

Rui Zhou

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SUMMARY

PhD student in Materials Science and Engineering with 7+ years of computational materials research experience in both academia and industry, specializing in battery materials (solid electrolytes, cathode materials) and simulation methods (DFT, MP2, MD, DEM). Strong programming and data analysis skills. Record of 10 peer-reviewed publications, 3 granted patents, and developed 3 software applications.

EXPERIENCE

PhD Researcher at Iowa State University

Ames, Iowa, USA | Jan 2023 - Present

- Perform first-principles simulations and MD simulations to study glassy and crystalline solid electrolytes (Li/Na thiophosphates, closo-hydroborates, metal oxyhalides), interfaces, phase transitions, and ion transport.
- Build machine-learning force fields with active learning workflow. Integrate with MP2 method to model C-H-O reaction.
- Contributed to studies on ceramics, metals, and semiconductors; Collaborate cross-functionally with experimental groups.

Simulation Engineer at Sunwoda Electric Vehicle Battery Co., Ltd.

Shenzhen, China | Dec 2020 - Dec 2022

- Applied physics-based simulations to lithium-ion battery R&D and manufacturing across atomic, particle, and cell levels
- Executed high-throughput DFT and force-field screening for NCM and LFMP-based cathode materials
- Modeled NCM and LFMP cathode calendaring process via Discrete Element Method (DEM)
- Applied back-box optimization algorithms (BO,PSO,DE) to optimize simulation model parameters and design variables
- Built autonomous parameter-identification workflows for DEM, electrochemistry (P2D, ECM), and FEM models to accelerate simulation cycles
- Developed machine learning models for battery power mapping and swelling force prediction.

EDUCATION

Iowa State University

Ames, Iowa, USA | Jan 2023 - (Expected 2026~2027)

PhD in Materials Science and Engineering

Washington University in St. Louis

St. Louis, Missouri, USA | Aug 2018 - Jan 2020

Master's in Materials Science and Engineering

Changchun University of Science and Technology

Changchun, China | Sep 2014 - Jun 2018

Bachelor's in Materials Science and Engineering

SKILLS

Simulation Tools: VASP, LAMMPS, ASE, GAMESS, Quantum ESPRESSO, LIGGGHTS, COMSOL

Programming: Python, Swift, MATLAB, C