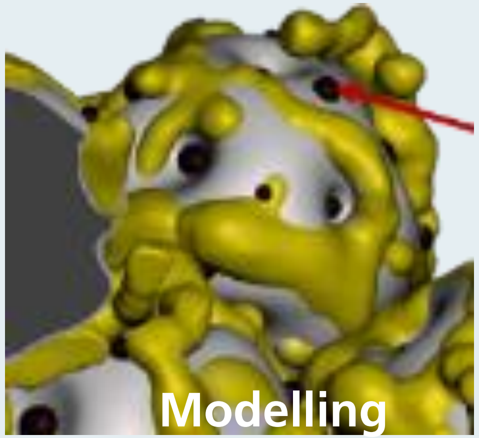
Key Performance Indicators 2024:

- 45 researchers plus students
- 9.2 Mio. € annual budget (w/o investments)
- 33% direct revenue by industry contract research
- > 500 m² laboratory area with 13 single cell test stations, 5 short stack test stations including temperature chamber (all fully automated for 24/7 operation)
- Focus on transport application

Enjoy our virtual lab tour



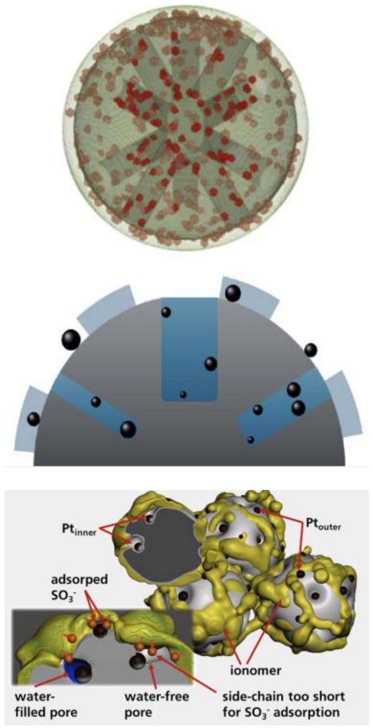


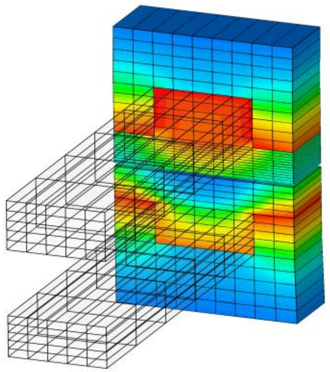


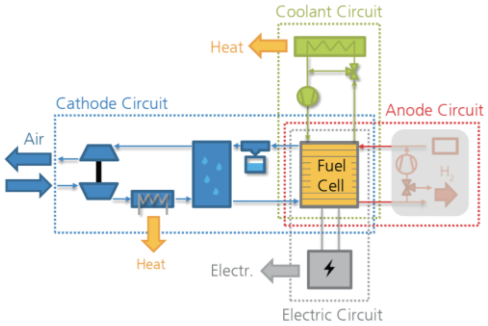
Team Modeling

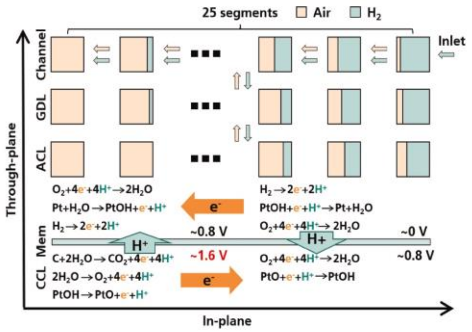
Electrode to System, Physics to AI

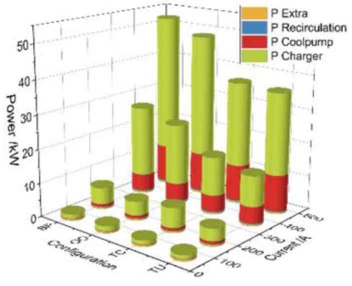
Physics models





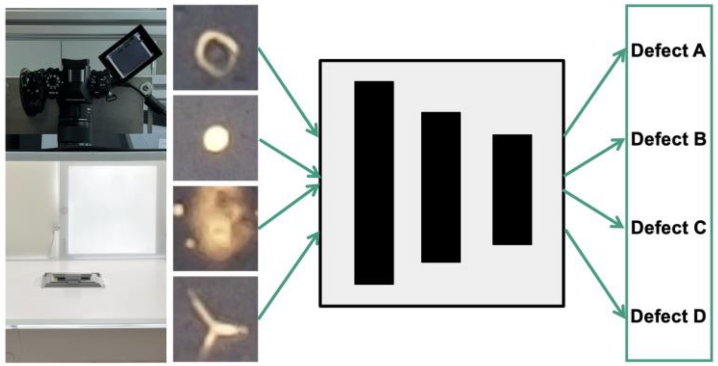


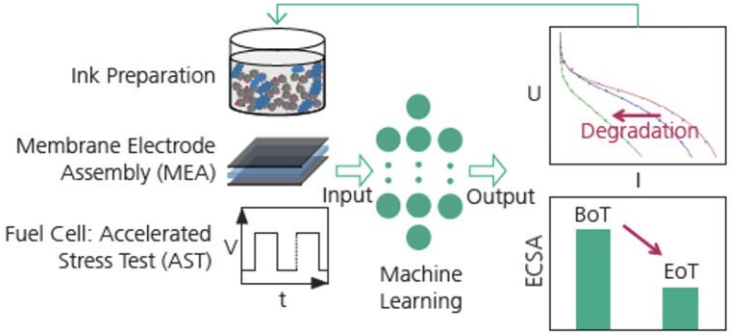




Electrode Single Cell System

AI





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Content

1. **Research Background**
2. **Data Generation**
   - Consistent Production
   - Consistent Characterization
3. **Model Training & Evaluation**
4. **Results & Disscussion**
5. **Conclusions**

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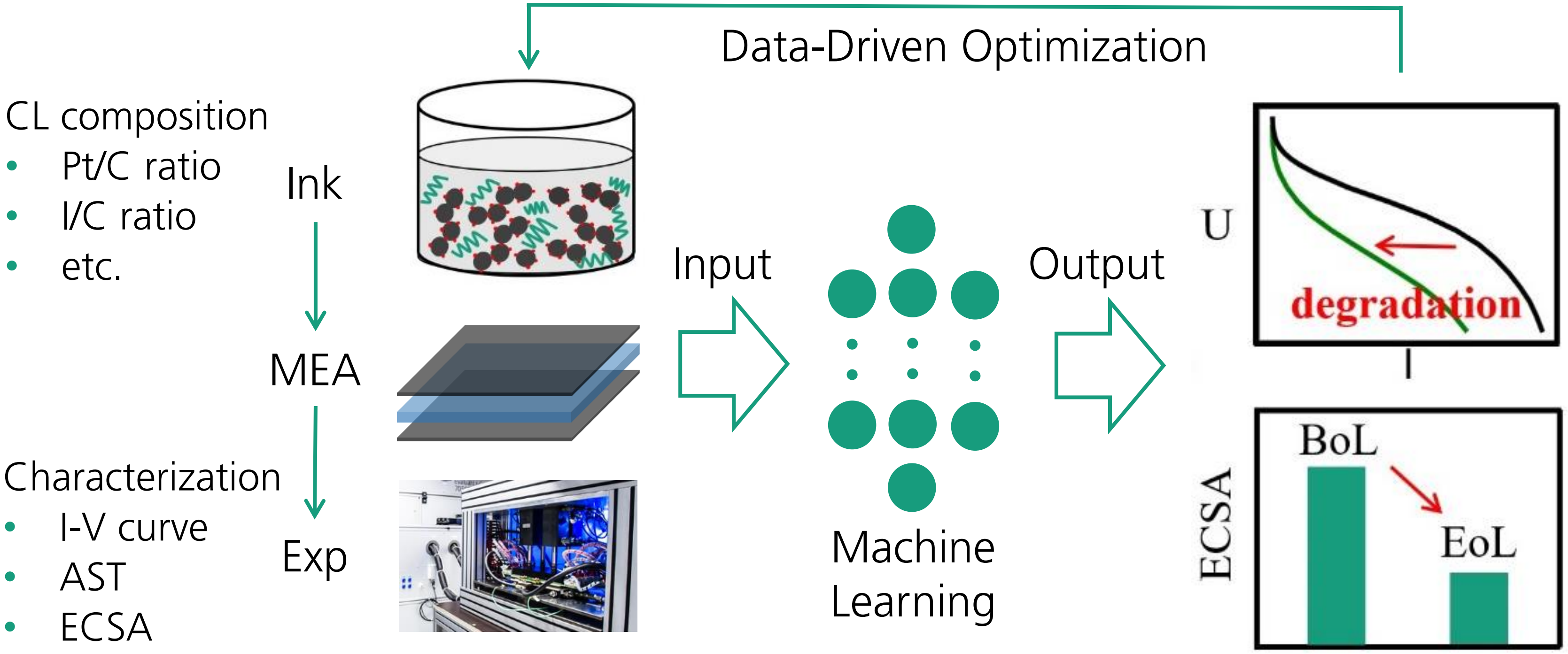
Research Background

Motivation

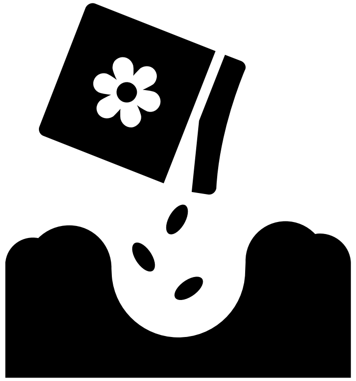
- The catalyst layer plays a critical role in determining the cost and commercial viability of PEM fuel cells.



- Understand the intricate interplay between CCL ink composition, performance, and durability.

Research Background

Uniqueness of Our AI



Data Acquisition → Data Cleaning → Data Featurization

↓

Model Selection → Model Evaluation → Model Deployment

Content

1. Research Background

2. **Data Generation**
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   - Consistent Characterization

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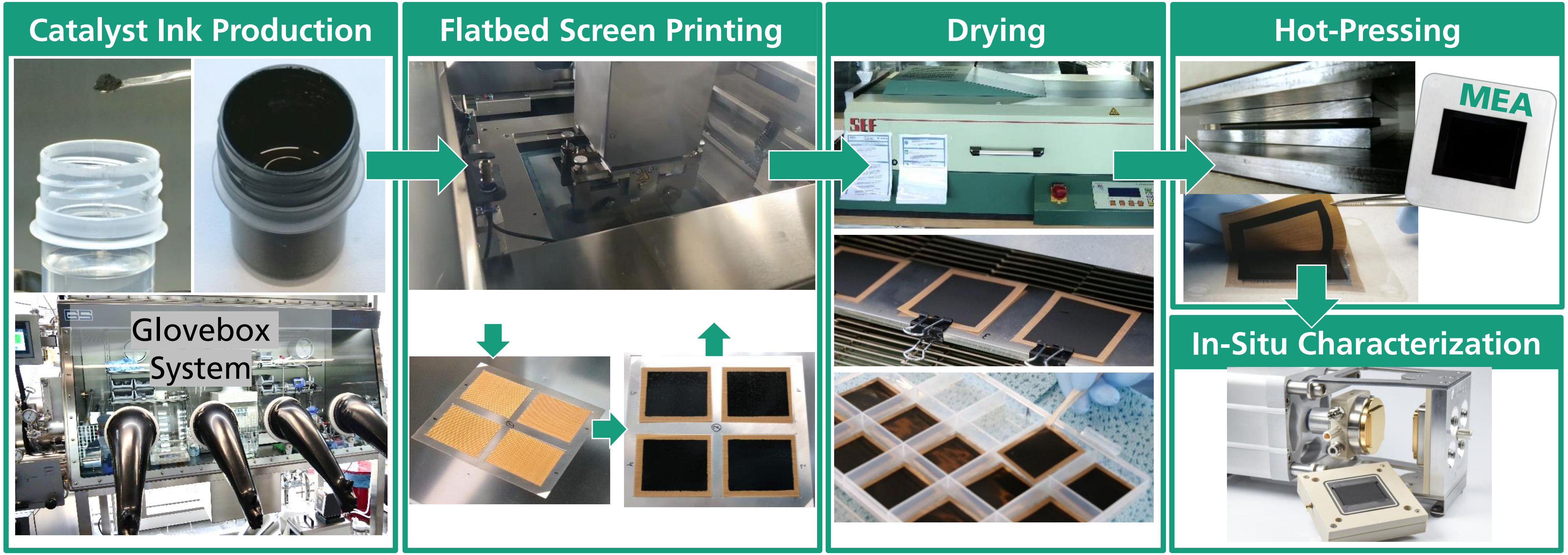
Data Generation
Consistent Production

- Our expertise in production guarantees consistent MEAs.



[1] Ney et al., European Coating Symposium ECS 2021, Challenges of Fabricating Catalyst Layers for PEM Fuel Cells using Flatbed Screen Printing, 2021

Data Generation

Ink Composition Design

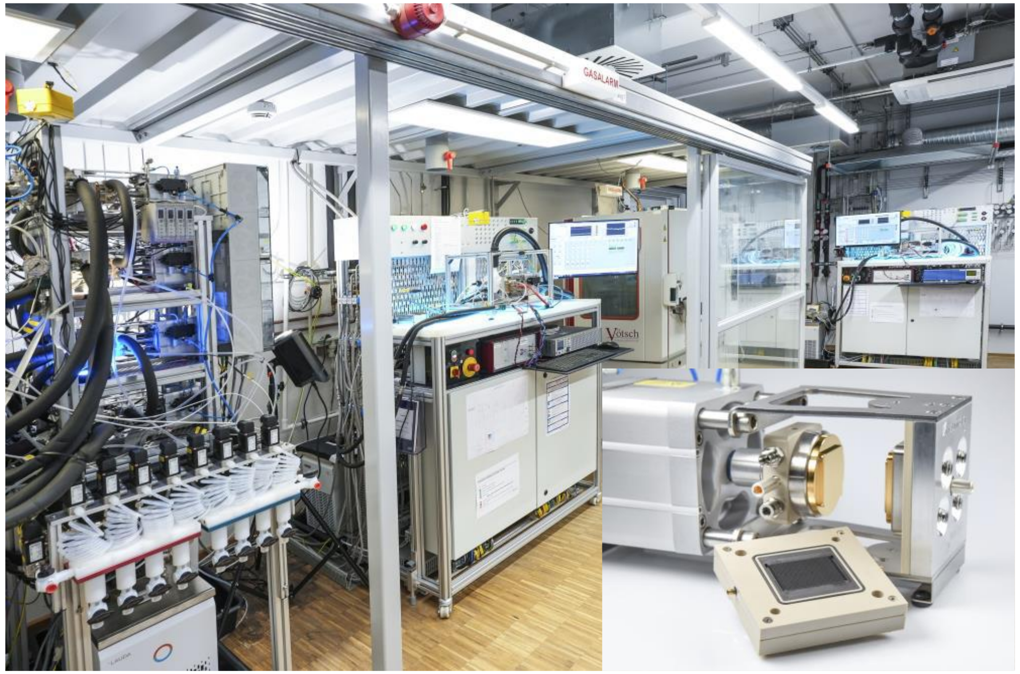
Variations	Group 1			Group 2					Group 3			
Pt/C ratio	50%			20%	30%	40%	50%	60%	50%			
I/C ratio	0.5	0.8	1.2	0.8					1.2			
Ionomer EW	790			790					720	790	830	980

- Cathode Pt loading: 0.4 ± 0.05mg cm^{-2}
- Cathode carbon support: High surface carbon
- Ionomer: Short side chain ionomer
- Membrane: GORE Membrane 18µm thickness

Data Generation

Consistent Characterization

- Comprehensive BoT and EoT characterization
- AST from DoE catalyst degradation protocol
- Fully automated testbench operation



Step Nr.		Protocol		Estimated test time [h]
1		BreakIn	Galvanostatic BreakIn, 2h @ 1.5 A/cm2	9
2			Recovery	
3			Potentiostatic BreakIn, 6h cycling between OCV, 0.6, 0.4 V	
4	0	BoT Characterization	Recovery (Table P.9)	25
	1		Limiting Current @ 4 pressures and 4 O2 concentrations (16 total)	
	2		Recovery	
	3		UI-Curves @ RH 100%	
	4		EIS H2/Air @ RH 100%	
	5		EIS H2/N2 @ RH 100%	
	6		Recovery	
	7		UI-Curves @ RH 70%	
	8		EIS H2/Air @ RH 70%	
	9		EIS H2/N2 @ RH 70%	
	10		Recovery	
	11		UI-Curves @ RH 40%	
	12		EIS H2/Air @ RH 40%	
	13		EIS H2/N2 @ RH 40%	
	14		Recovery	
	15		CV @ 100mV/s	
	16		LSV @ 1mV/s	
5		Catalyst Aging (DoE protocol) - Cycle Steps: 10,100,1k,3k,5k,10k,20k,30k	Degradation protocol: potential cycles 0.6 - 0.95 V (Table P.1)	71
			CV @ 100mV/s	
			H2/N2 @ RH100%	
			Recovery	
			UI-Curves @ RH 100% (only after 1k, 5k,10k cycles)	
6	0-16	EoT Characterization	same as BoT	25
				130

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Data Generation

Characterization Design

Variations	I/C ratio	Pt/C ratio	Ionomer EW
Operating RH	40% · 70% · 100%	40% · 70% · 100%	40% · 70% · 100%
AST potential	0.6~0.95 V · 0.6~1.15 V	0.6~0.95 V · 0.6~1.15 V	0.6~0.95 V · 0.6~1.15 V
AST RH	40% · 70% · 100%		

- Prioritizing the right features is crucial
- An algorithm was developed for data processing, which is essential for effective training
- 49 MEAs, 294 polarization curves (~6700 data points)

Content

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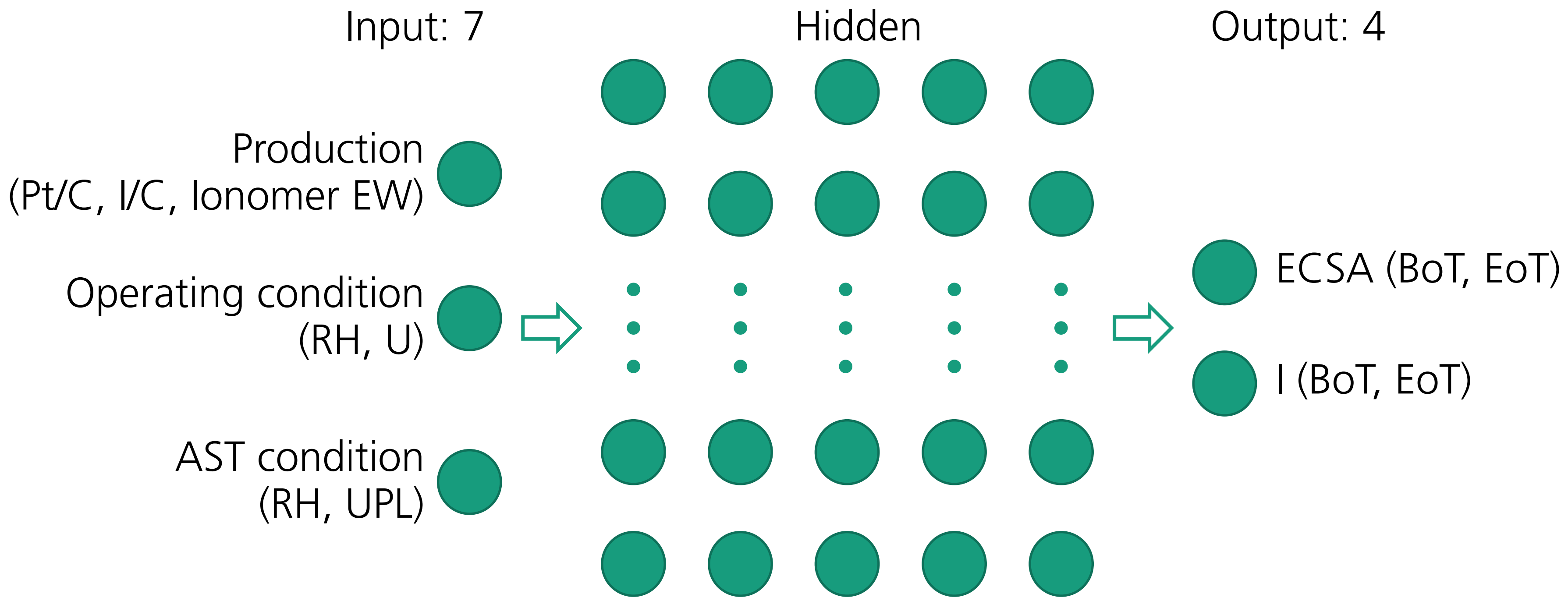
Model Training & Evaluation

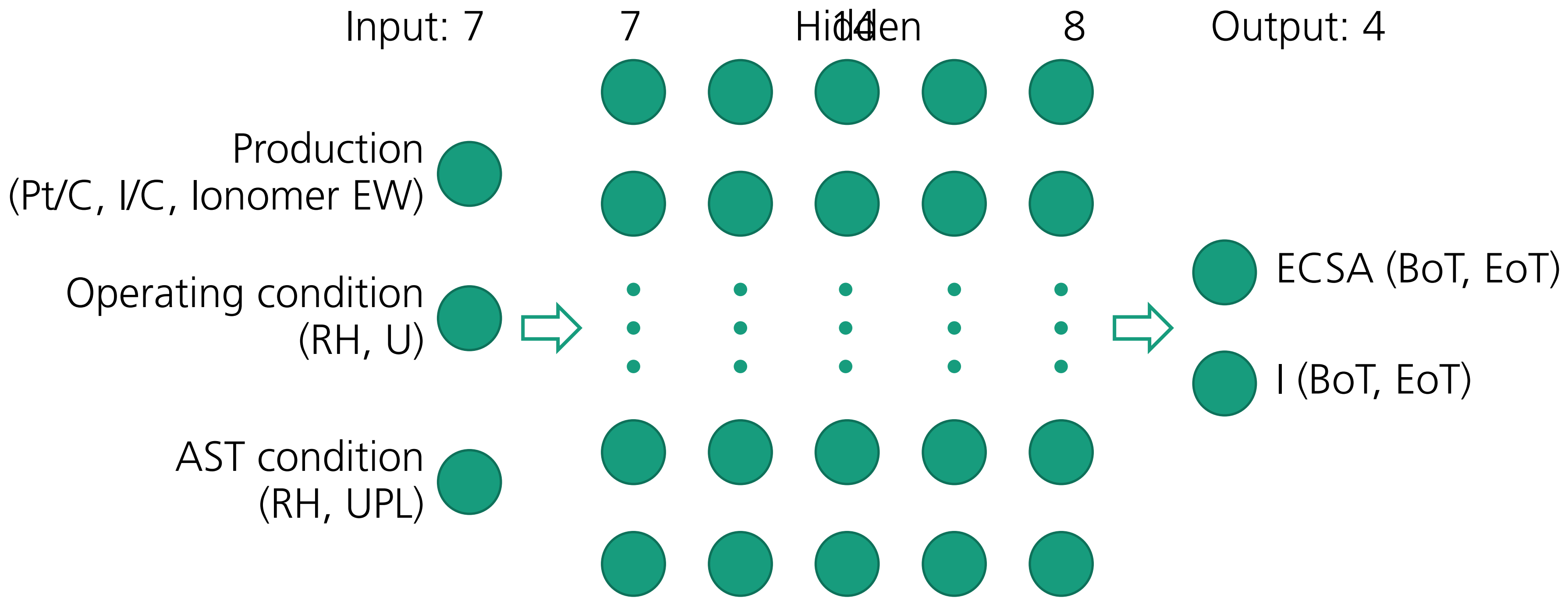
ANN: A Versatile Solution



- Pros: Multi-output, Nonlinear Approximation Power, Scalability

Model Training & Evaluation

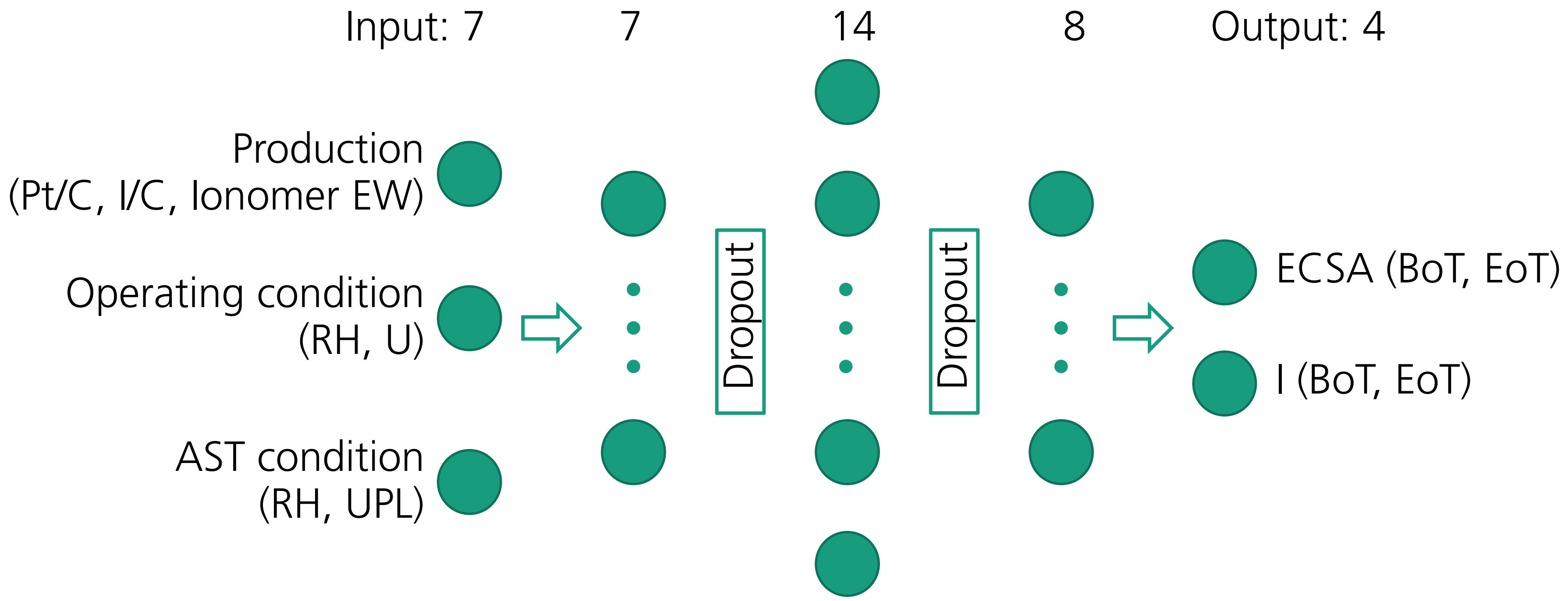
Balanced Model



- Pros: Multi-output, Nonlinear Approximation Power, Scalability
- Model is finely tuned for effective learning without unnecessary complexity

Model Training & Evaluation

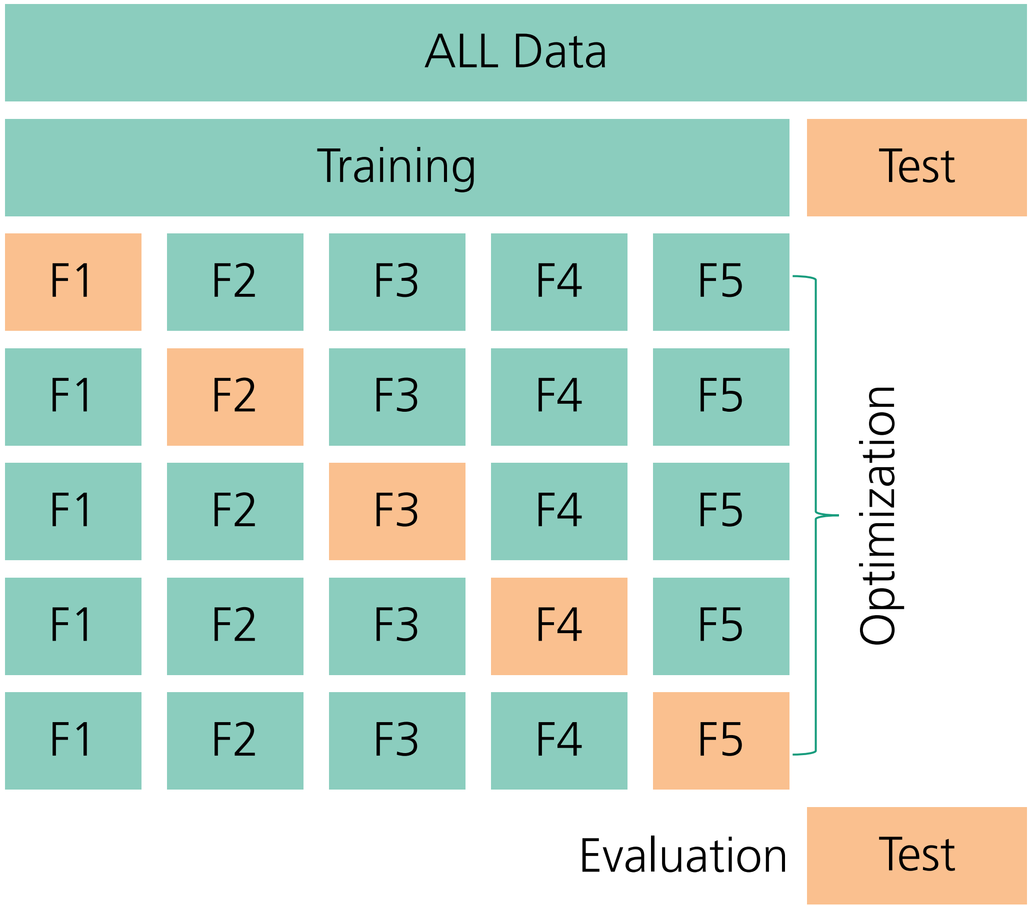
Improved Generalization



- Pros: Multi-output, Nonlinear Approximation Power, Scalability
- Model is finely tuned for effective learning without unnecessary complexity
- “Dropout” and “L2 regularization“ are added to improve generalization

Model Training & Evaluation

Cross Validation

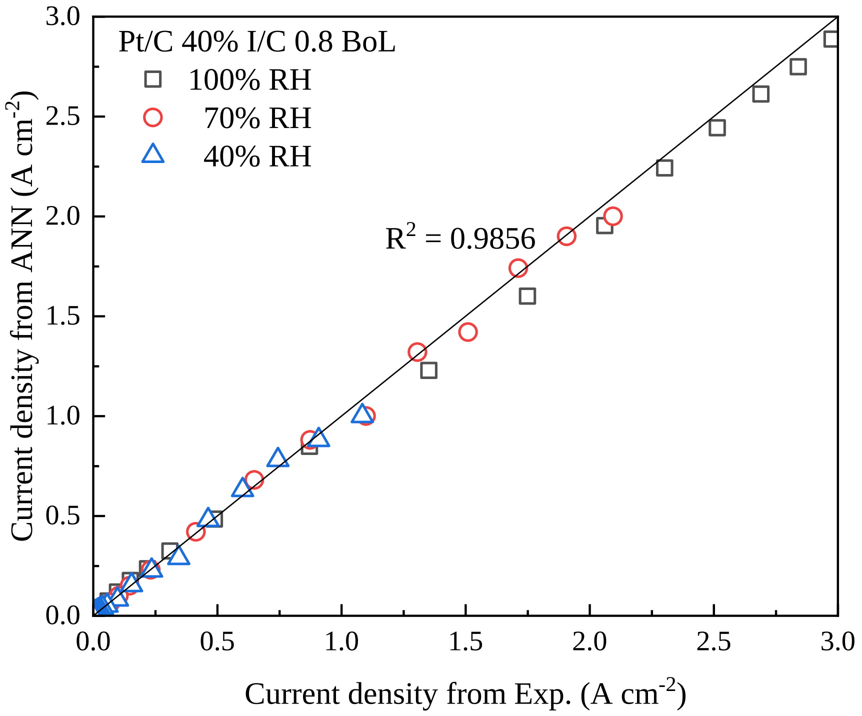


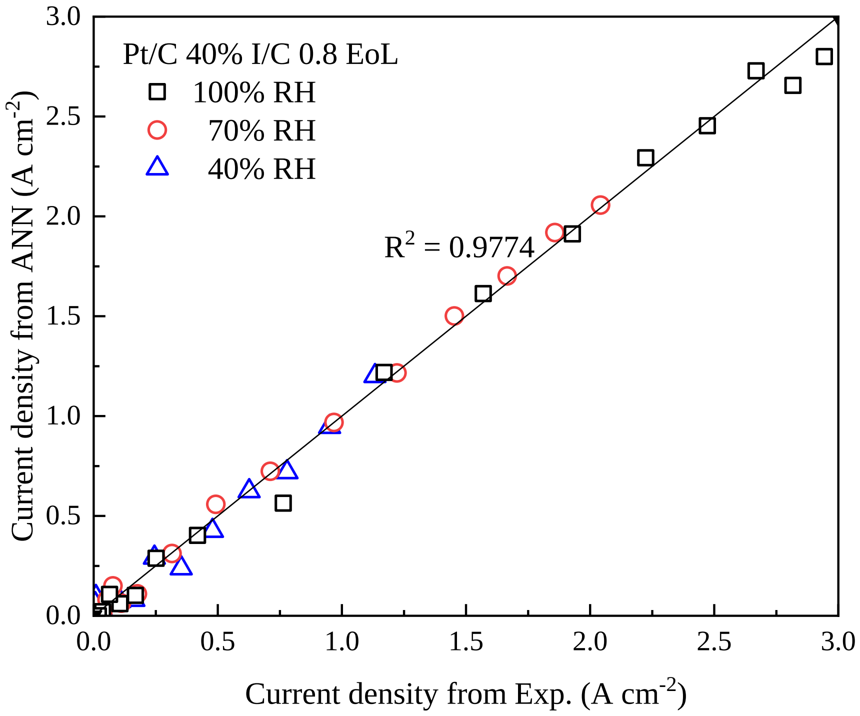
- K-fold cross-validation is employed to further ensure the NN model achieves robust generalization performance.
- Assisting in identifying the optimal NN architecture
- Activation function: ReLU
  Optimizer: adam
  Loss function: Mean Squared Error
- Accelerated by GPU computing

Model Training & Evaluation

R-Squared Analysis

ANN predictions vs experimental data

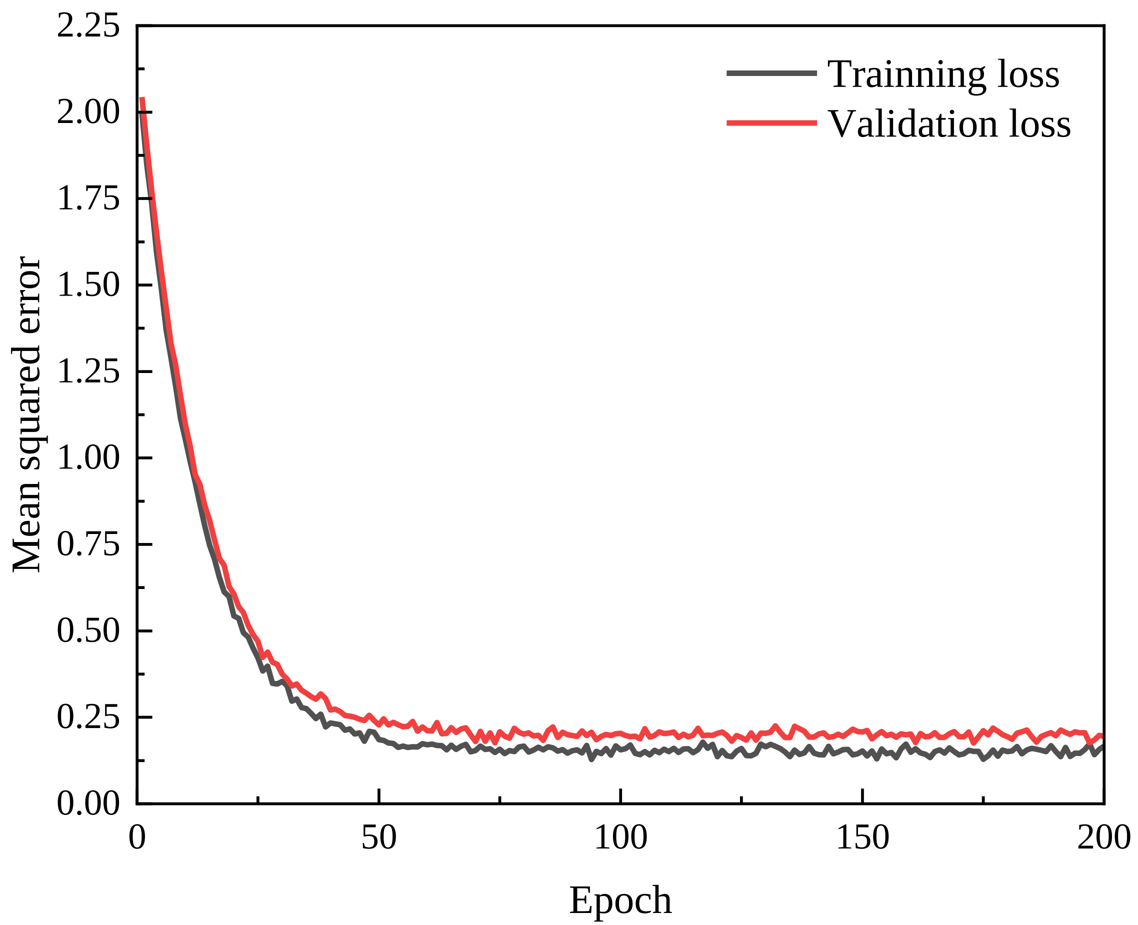




- The model shows strong predictive capabilities, as evidenced by R-squared values of 0.9856 and 0.9774 for BoL and EoL comparisons, respectively, which is valuable for lifespan optimization.

Model Training & Evaluation

Learning Curve



- A steady decrease in training loss over time indicates the model is successfully learning from the data, refining its understanding of the underlying patterns.
- Validation loss trend implies the model is generalizing well, not simply memorizing the training data.
- Stable convergence and a minimal gap between training and validation loss confirm effective learning and the absence of overfitting.

Content

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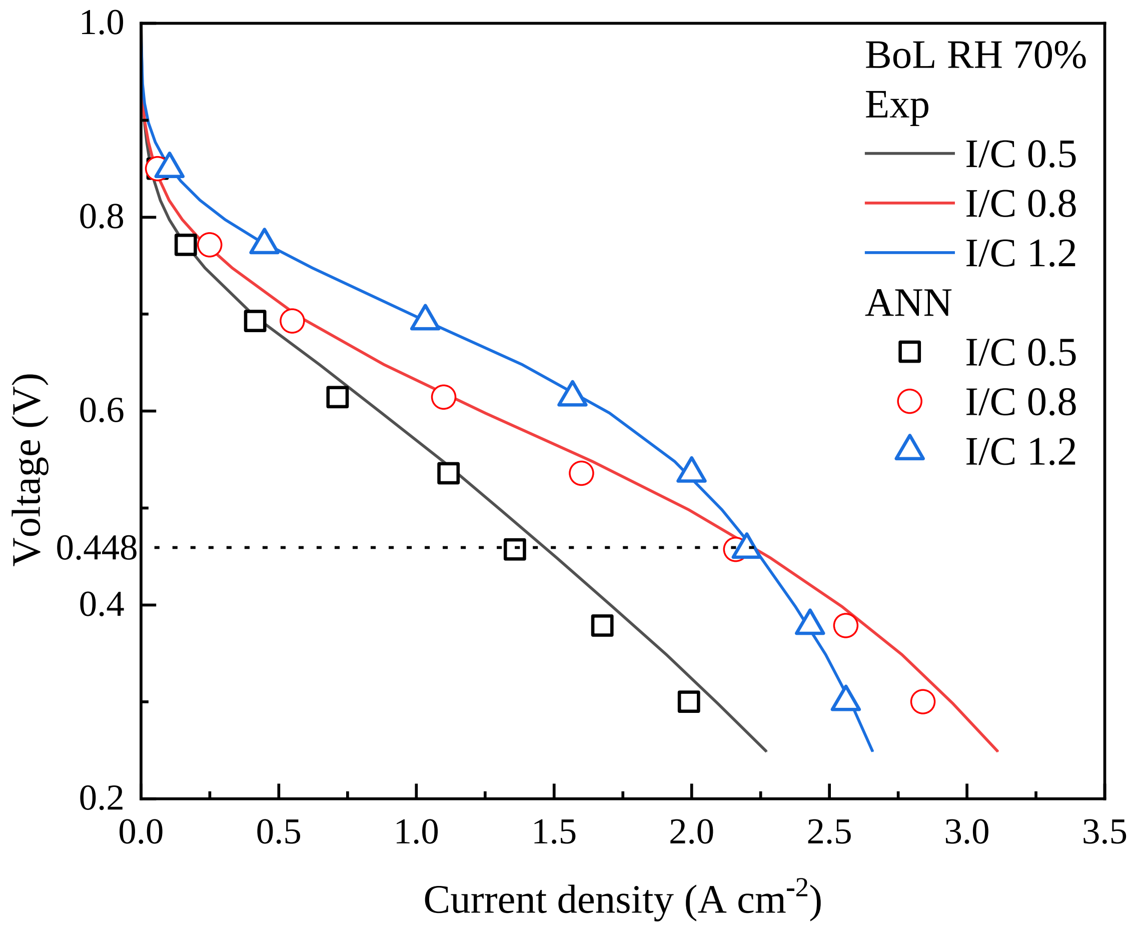
Results

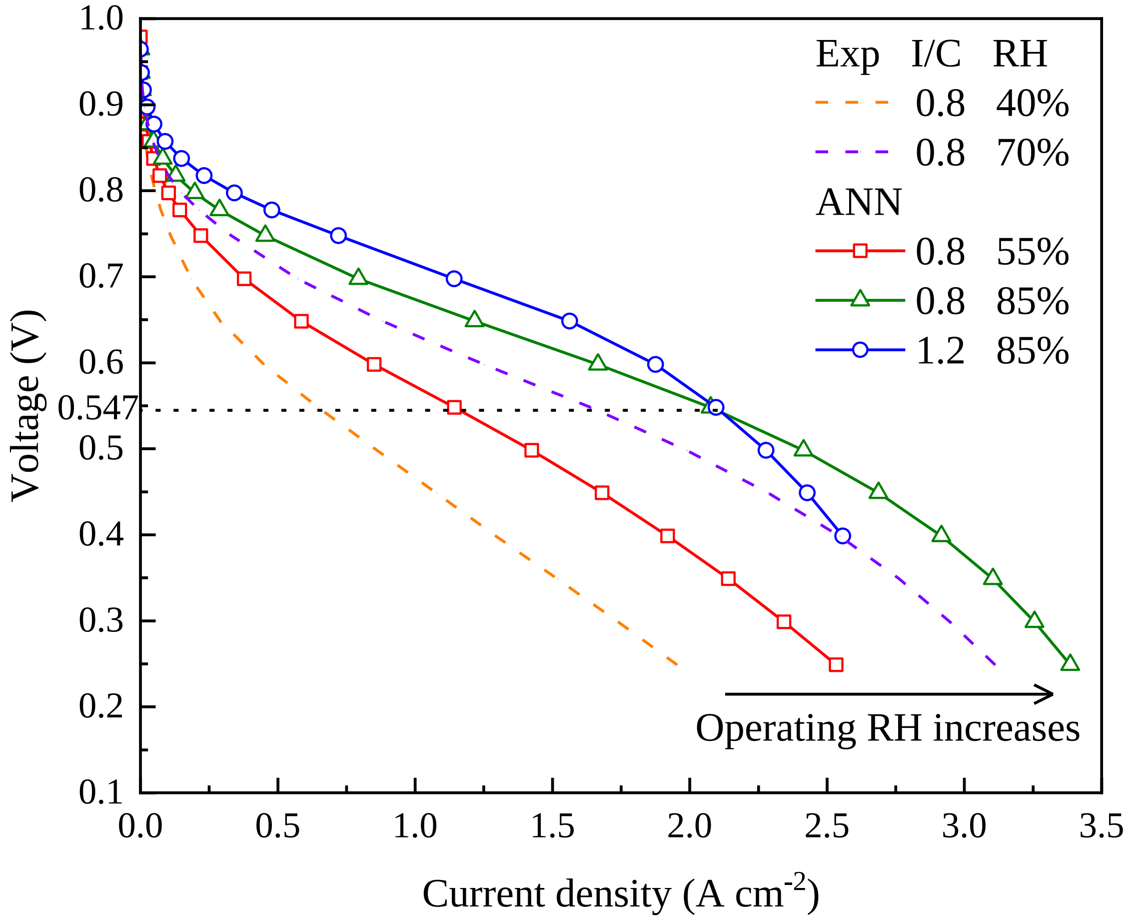
BoT Performance Validation



- The predicted data points closely align with the experimental curves, demonstrating the model's accuracy in capturing the performance behavior.
- In 70 % RH, higher I/C ratios generally lead to improved performance in the medium to high voltage operating region due to a lower R_{proton}.
- Below 0.448 V, the I/C 0.8 cell outperforms the I/C 1.2 cell. This is due to the increased likelihood of flooding at high current density with increased ionomer content, hindering mass transport.

Results

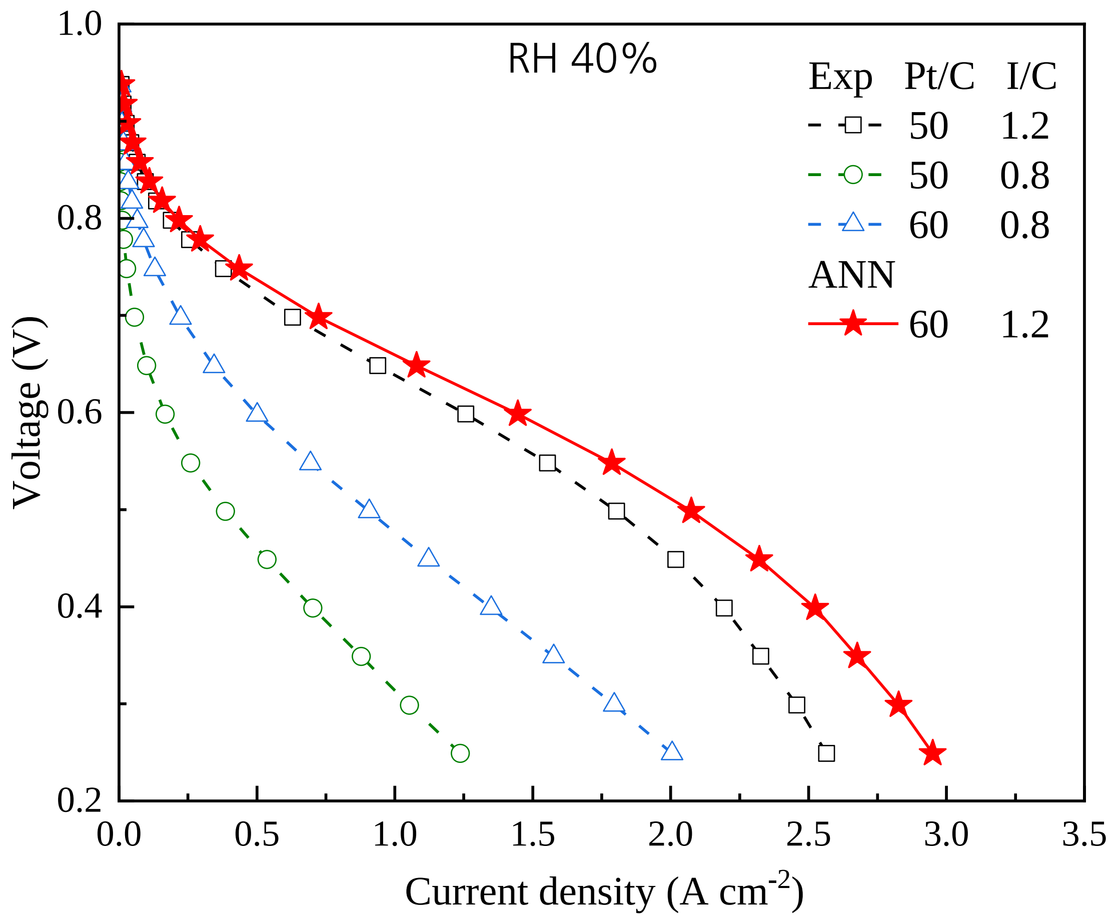
BoT Performance Forecasting (Unseen Conditions)



- Predicted polarization curves adeptly capture the operating behavior of the fuel cells.
- The I/C 0.8 cell shows a better performance under a higher RH due to the reduced R_{proton}, which agrees with experimental findings.
- As with increased humidity comes a greater risk of flooding, the I/C 0.8 cell outperforms the I/C 1.2 cell from a higher voltage of 0.547 V. The ability to predict performance under unseen humidity conditions demonstrates the model's robustness.

Results

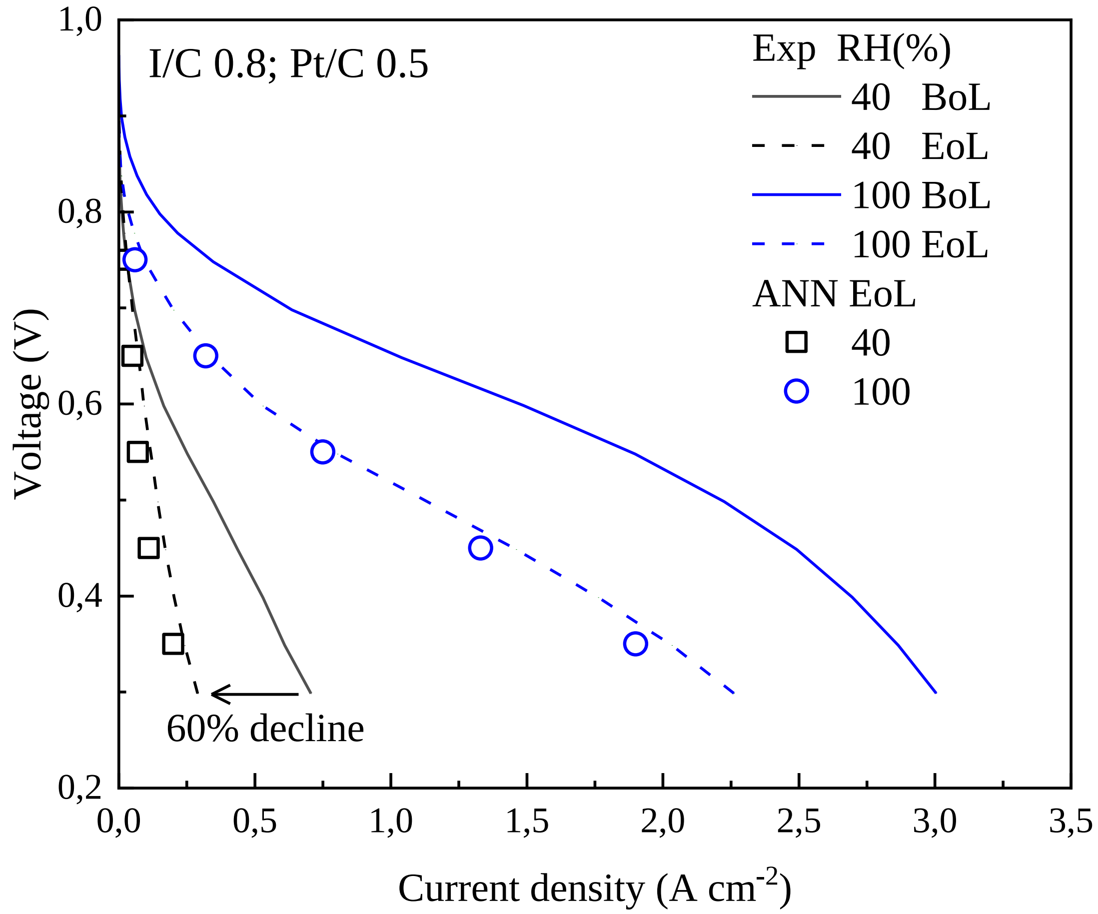
Optimizing ink composition



- By evaluating all Pt/C (20–60%) and I/C (0.5–1.2) ratios, the model predicts an optimal composition (Pt/C 60%, I/C 1.2) that surpasses the best experimental results (Pt/C 50%, I/C 1.2) at 40% RH.
- A well-trained ML model significantly enhances data analysis, reveals intricate patterns, and efficiently guides users to optimal solutions, serving as a critical asset for industrial applications.

Results

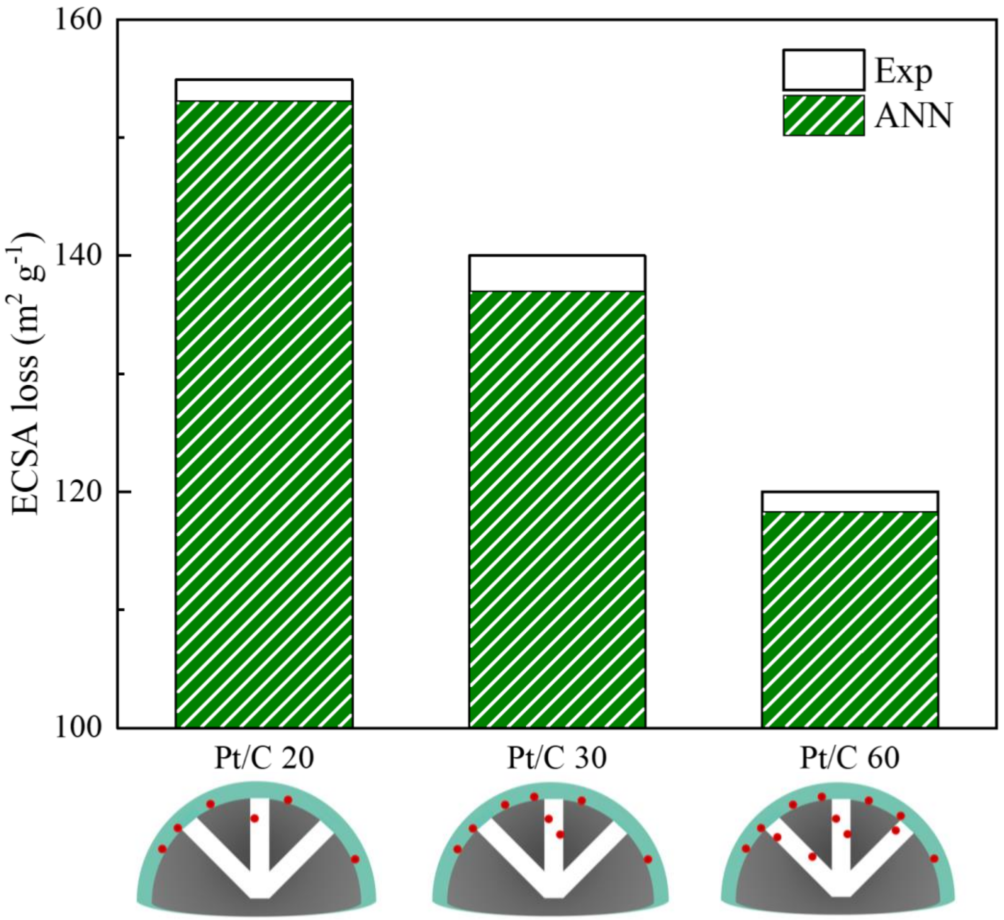
EoT Performance Forecasting



- ANN results closely match experimental data, validating the model's accuracy for EoT performance.
- Despite degradation, the cell performs well at 100% RH but loses 60% limiting current density at 40% RH. This suggests that internal Pt sites remain active at high RH, while most external Pt particles become non-functional, indicating most Pt loss occurs externally.

Results

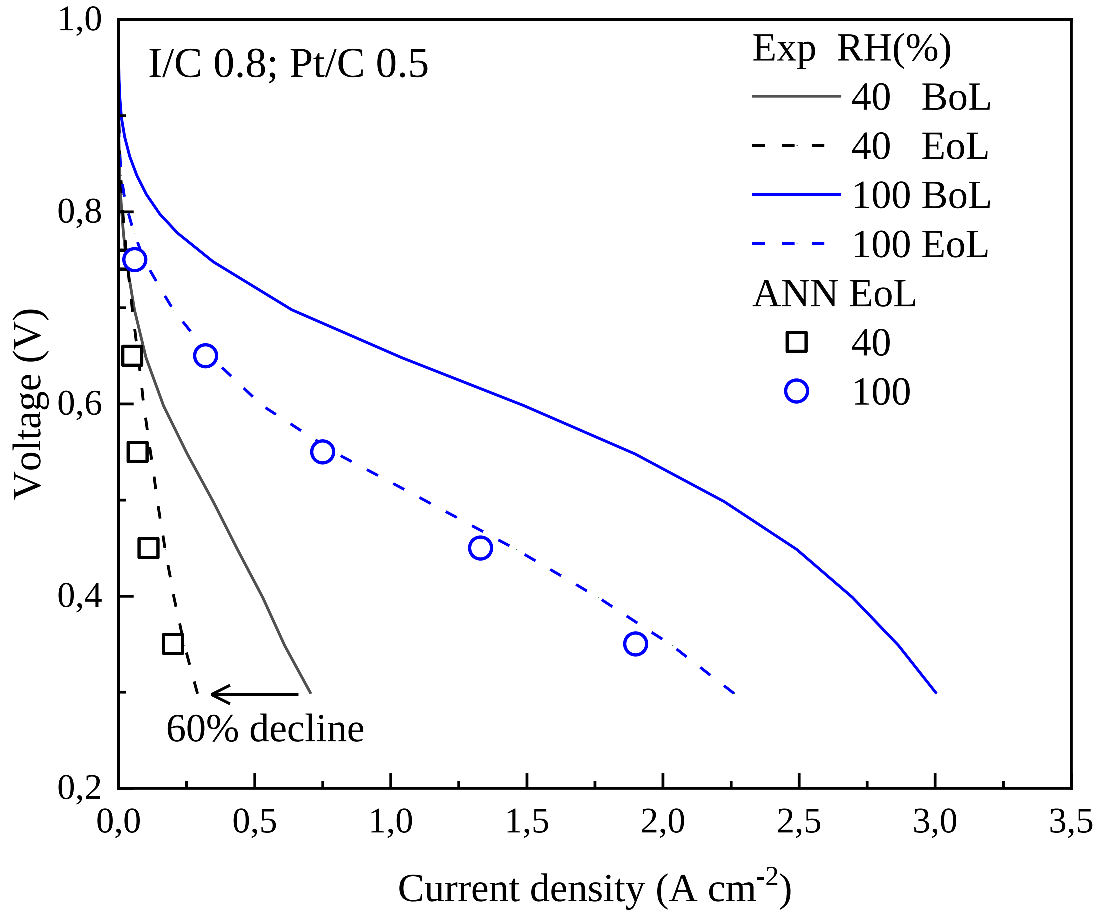
EoT ECSA Forecasting



- ANN results closely match experimental data, validating the model's accuracy for EoT performance.
- Despite degradation, the cell performs well at 100% RH but loses 60% limiting current density at 40% RH. This suggests that internal Pt sites remain active at high RH, while most external Pt particles become non-functional, indicating most Pt loss occurs externally.
- Increasing the Pt/C ratio leads to lower ECSA loss, and the data suggests more internal Pt under a higher Pt/C ratio for this HSC material.

Results

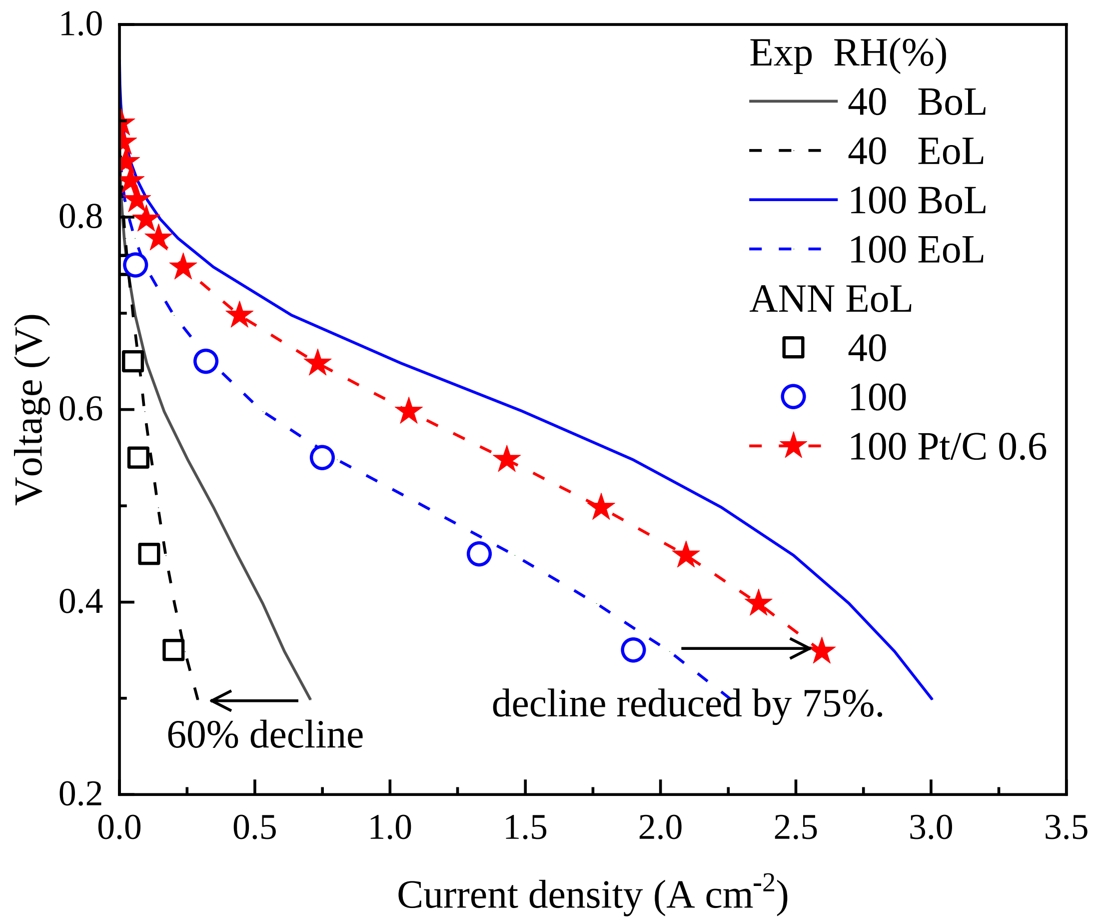
EoT Performance Optimization



- Based on these findings, it can be inferred that the ink composition with a 0.6 Pt/C ratio is likely to show a better EoL performance in high RH condition.

Results

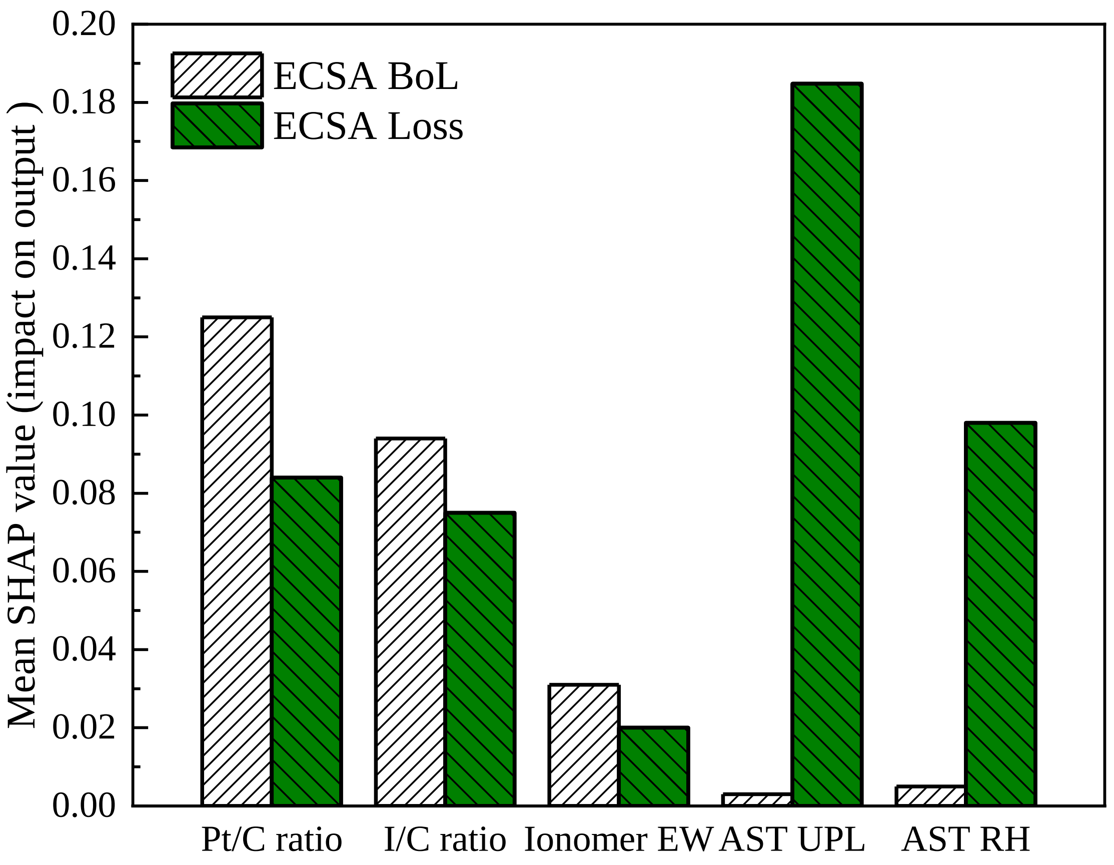
EoT Performance Optimization



- Based on these findings, it can be inferred that the ink composition with a 0.6 Pt/C ratio is likely to show a better EoL performance in high RH condition.
- The ANN prediction confirms a substantial performance increase for Pt/C 0.6 under high RH, reducing performance decline by 75 %.
- These results highlight the model's ability to provide valuable insights into degradation mechanisms and material properties, supporting CL optimization.

Results

Impact Analysis of Variables



- SHAP analysis helps to understand the impact of each input factor on each output factor.
- The AST conditions play a major role in ECSA loss, based on the present dataset, the model shows the UPL exerts a more significant impact than RH.
- This allows to prioritize mitigation strategies for minimizing degradation and to streamline the CL development process.

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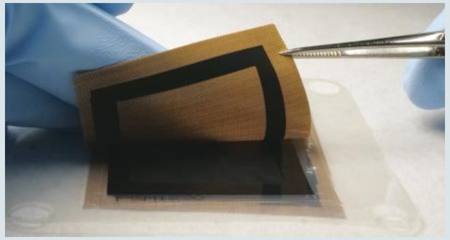
Conclusions

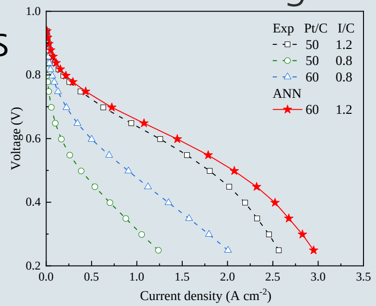
Our expertise in production and characterization ensures high-quality data.



Production Characterization

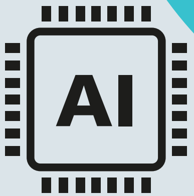
Our expertise in modeling ensures effective learning.

Efficient prediction streamlines production optimization, making it a valuable industry tool.



Reliable Prediction

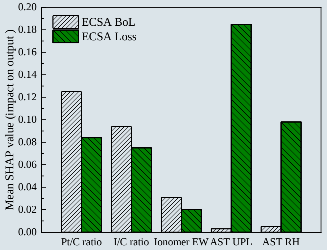
The model's reliability may decrease with out-of-range input data;
however, its capabilities will grow powerfully as the dataset expands.



Robust development support

Deep insights from data

The model also shows a significant advantage in data mining, offering valuable insights into complex data patterns that are difficult to interpret intuitively.



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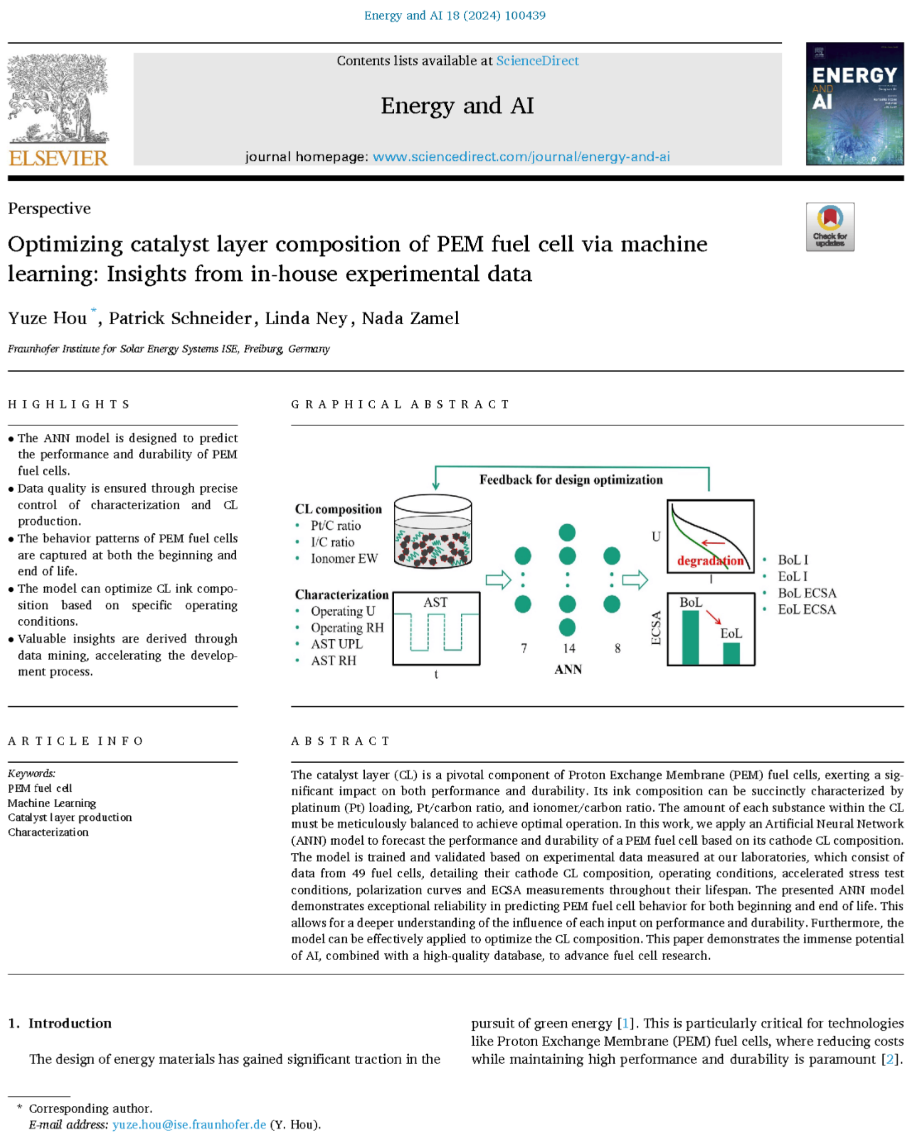
For more information about this work

- Link to this work

  https://doi.org/10.1016/j.egyai.2024.100439

- Link to more recent works from our department

  https://www.ise.fraunhofer.de/en/business-areas/hydrogen-technologies/fuel-cell.html



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Perspective

Optimizing catalyst layer composition of PEM fuel cell via machine learning: Insights from in-house experimental data

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H I G H L I G H T S

- The ANN model is designed to predict the performance and durability of PEM fuel cells.
- Data quality is ensured through precise control of characterization and CL production.
- The behavior patterns of PEM fuel cells are captured at both the beginning and end of life.
- The model can optimize CL ink composition based on specific operating conditions.
- Valuable insights are derived through data mining, accelerating the development process.

G R A P H I C A L   A B S T R A C T

A R T I C L E   I N F O

Keywords:
PEM fuel cell
Machine Learning
Catalyst layer production
Characterization

A B S T R A C T

The catalyst layer (CL) is a pivotal component of Proton Exchange Membrane (PEM) fuel cells, exerting a significant impact on both performance and durability. Its ink composition can be succinctly characterized by platinum (Pt) loading, Pt/carbon ratio, and ionomer/carbon ratio. The amount of each substance within the CL must be meticulously balanced to achieve optimal operation. In this work, we apply an Artificial Neural Network (ANN) model to forecast the performance and durability of a PEM fuel cell based on its cathode CL composition. The model is trained and validated based on experimental data measured at our laboratories, which consist of data from 49 fuel cells, detailing their cathode CL composition, operating conditions, accelerated stress test conditions, polarization curves and ECSA measurements throughout their lifespan. The presented ANN model demonstrates exceptional reliability in predicting PEM fuel cell behavior for both beginning and end of life. This allows for a deeper understanding of the influence of each input on performance and durability. Furthermore, the model can be effectively applied to optimize the CL composition. This paper demonstrates the immense potential of AI, combined with a high-quality database, to advance fuel cell research.

1. Introduction

The design of energy materials has gained significant traction in the pursuit of green energy [1]. This is particularly critical for technologies like Proton Exchange Membrane (PEM) fuel cells, where reducing costs while maintaining high performance and durability is paramount [2].

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Following Webinar Topics

- **Screen Printing of Catalyst Layers for PEM Fuel Cells**
  Linda Ney, Production
  September 24, 2025

- **Tolerance of Silicon Oxide Coated Pt/C Catalyst toward Contamination in the Hydrogen Feed**
  Dr. Sebastian Prass, Characterization
  October 15, 2025

- **In-Situ Characterization of Cathode Catalyst Degradation in PEM Fuel Cells**
  Patrick David Schneider, Characterization
  November 19, 2025

- **Modeling the Morphology of Porous Carbon Supports of PEMFC**
  Anne-Christine Scherzer, Modeling
  December 10, 2025

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Workshop / June 30, 2025 - July 01, 2025

International Workshop on Fuel Cell MEA

The **International Workshop on Fuel Cell MEA** will take place on **June 30 and July 1, 2025.** This event will be hosted both onsite at Fraunhofer ISE in Freiburg, Germany, and online.

In our workshop we will focus on the interaction of ionomer with the catalyst in a fuel cell membrane electrode assembly (MEA) and its effects on performance and life-time. We will concentrate on low temperature PEM fuel cells for mobile applications.

Why should you attend?

- **Gain Comprehensive Insights**: Understand the effects of ionomer type and ionomer to carbon ratio on fuel cell performance and fuel cell long-term operation.
- **Connect with Experts**: Engage in meaningful discussions with leading experts from industry and academia, including **Prof. Jasna Jankovic** (University of Connecticut), **Prof. Anna Fischer** (University of Freiburg), **Prof. Marian Chatenet** (Grenoble Institute of Technology) and **Prof. Marc Secanell** (Newcastle University).
- **Explore Real-World Applications**: Learn about successful use cases and current trends in MEA architectures from an international perspective.
- **Discuss Challenges and Solutions**: Share your design criteria for MEAs and collaborate on strategies for your projects during panel discussions with experts.
- **Experience Cutting-Edge Research**: Join us for a lab tour at Fraunhofer ISE to see state-of-the-art experimental setups.

Register now!

REGISTRATION FORM

Save the date!

ADD TO CALENDAR

June 30 – July 01

Registration still open!

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Thank You for Your Attention! Q & A

Dr. Yuze Hou
yuze.hou@ise.fraunhofer.de

Feedback questionnaire