Ziqi Wang

ziqiw@umich.edu · (617) 309-9097 · linkedin.com/in/ziqi-wang · https://eeg.engin.umich.edu/ziqiwang/ · arxiv.org/abs/2507.14267

Trustworthy scientific LLM agent researcher. First author of DREAMS.

EDUCATION

Ph.D., Mechanical Engineering and Scientific Computing 2021–2026 (expected)
Carnegie Mellon University & University of Michigan · Advisor: Prof. Venkatasubramanian Viswanathan

B.S., Mechanical Engineering & B.S., Computer Science 2016–2021
University of Michigan & Florida Institute of Technology

RESEARCH EXPERIENCE

DREAMS First author · arXiv 2025

Fully autonomous LLM agent that runs expert-level materials simulations

- Reached human-expert accuracy on multi-step autonomous workflows: reproduced a long-debated surface-chemistry benchmark (CO/Pt(111)) to within 0.2% and matched expert structures on all 27 systems of a crystal benchmark, where a single-agent baseline failed every run and a multi-agent baseline missed by 389%.
- Canvas: a shared communication-and-memory scheme with report-based history compression for long-horizon runs; benchmarked against single- and multi-agent baselines on accuracy, success rate, and token cost, using up to ~3x fewer tokens on long-horizon tasks.
- Deterministic and LLM-based safety guards validate every parameter against customizable rule levels and user-defined sensitive parameters; tuned on an adversarial harness of 145 scenarios from real DFT runs, best judge at 1 false positive and 3 false negatives (n=145) across five frontier LLMs.
- Full traceability: every result registered with its inputs and outputs, verified by reference ID, and linked to its sources through a provenance DAG, each claim backed by an ID-annotated reasoning chain, enabling recursive debugging of long runs.

DREAMS-OER Manuscript in preparation

Autonomous agent for open-ended catalyst discovery over a ~380,000-material space

- Scaled the agent from a single fixed task to open-ended search over ~380,000 candidate materials (Google DeepMind's GNoME set, DFT via VASP), choosing what to study next (material, surface, site, three intermediates) from accumulated evidence rather than a fixed plan. (Demonstrated on behavioral runs; production screening in progress.)
- Grounded decisions in retrieval-augmented (RAG) literature results and a multi-level relational experiment log that enables efficient information retrieval and progress tracking across hundreds of partial, interdependent studies.
- Gave the agent live time- and compute-budget awareness to submit work opportunistically, keep the cluster busy while reasoning, and re-plan under pressure, completing a bounded 7-hour study without overrunning.
- Caught workers specification-gaming a queue-occupancy target, submitting jobs to satisfy the metric without analyzing results; fixed it structurally with a disposition gate making engagement with every completed result a verifiable predicate before rest, plus a runaway-loop guard.

Alloy Thermodynamics and Phase Behavior with Machine-Learning Interatomic Potentials Manuscript in preparation

- Built a committee-based active-learning loop to fine-tune universal MLIPs (MACE, NequIP, GRACE, MatterSim) into low-cost surrogates for the Li-Mg alloy system, cutting prediction error by roughly 5x versus off-the-shelf models; stress-weighted training gave the largest gains on hard second-derivative properties.
- Ran LAMMPS molecular dynamics melting/solidification campaigns with MLIPs and classical potentials to locate melting temperatures across composition for binary and ternary lithium alloys.
- Mapped solid-phase boundaries of binary alloys with canonical and semi-grand canonical Monte Carlo, using cluster-expansion models and LAMMPS with MLIPs and classical potentials.
- Computed free energies by thermodynamic integration to an Einstein crystal; constructed phase diagrams via thermodynamic integration, metadynamics, heat capacity, and moving-interface methods.
- Quantified non-linear excess effects in stiffness and atomic-transport barriers across alloy composition.

PUBLICATIONS & PREPRINTS

- **Z. Wang**, H. Huang, H. Zhao, C. Xu, S. Zhu, J. Janssen, V. Viswanathan. "DREAMS: Density Functional Theory Based Research Engine for Agentic Materials Simulation." arXiv:2507.14267 (2025).
- A. M. Yao, S.-J. Kim, V. D. Veeraraghavan, **Z. Wang**, S. Gasilov, A. Kastengren, Y.-M. Chiang, P. Fenter, V. Viswanathan. "Effective Li-Ion Transport Quantification in Composite Cathodes for All-Solid-State Batteries via Multiscale Modeling and Experiments." Chem. Mater. 37, 9260–9267 (2025).

TECHNICAL SKILLS

Agentic AI / LLM: multi-agent system design, harness design, SKILL design, guardrail and provenance systems, agent evaluation and benchmarking, RAG, LangGraph, LangChain.
Machine Learning: PyTorch, machine learning interatomic potentials (MACE, NequIP, MatterSim, GRACE, SchNet), graph neural networks, active learning
Atomistic Simulation: DFT (Quantum ESPRESSO, VASP), ASE, molecular dynamics (LAMMPS), Monte Carlo, cluster expansion, thermodynamic integration, nudged elastic band
Computing: Python, C++, HPC / SLURM, Git

HONORS & AWARDS

- Selected for Anthropic AI for Science Program (2026)
- University Honors, University of Michigan (2019, 2020, 2021)