Ruijie (Ray) Zhu

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Education

University of Chicago Chicago, IL 09/2023–06/2028

PhD student in Molecular Engineering | GPA: 3.84/4

Selected Coursework: quantum molecular and materials modeling, classical molecular and materials modeling, electrochemical principles and methods, thermodynamics and statistical mechanics, math methods in molecular engineering

Northwestern University Evanston, IL 09/2021–12/2022

MS in Materials Science and Engineering | GPA: 3.92/4

Selected Coursework: computational materials science, advanced physics of materials, chemical and statistical thermodynamics of materials, crystalline and noncrystalline materials, phase transformations in materials

Shanghai University Shanghai, China 09/2019–12/2022

MS in Materials Science and Engineering | GPA: 89/100

Selected Coursework: computational materials design, materials information and data science, materials thermodynamics and kinetics, structure property and application of materials, thermoelectric materials and devices

Shanghai University Shanghai, China 09/2015–06/2019

BS in Materials Physics, Qianweichang College | GPA: 3.75/4

Selected Coursework: computational materials science, physical chemistry, solid state physics, physical properties of materials, nanostructures and nanomaterials

Publication

- Hilal Daglar, Zihui Zhou, **Ray Zhu**, Pragya Parihar, Ijla Siepmann, Omar Yaghi, and Laura Gagliardi. "Discovery of Stacking Heterogeneity, Layer Buckling, and Residual Water in COF-999-NH2 and Implications on CO2 Capture" *Journal of the American Chemical Society* (2025).

- King, Daniel, Daniel Grzenda, **Ray Zhu**, Nathaniel Hudson, Ian Foster, and Laura Gagliardi. "Cartesian Equivariant Representations for Learning and Understanding Molecular Orbitals" *PNAS* (2025).

- Bayesian optimization hackathon contributors (including **Ruijie Zhu**) "Bayesian Optimization Hackathon for Chemistry and Materials" *ChemRxiv* (2025)

- Griesemer, Sean D., Bianca Baldassarri, **Ruijie Zhu**, Jiahong Shen, Koushik Pal, Cheol Woo Park, and Chris Wolverton. "Wide-ranging predictions of new stable compounds powered by recommendation engines." Science Advances 11, no. 1 (2025): eadq1431.

- LLM hackathon contributors (including **Ruijie Zhu**) "Reflections from the 2024 Large Language Model (LLM) Hackathon for Applications in Materials Science and Chemistry" *Arxiv* (2024)

- Park, Hyun, Xiaoli Yan, **Ruijie Zhu**, Eliu A. Huerta, Santanu Chaudhuri, Donny Cooper, Ian Foster, and Emad Tajkhorshid. "A generative artificial intelligence framework based on a molecular diffusion model for the design of metal-organic frameworks for carbon capture.v *Communications Chemistry 7* (2024).

- Hyun Park, **Ruijie Zhu**, Eliu Huerta, Santanu Chaudhuri, Emad Tajkhorshid, and Donny Cooper. "End-to-end AI Framework for Interpretable Prediction of Molecular and Crystal Properties." *Machine Learning: Science and Technology* (2023).

- Yihang Li, **Ruijie Zhu**, Yuanqing Wang, Lingyan Feng, Yi Liu."Center-environment deep transfer machine learning across crystal structures: from spinel oxides to perovskite oxides", *npj Computational Materials* (2023).

- TRI Consortium (including **Ruijie Zhu**) "Materials cartography: A forward-looking perspective on materials representation and devising better maps", *APL Machine Learning* (2023).

- **Ruijie Zhu**. "Correlating research octane numbers of gasoline surrogates with high temperature oxidation characteristics." *Arxiv* (2022).

Research Experience

Developing autonomous agents for protein design 09/2025-Pres.

Advisor: Arvind Ramanathan

- Integrate cheminformatics tool and model context protocol (MCP) into the agent system for tool calling

Modeling CO_2 speciation in amine-functionalized reticular frameworks 01/2024-06/2025

Advisor: Laura Gagliardi

- Performed DFT single point calculations for input dataset generation for MACE-MP-0b model fine-tuning
- Performed metadynamics simulations for modeling CO_2 chemisorption in amine-functionalized covalent organic frameworks (COFs)
- Performed density functional theory (DFT) calculations to evaluate binding energies of CO_2 and H_2O in amine-functionalized metal organic frameworks (MOFs)
- Performed grand canonical Monte Carlo (GCMC) simulations for CO_2 adsorption isotherms of MOFs

Accelerated discovery of i-MAX phases using HT-DFT calculations 09/2021–12/2022

Advisor: Christopher Wolverton

- Generated a combinatorial search space of in-plane ordered MAX phases (i-MAX) via prototype decoration
- Performed 7,774 high-throughput DFT calculations for the thermodynamic stabilities of i-MAX phases
- Discovered 295 new thermodynamically stable i-MAX phases that have not yet been experimentally synthesized

Predicting formation energy of inorganic crystals using machine learning 09/2019–09/2021

Advisor: Yi Liu

- Generated elemental and structural machine learning features for ICSD crystals using Center-Environment (CE) model
- Performed formation energy prediction using XGBoost model with generated CE features
- Benchmarked prediction accuracy of XGBoost model with CE features against Magpie features

Correlating RONs of gasoline surrogates with combustion characteristics 07/2015–09/2019

Advisor: Yi Liu

- Performed high temperature combustion molecular dynamics simulations of hydrocarbons using ReaxFF force field
- Performed fragment analysis of radicals generated during combustion simulations
- Identified that the number of hydroxyl radicals at the equilibrium state is inversely correlated to RON

Work Experience

Research Mentor (Remote), Francis W. Parker School, IL 11/2025–Pres.

- Mentored three middle school students for participation in Presidential AI challenge
- Ideation, and of related to pollutatnt monitering in water

Computational Chemistry and Materials Science (CCMS) Summer Institute Fellow, Lawrence Livermore National Laboratory 06/2023–08/2023

Advisor: Fei Zhou

Project: Structure generation using probabilistic models

- Applied diffusion model to generate ground state structures of Lennard-Jones clusters
- Performed conditional generation of amorphous carbon under extreme conditions using diffusion model
- Employed entropy maximization method to conditionally generate amorphous carbon

Predoctoral Appointee, Argonne National Laboratory 04/2023–05/2023

Advisor: Eliu Huerta

Project: Rational high-throughput design of metal-organic frameworks using diffusion models

- Adopted a diffusion model named `DiffLinker` to generate novel MOF linkers
- Devised a computational framework to generate novel and chemically diverse MOFs in high-throughput
- Co-authored a paper on using diffusion model for high-throughput MOF design

Research Aide Technical, Argonne National Laboratory 06/2022–03/2023

Advisor: Eliu Huerta

Development of a FAIR AI framework for molecular and crystal property prediction

- Performed hyperparameter tuning of PhysNet model with homo and zpve as target properties using DeepHyper
- Performed model training, interpretable inference and benchmarking of graph neural networks on ThetaGPU and Delta supercomputers
- The work was a part of DOE Braid: Data Flow Automation for Scalable and FAIR Science project

Generating new MOF structures for Direct Air Capture (DAC) application

- Performed statistical analysis of the hMOF database to identify key structural features of high-performing MOFs
- Constructed isoreticular optimization framework for new MOF generation with organic linkers from diffusion model
- Trained modified CGCNN model with adjacency list format node and endge embeddings for accurate prediction of MOF CO_2 working capacity
- This work was a part of DOE HPC4EnergyInnovation (HPC4EI) project

Science Olympiad Coach, Marie Murphy School, IL 11/2022-05/2023

- Developed course materials for Science Olympiad coaching (Crave the Wave, Division B)
- Co-taught fundamentals of different kinds of waves (mechanical and electronic) and their characteristics
- Hosted practice test review sessions to help the students prepare for regional invitationals

Research Mentor (Remote), Troy High School, CA 06/2022–07/2022

- Mentored two URM students from Troy High School during their summer internship at Northwestern
- Hosted hands-on coding sessions on data analysis using Python and crystal structure visualization using VESTA

Graduate Teaching Assistant, MGI, Shanghai University 08/2020–11/2020

- Coordinated with the instructor and students to prepare for solid state physics class
- Graded homework assignments and delivered student performance evaluation
- Hosted course material review sessions to help the students prepare for final exam

Entrepreneurship

I-Corps Fall 2024 cohort, University of Chicago 10/2024–12/2024

As the conceptualizer of CatalyzeQ, we developed a computational platform concept for technoeconomic analysis of electrocatalysts for CO_2 reduction through the Polsky I-Corps program. Engaged in customer discovery and business model validation to assess the commercial potential of this innovation.

Reviewer Activity

Reviewer for Machine Learning: Science and Technology and ACM Transactions on Knowledge Discovery from Data journals

Awards & Honors

NSF-NRT AI-enabled Molecular Engineering of Materials and Systems (AIMEMS) for Sustainability Trainees	2024
1st Place, AI4Science Hackathon, DeepVerse	2024
Reincarnate Prize, Large Language Model (LLM) Hackathon For Materials and Chemistry, University of Chicago	2024
6th Place, Bayesian Optimization Hackathon for Chemistry and Materials, Acceleration Consortium	2024
(Contributor) HPCwire Editors' Choice Award for Best Use of High-Performance Data Analysis & Artificial Intelligence	2024
1st Place, Argonne Leadership Computing Facility AI Hackathon	2022
Outstanding Student Award, Materials Genome Initiative, Shanghai University	2019
Outstanding Graduates of Shanghai	2019
Excellence & Innovation Award, Shanghai University	2017
Meritorious Winner, Mathematical Contest in Modeling	2017
Bronze Medal, The University Physics Competition	2017

Membership

Member of Trillion Parameter Consortium (TPC)	2024
Member of The Materials Research Data Alliance (MaRDA)	2022

Conference Presentation

Catalyst Design for Decarbonation Center (CD4DC) all hands meeting, University of Chicago, Chicago, IL	10/2023
The 15th AIChE Midwest Regional Conference, University of Illinois Chicago, Chicago, IL	04/2023
Artificial Intelligence for Materials Science (AIMS) Workshop (lightning talk), Remote	02/2023

Poster Presentation

NRT annual meeting, Colorado School of Mines, Golden, CO 03/2026
Catalyst Design for Decarbonation Center (CD4DC) all hands meeting, University of Chicago, Chicago, IL 10/2024
Materials Research Data Alliance (MaRDA) Annual Meeting 02/2023
Artificial Intelligence for Materials Science (AIMS) Workshop 07/2022
Materials Research Data Alliance (MaRDA) Annual Meeting 02/2022

Skills

Computational Biology, Computational Materials Science, Materials Informatics, High Performance Computing, High-throughput DFT Calculation, Molecular Dynamics
Programming: Python, Bash, LaTeX, HTML, CSS, Flask