

# Rui Ding

University of Chicago  
Argonne National Laboratory



## EDUCATION

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<b>Argonne National Laboratory</b>	Sep 2023
Resident Associate	
<i>Host: Junhong Chen</i>	
<b>The University of Chicago</b>	Sep 2023
The Eric and Wendy Schmidt AI in Science Postdoctoral Fellowship	Chicago
<i>Advisor: Junhong Chen &amp; Yuxin Chen</i>	
<b>Hongkong University of Science and Technology</b>	Oct 2022 - Apr 2023
Material Science Doctor Department of Chemical and Biological Engineering	
<i>PG Visiting Internship Student Co-mentor: Minhua Shao (kemshao@ust.hk)</i>	
<b>Nanjing University</b>	Sep 2018 - Jun 2023
Material Science and Engineering Doctor College of Engineering and Applied Science	Nanjing
<i>China Optical Valley Scholarship for Doctoral Students (2022)</i>	
<i>Bojiao Scholarship for Doctoral Students (2021)</i>	
<i>National Scholarship for Doctoral Students in China (2020)</i>	
<b>Nanjing University</b>	Sep 2014 - Jun 2018
Renewable Science and Engineering Bachelor College of Engineering and Applied Science	Nanjing
<i>GPA: 4.63/5.0 (top 2 in the department)</i>	

## ADVISORS

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### Junhong Chen, Prof. Dr.

junhongchen@uchicago.edu; junhongchen@anl.gov

*Crown Family Professor of Molecular Engineering and Lead Water Strategist at Argonne National Laboratory  
University of Chicago*

### Yuxin Chen, Prof. Dr.

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*Assistant Professor  
Department of Computer Science  
University of Chicago*

## PUBLICATIONS (FIRST AUTHOR/CO-FIRST AUTHOR#)

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- Rui Ding**, Jia Li\*, Jianguo Liu\* et. al. Designing AI-aided analysis and prediction models for nonprecious metal electrocatalyst-based proton exchange membrane fuel cells, *Angew. Chem. Int. Ed.*, 2020, 59, 19175-19183.
- Rui Ding**, Jia Li\*, Jianguo Liu\* et. al. Machine Learning-Guided Discovery of Underlying Decisive Factors and New Mechanisms for the Design of Nonprecious Metal Electrocatalysts, *ACS Catal.*, 2021, 11, 9798
- Rui Ding**, Jianguo Liu\* et. al. Unlocking New Insights for Electrocatalyst Design: A Unique Data Science Workflow Leveraging Internet-Sourced Big Data, *ACS Catal.*, 2023, accepted
- Rui Ding**, Jia Li\*, Jianguo Liu\* et. al. Applying machine learning to boost the development of high-performance membrane electrode assembly for proton exchange membrane fuel cells, *J. Mater. Chem. A*, 2021, 9, 6841-6850 (inside cover)
- Rui Ding**, Jia Li\*, Jianguo Liu\* et. al. Facile Grafting strategy synthesis of single-atom electrocatalyst with enhanced ORR

performance, *Nano Res.* , 2020, 13, 1519-1526. (back cover)

6. **Rui Ding**, Guoxiong Wang\*, Jianguo Liu\* et. al. Inspecting design rules of metal-nitrogen-carbon catalysts for electrochemical CO<sub>2</sub> reduction reaction: From a data science perspective, *Nano Res.* , 2023, 16, 264–280

7. **Rui Ding**, Xuebin Wang, Jia Li\*, Jianguo Liu\* et. al. Atomically Dispersed, Low-Coordinate Co–N Sites on Carbon Nanotubes as Inexpensive and Efficient Electrocatalysts for Hydrogen Evolution, *Small*, 2021, 18, 2105335

8. **Rui Ding**, Xuebin Wang, Jia Li\*, Jianguo Liu\* et. al. Guiding the Optimization of Membrane Electrode Assembly in a Proton Exchange Membrane Water Electrolyzer by Machine Learning Modeling and Black-Box Interpretation, *ACS Sustainable Chem. Eng.* 2022, 10, 14, 4561–4578

9. **Rui Ding**, Xuebin Wang, Jia Li\*, Jianguo Liu\* et. al. Application of Machine Learning in Optimizing Proton Exchange Membrane Fuel Cells: A Review, *Energy and AI*, 2022, 9, 100170.

10. **Rui Ding**, Yawen Chen., Jia Li\*, Jianguo Liu\* et. al. Machine learning utilized for the development of proton exchange membrane electrolyzers, *J. Power Sources*, 2023, 556, 232389

11. **Rui Ding**#, Wenjuan Yin#, Jia Li\*, Jianguo Liu\* et. al. Effectively Increasing Pt Utilization Efficiency of the Membrane Electrode Assembly in Proton Exchange Membrane Fuel Cells through Multiparameter Optimization Guided by Machine Learning, *ACS Appl. Mater. Interfaces*, 2022, 14, 6, 8010–8024 (project leader, machine learning works)

12. **Rui Ding**#, Wenjuan Yin#, Jia Li\*, Jianguo Liu\* et. al. Boosting the optimization of membrane electrode assembly in proton exchange membrane fuel cells guided by explainable artificial intelligence, *Energy and AI*, 2021, 5, 100098. (project leader, COMSOL modelling and machine learning works)

## RESEARCH EXPERIENCE

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### Development of Single-Atom Electrocatalyst

Material Design/Synthesis/Characterization/Electrochemical Test

DFT Theoretical Simulation of Catalytic Process

### Application of Machine Learning in PEMFC/PEMEC

Database Preparation&Data Preprocessing

Script Writing for Training Machine Learning Models

Interpretation of Machine Learning Prediction Results.

### Development of Organic Additives in Proton Exchange Membrane

DFT Simulation of Organic Molecules

## SKILLS

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### Machine Learning:

Python Scripts; R Scripts; Linux Shell Scripts; Proficient in the Use of Machine Learning Related Packages and Frameworks: *Tensorflow, Keras, Pytorch, Scikit-learn, XGBoost, CatBoost, LightGBM* ect.

Natural Language Processing Pipeline and Large Language Model Fine-Tuning

### Experimental:

Nano-material Synthesis, Electrochemical Testing; Material Characterization

### Theoretical Simulation:

First Principle Simulation: *VASP*; Quantum Chemistry: *Gaussian*; Multiphysics Simulation: *COMSOL*

### English Level:

IELTS: 7.0 Listening/Reading/Writing/Speaking: 8.0/8.0/6.5/6.0 (2022/02/27)

## ACADEMIC REPORTS

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### The 32nd Annual Meeting of the Chinese Chemical Society

Apr 2021

Oral Report

Zhu Hai; China

A New Generation of Electrochemical Energy Research Paradigm with Artificial Intelligence

### The 9th China Hydrogen Energy Doctoral Forum

Sep 2021

Oral Report

Wu Han; China

Machine learning's participation in the design of high-performance fuel cell membrane electrode assemblies

### The 5th China Frontier Forum on Electrochemical Energy Technology

Oct 2021

Oral Report

Gui Yang; China

Application of machine learning in the study of key materials for fuel cells