RUI ZHOU

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EDUCATION

IOWA STATE UNIVERSITY   Ames, IA
  Ph.D., Materials Science and Engineering   expected 2027

WASHINGTON UNIVERSITY IN ST. LOUIS   St. Louis, MO
  M.S., Materials Science and Engineering   December 2019

CHANGCHUN UNIVERSITY OF SCIENCE AND TECHNOLOGY   Jilin, China
  B.Eng., Materials Science and Engineering   June 2018

RESEARCH EXPERIENCE

IOWA STATE UNIVERSITY   Ames, IA
Graduate Research Assistant   January 2023 - Present
> Use first-principal calculation and machine learning forcefield to study structure and transport behavior of solid-state electrolyte materials and structural materials

WASHINGTON UNIVERSITY IN ST. LOUIS   St. Louis, MO
Graduate Research Assistant   August 2018 – December 2019
> Study the influence of the surface properties on the thermal and mass transfer behavior of water evaporation using MD simulations
> Optimize the shape of micropillar array to improve its evaporation and cooling

PROFESSIONAL EXPERIENCE

Sunwoda Electric Vehicle Battery Co., ltd   Shenzhen, China
Simulation Engineer   December 2020 - December 2022
> Developing simulation-based methods to improve battery development and manufacturing focusing on safety, stability, and energy density.
> Developing numeric models to detect lithium-plating and predict the swelling force
> Developing tools to fit model parameters to experiment data with lower cost

PUBLICATIONS

R Zhou, K Luo, Q An. *Data-Driven Atomistic Modeling of Crystalline and Glassy Solid-State Electrolytes*. Chemical Communications, 2025

K Luo, **R Zhou**, Q An. *Mechanistic insights into photoplasticity of CdTe*. International Journal of Mechanical Sciences, 2025

J Zheng, …, **R Zhou**, … H Wang. *dpdata: A Scalable Python Toolkit for Atomistic Machine Learning Data Sets*. Journal of Chemical Information and Modeling, 2025

R Zhou, K Luo, L Fei, Q An. *Unraveling Superionic Conductivity in $Na_2B_{12}H_{12}$: Molecular Dynamics Study of Phase Transition, Anion Reorientation, and Ionic Conductivity via Machine Learning Force Field*. ACS Electrochemistry, 2025

K Luo, **R Zhou**, Q An. *Unraveling Photoplasticity in ZnS: Enhanced Peierls Stress under Photoexcitation using Machine Learning Potentials*. ACS Materials Letters, 202

K Luo, **R Zhou**, SW Martin, Q An. *Flexible doorway controlled Na+ ionc diffusion in NaPSO glassy electrolytes from machine-learning force field simulations*. Journal of Materials Chemistry A, 2024

R Zhou, K Luo, SW Martin, Q An. *Insights into Lithium Sulfide Glass Electrolyte Structures and Ionic Conductivity via Machine Learning Force Field Simulations.* ACS Applied Materials & Interfaces, 2024

J Liu, K Luo, **R Zhou**, Q An. *Understanding the Role of 1/2 ⟨110⟩ Dislocations in Deformation Mechanisms of Single-Crystal High-Entropy Carbide Ceramics from Machine Learning Force Field Simulations*. ACS Applied Engineering Materials, 2024

H Wang, C Yuan, **R Zhou**, Q Duan, Y Li. *Self-sacrifice template formation of nitrogen-doped porous carbon microtubes towards high performance anode materials in lithium ion batteries*. Chemical Engineering Journal, 2017

J Guo, J Liu, H Dai, **R Zhou**, T Wang, C Zhang, S Ding, H Wang. *Nitrogen doped carbon nanofiber derived from polypyrrole functionalized polyacrylonitrile for applications in lithium-ion batteries and oxygen reduction reaction*. Journal of colloid and interface science, 2017

PATENTS

"Ternary material and preparation method thereof, lithium ion battery and power utilization equipment"
    (Granted) CN114744187B. Date of Application: June 2022
"Method, system, equipment and storage medium for optimizing particle size of material particles"
    (Granted) CN114169233A. Date of Application: Nov 2021
"Simulation optimization design method, system, equipment and medium for battery material mixing proportion"
    (Pending) CN115579085A. Date of Application: Oct 2022
"Parameter identification method, system, device and medium for secondary battery physical model"
    (Granted) CN115392123A. Date of Application: Aug 2022