RUI DING

Research Interests: Nanomaterials for Energy Applications, Machine Learning in Materials Science
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EDUCATION

The University of Chicago
The Eric and Wendy Schmidt AI in Science Postdoctoral Fellowship, ***Sept. 2023 – Now***
Argonne National Laboratory
Resident Associate (Host: Junhong Chen), ***Sept. 2023 – Now***
Advisors:
Junhong Chen, Prof. Dr. (junhongchen@uchicago.edu; The University of Chicago-Pritzker School of Molecular Engineering; Argonne National Laboratory)
Yuxin Chen, Prof. Dr. (chenyuxin@uchicago.edu; The University of Chicago-Department of Computer Science)
Nanjing University, **China**
Doctor of Engineering, College of Engineering and Applied Science, ***Sept. 2018 – Jun. 2023***
Hongkong University of Science and Technology, **Hong Kong**
PG Visiting Internship Student, Department of Chemical and Biological Engineering, ***Oct. 2022 – Apr. 2023***
Nanjing University, **China**
Bachelor of Engineering, College of Engineering and Applied Science, ***Sept. 2014 – Jun. 2018***

RESEARCH EXPERIENCE

The University of Chicago
As the Eric and Wendy Schmidt AI in Science Postdoctoral Fellow (Sept. 2023 – Now)
Argonne National Laboratory
As the Resident Associate (Host: Junhong Chen; Sept. 2023 – Now)

Summary of Research Work:

- Proposed the 'Broad-scope Reasoning Artificial Intelligence for Nano-micro material and devices Identification, Assessment, and Categorization' (BRAINIAC) Project, which focuses on enhancing materials discovery and device innovation using advanced data collection and machine learning in collaborative experimental frameworks.
- BRAINIAC aims to integrate a vast multi-fidelity dataset with sophisticated graph neural network and self-driven AI research agent. BRAINIAC supports the identification and optimization of materials for various applications, typically including sensors and catalysts for renewable energy and environmental science.
- Participate in the NSF-funded Manufacturing ADvanced Electronics through PrintingUsing Bio-based and Locally Identifiable Compounds (MADE-PUBLIC) Project as the Designer of the Data Portal to Facilitate Knowledge Transfer as well as a cyber-manufacturing platform.

Nanjing University
As Ph.D. Candidate and Research Assistant (Sept. 2018 – Jun. 2023)

Summary of Research Work:

- Investigation of Application of Machine Learning in Proton Exchange Membrane Fuel Cell/Water Electrolyzer Related Material and Component Systems' Discovery and Optimization
  Focused on developing electrocatalysts for renewable energy applications, emphasizing material design, synthesis, characterization, electrochemical testing, and computational modeling.

PAPERS, PUBLICATIONS, AND INVENTION DISCLOSURE (FIRST/ FIRST CO-AUTHOR#)

After joining Schmidt Postdoctoral Program (Sept. 2023 – Feb. 2025):

1. **Rui Ding**[#], Rodrigo P. Ferreira[#], Yuxin Chen, Junhong Chen, Deep Research with Local–Web RAG: Toward Automated System-Level Materials Discovery, accepted by Conference on Neural Information Processing Systems (**NeurIPS**) **2025 AI4Mat** Workshop (non-archival).
2. Rodrigo P. Ferreira[#], **Rui Ding**[#], Rapti Ghosh, Haihui Pu, Junhong Chen, Neuromorphic Random Walk for Experimental Phosphate Adsorption Modeling, accepted by Conference on Neural Information Processing Systems (**NeurIPS**) **2025 ML4PS** Workshop (non-archival).).
3. **Rui Ding**, Jianguo Liu, Kang Hua, Xuebin Wang, Xiaoben Zhang, Minhua Shao, **Yuxin Chen**[*]**, and Junhong Chen**[*] Leveraging Data Mining, Active Learning, and Domain Adaptation in a Multi-Stage, Machine Learning-Driven Approach for the Efficient Discovery of Advanced Acidic Oxygen Evolution Electrocatalysts, (arXiv:2407.04877; ***Sci. Adv.*** **2025, 11, eadr9038**,)
4. **Rui Ding, Junhong Chen**[*], **Yuxin Chen**[*], Jianguo Liu, Yoshio Bando, Xuebin Wang[*] Unlocking the Potential: Machine Learning Applications in Electrocatalyst Design for Electrochemical Hydrogen Energy Transformation, (***Chem. Soc. Rev.*****, 2024, 53, 11390-11461***,* https://doi.org/10.1039/D4CS00844H invited to contribute **journal cover**)
5. **Rui Ding,** Haihui Pu, Kuldip Kumar, Jonathan S. Grabowy, Dominic A. Brose, Maria Chan, Seth B. Darling, Andrew Ferguson, **Yuxin Chen**[*], **Junhong Chen**[*] Leveraging Artificial Intelligence and Machine Learning to Accelerate Material Discovery in Water Applications, (Under Review by *Nat. Water*)
6. Rodrigo P. Ferreira[#], **Rui Ding**[#], Fengxue Zhang, Haihui Pu, Claire Donnat, **Yuxin Chen, Junhong Chen**[*] (***Molecular Systems Design & Engineering 2025****, 10.1039/D4ME00203B, Cover Art)*
7. (Invention Disclosure) **Rui Ding**, **Junhong Chen**, **Yuxin Chen** Broad-scope Reasoning Artificial Intelligence for Nano-micro material and devices Identification, Assessment, and Categorization (BRAINIAC) Polsky Center for Entrepreneurship and Innovation-The University of Chicago (In Preparation)

Ph.D. Period (Sept. 2018 – Jun. 2023):

1. **Rui Ding**, Ran Wang, Yiqin Ding, Wenjuan Yin, Yide Liu, Jia Li[*], Jianguo Liu[*] 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.
2. **Rui Ding**, Yawen Chen, Ping Chen, Ran Wang, Jiankang Wang, Yiqin Ding, Wenjuan Yin, Yide Liu, Jia Li[*], Jianguo Liu[*] Machine Learning-Guided Discovery of Underlying Decisive Factors and New Mechanisms for the Design of Nonprecious Metal Electrocatalysts, **ACS Catal.**, 2021, 11, 9798
3. **Rui Ding**, Xuebin Wang, Aidong Tan, Jia Li[*], Jianguo Liu[*] Unlocking New Insights for Electrocatalyst Design: A Unique Data Science Workflow Leveraging Internet-Sourced Big Data, **ACS Catal.**, 2023, 13, 13267–13281.
4. **Rui Ding**, Yiqin Ding, Hongyu Zhang, Ran Wang, Zihan Xu, Yide Liu, Wenjuan Yin, Jiankang Wang, Jia Li[*], Jianguo Liu[*] 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)
5. **Rui Ding**, Yide Liu, Zhiyan Rui, Jia Li[*], Jianguo Liu[*], Zhigang Zou Facile Grafting strategy synthesis of single-atom electrocatalyst with enhanced ORR performance, **Nano Res.**, 2020, 13, 1519-1526. (back cover)
6. **Rui Ding**, Meng Ma, Yawen Chen, Xuebin Wang, Jia Li[*], Guoxiong Wang[*], Jianguo Liu[*] Inspecting design rules of metal-nitrogen-carbon catalysts for electrochemical CO_2 reduction reaction: From a data science perspective, **Nano Res.**, 2023, 16, 264–280
7. **Rui Ding**, Yawen Chen, Xiaoke Li, Zhiyan Rui, Kang Hua, Yongkang Wu, Xiao Duan, Xuebin Wang, Jia Li[*], Jianguo Liu[*] 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**, Yawen Chen, Zhiyan Rui, Kang Hua, Yongkang Wu, Xiaoke Li, Xiao Duan, Xuebin Wang, Jia Li[*], Jianguo Liu[*] 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**, Shiqiao Zhang, Yawen Chen, Zhiyan Rui, Kang Hua, Yongkang Wu, Xiaoke Li, Xiao Duan, Xuebin Wang, Jia Li[*], Jianguo Liu[*] Application of Machine Learning in Optimizing Proton Exchange Membrane Fuel Cells: A Review, **Energy and AI**, 2022, 9, 100170.

10. **Rui Ding,** Yawen Chen, Zhiyan Rui, Kang Hua, Yongkang Wu, Xiaoke Li, Xiao Duan, Jia Li[*], Xuebin Wang[*], Jianguo Liu[*] Machine learning utilized for the development of proton exchange membrane electrolyzers, **J. Power Sources**, 2023, 556, 232389.
11. **Rui Ding[#],** Wenjuan Yin[#], Gang Cheng, Yawen Chen, Jiankang Wang, Xuebin Wang, Min Han, Tianren Zhang, Yinliang Cao, Haimin Zhao, Shengping Wang, Jia Li[*], Jianguo Liu[*] 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
12. **Rui Ding[#]**, Wenjuan Yin[#], Gang Cheng, Yawen Chen, Jiankang Wang, Ran Wang, Zhiyan Rui, Jia Li[*], Jianguo Liu[*] Boosting the optimization of membrane electrode assembly in proton exchange membrane fuel cells guided by explainable artificial intelligence, **Energy and AI**, 2021, 5, 100098.

CONFERENCE PRESENTATIONS, WORKSHOPS, AND PROFESSIONAL ENGAGEMENTS

1. Rui Ding (2025) "Hierarchical Deep Research with Local–Web RAG: Toward Automated System-Level Materials Discovery" – Poster, San Diego, CA, December 6, 2025
2. Rodrigo Ferreira, Rui Ding (2025) "Neuromorphic Random Walk for Experimental Phosphate Adsorption Modeling" – Poster, December 6, San Diego, CA, December 7, 2025
3. Rui Ding (2025) Abstract #I01B-1845 "Leveraging Data Mining, Active Learning, and Domain Adaptation for Efficient Discovery of Advanced Oxygen Evolution Electrocatalysts" – Poster, **248th Electrochemical Society Meeting**, Chicago, IL, October 13, 2025
4. Rui Ding (2025) "Application of Versatile Machine Learning Approaches to Facilitate the Discovery of Nano-Materials/Devices in Renewable Energy" – **Gordon Research Seminar on Nanomaterials for Applications in Energy Technology**, Ventura, CA, February 23–28, 2025
5. Rui Ding (2025) "Expediting Field-Effect Transistor Chemical Sensor Design with Neuromorphic Spiking Graph Neural Networks (Extended Abstract)" – **ACM ICONS 2025: International Conference on Neuromorphic Systems**, Seattle, WA, July 29–31, 2025
6. Rui Ding (2025) "Journey to a Nanomaterials/Devices Copilot" – **Knowledge-Guided Machine Learning Workshop**, University of Michigan, Ann Arbor, MI, August 4–8, 2025
7. Rui Ding (2025) **Schmidt Sciences Entrepreneurship Retreat**, Cold Spring Harbor Laboratory, NY, September 28–October 1, 2025
8. Rui Ding (2024) "Hunting for Rare High-Performance Electrocatalysts: A Multi-Stage ML Approach to Discover Extreme Performers in Acidic Oxygen Evolution" **– NSF Workshop on Data-driven Modeling and Prediction of Rare and Extreme Events**, University of Chicago, Chicago, IL, 2024
9. Rui Ding (2024) "Leveraging Data Mining, Active Learning, and Domain Adaptation in a Multi-Stage, Machine Learning–Driven Approach for the Efficient Discovery of Advanced Acidic Oxygen Evolution Electrocatalysts" – **AI for Multidisciplinary Exploration and Discovery Workshop (Heterogeneous Catalysis)**, Big Ten Conference Center, Rosemont, IL, 2024
10. Rui Ding (2024) "Leveraging Data Mining, Active Learning, and Domain Adaptation in a Multi-Stage, Machine Learning–Driven Approach for the Efficient Discovery of Advanced Acidic Oxygen Evolution Electrocatalysts" – **AI+Science Summer School 2024**, University of Chicago, Chicago, IL, 2024
11. Rui Ding (2024) "Cybermanufacturing Platform of MADE-PUBLIC Project" – **NSF MADE-PUBLIC Project Annual Retreat**, Northwestern University, Evanston, IL, 2024
12. Rui Ding (2024–2026) Host Representative, AI+ Science Schmidt Fellows Speaker Series, University of Chicago
13. Rui Ding (2021) "A New Generation of Electrochemical Energy Research Paradigm with Artificial Intelligence" – 32nd Annual Meeting of the Chinese Chemical Society, Zhuhai, China, 2021

RESEARCH MENTORSHIP

Research Experience for Nigerian Undergraduates (RENEU), University of Chicago (Cohort 2025)
Mentee: Covenant Amoo; Project: Knowledge Extraction using LLM for Field-Effect Transistor-Based Sensor (2025)
Research Experience for Nigerian Undergraduates (RENEU), University of Chicago (Cohort 2024)
Assisted in Mentoring Mentee: Abdulafeez Olaitan; Project: Dynamic Reshaping of Nanodroplet Under Electron Beam Radiation(2024)

2025 AI+Science Hackathon, University of Chicago (2025) April 15 – 29. Project: characterizing new materials using AI. Mentoring a team of 4 undergraduate members.
LLM Hackathon for Applications in Materials Science & Chemistry, **Physical Sciences and Engineering, Argonne National Lab (2025)** September 11 – 12. Project: V-RAPIDS

RESEARCH FUNDING& AWARDS

1. 2024 AI+Science Research Initiative, Data Science Institute, University of Chicago, 2024
"BRAINIAC: A Revolutionary Approach to Nano-Micro Material and Device Optimization"
2. Service Unit Award from Center for Nanoscale Materials, Argonne National Laboratory, 2024
"Accelerated Discovery of Multifunctional Probes for PFAS Detection through Integrated Graph Neural Networks and Active Learning-Enhanced Simulations"
3. Service Unit Award from NSF ACCESS Program, 2024
"BRAINIAC: An AI-Driven Framework for Accelerating Nano-Micro Materials Discovery and Device Innovation" (MAT240097)
4. Service Unit Award from Argonne ALCF, 2024
"BRAINIAC" (MAT240097)

SKILLS

- **Traditional Machine Learning:**
- Python Scripts; R Scripts; Linux Shell Scripts; Experienced with various machine learning frameworks, including Tensorflow, Pytorch, and Scikit-learn;
- **Natural Language Processing:**
- NLP Pipeline and Large Language Model Fine-Tuning/AI agent framework building
- **Material Science Experimental:**
  Nano-material Synthesis, Electrochemical Testing; Material Characterization
- **Material Science Theoretical Simulation:**
  First Principle Simulation: VASP; Quantum Chemistry: Gassausian ; Multiphysics Simulation: COMSO

REFERENCES

Junhong Chen
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