

Tianhao (Tyan) Li

Baltimore, MD | (+1) 410-908-3216 | tli114@jh.edu | tianhao-li.com | linkedin.com/in/tyanli | [Google Scholar](https://scholar.google.com/citations?user=...)

SUMMARY

Ph.D. candidate researching data-efficient and reliable machine learning for scientific discovery: selecting training data to adapt foundation models under distribution shift, uncertainty-aware surrogate screening, and evaluation beyond proxy metrics. At Amazon, built a multi-agent AI co-scientist with tool-using, citation-grounded retrieval and LLM-as-a-judge evaluation. Built data infrastructure behind a 243K-entry simulation database and a 3.4M-structure open dataset.

EDUCATION

Johns Hopkins University

Ph.D. in Materials Science and Engineering

- Advisor: Prof. Corey Oses
- **Amazon AI PhD Fellow** (2025 – 2027)

Baltimore, MD

Sept. 2023 – Expected 05/2028

Duke University

M.S. in Materials Science and Engineering

Durham, NC

Sept. 2021 – Aug. 2023

Changsha University of Science and Technology

B.S. in Materials Science and Engineering

Changsha, China

Sept. 2016 – Jun. 2020

INDUSTRY EXPERIENCE

Amazon

Applied Scientist Intern — Agentic AI for Scientific Discovery

Seattle, WA

Jun. 2026 – Sep. 2026

- Built a multi-agent AI co-scientist for scientific hypothesis generation: literature-grounded generation, reflection, Elo-rated pairwise tournaments, and evolution agents, with a scientist- and lab-in-the-loop feeding expert review, simulation, and experimental results back into ranking.
- Built a tool-using literature agent through three architectures: single-agent search-and-write loop → citation-graph crawler with a recall-based stopping rule → map-reduce full-text reading over thousands of papers, with quote-level attribution so every finding cites a verbatim passage from a retrieved source.
- Designed the evaluation protocol: an independent LLM-as-a-judge scoring structured hypotheses (claim strength, reasoning, counterexample) on separate grounding and reasoning axes; tournament safeguards (review-gated entry, Elo reliability by unique opponents, no repeat matches); a Recall@K retrieval benchmark from survey bibliographies; and blinded-rediscovery runs with leakage checks, where top-ranked hypotheses independently recovered the design family already used in production (preliminary).

RESEARCH EXPERIENCE

Johns Hopkins University, Entropy for Energy Laboratory

Graduate Research Assistant

Baltimore, MD

Sept. 2023 – Present

Data-Efficient Fine-Tuning of Foundation Models for Atomistic Simulation

2024 – Present

- Pretrained graph neural network (GNN) foundation models for atomistic simulation degrade on out-of-distribution, highly disordered materials, where labels from expensive physics simulations are scarce; framed adaptation as selecting training data from a ~150K-sample pool of related structures.
- Developed a similarity-guided data-selection loop that tunes its threshold until out-of-distribution validation error meets target: 109 selected samples fine-tune the model to 29 meV/atom error (target <30), whereas random selection saturates near 50 meV/atom and degrades as more data is added.
- Analyzed the GNN latent space to explain why the selected data transfers, then deployed the adapted model across millions of calculations for large-scale materials screening, with a two-stage sampling scheme needing about one-fifth of the original cost.

Benchmarking Atomistic Foundation Models Beyond Proxy Metrics

2025 – 2026

- Co-developed a 1,500-system benchmark of four foundation models (MACE, CHGNet, eSEN, UMA) showing that standard structural-accuracy benchmarks are a poor proxy for downstream electronic-structure accuracy (Pearson $r = 0.03$ – 0.24 between the two errors); using the models to pre-optimize structures still makes reference quantum-mechanical simulations converge 3 – $7\times$ faster (11 – $15\times$ for MACE).
- Co-authored a study of how 15 attention-based models transfer from training data to long-running dynamic simulations in deployment; deployment tests exposed failures that static test-set errors missed.

- Trained random-forest surrogate models on >20K physics simulations (427 alloy compositions) to predict four activity and stability metrics (5-fold CV test $r^2 > 0.8$, up to 0.99), extending coverage 50 $\times$ to 26,334 candidates that would otherwise need >1M simulations.
- Combined multi-objective ranking (activity, stability, cost, supply risk) with per-tree uncertainty (0.66 vs. 0.28 for inputs containing unseen vs. seen chemical elements) to flag out-of-domain predictions; identified 40 platinum-free fuel-cell catalyst candidates and released [open-source code](#).

Scientific Data & LLM Infrastructure

2023 – Present

- Built and operate an automated high-throughput simulation workflow on HPC clusters (Slurm/Bash) feeding the lab's CHAOS database, now ~243K entries behind a public search API and LLM agent; co-developed CHAOS-MatForge, an open [Hugging Face](#) dataset of 3.4M simulation-labeled atomic structures for ML training.
- Productionized the lab's Django/MongoDB materials-data platform (Docker deployment, security hardening, automated backups, vector search, CHAOS data import), and added embedding-based retrieval (RAG) to the CHAOS-GPT natural-language query prototype.

SKILLS

LLM & Agentic AI: multi-agent orchestration, tool calling, RAG, embedding/vector search, prompt engineering, LLM-as-a-judge evaluation, citation grounding

Machine Learning: PyTorch, TensorFlow, scikit-learn; graph neural networks and ML interatomic potentials (CHGNet, MACE, DeePMD-kit); active learning and data selection; surrogate modeling; uncertainty estimation

Software & Infrastructure: Python, C++, Bash, SQL; Linux/HPC (Slurm), Docker Compose, Django, MongoDB, SQLite, Git, pytest

Scientific Computing: DFT (VASP, AFLOW), LAMMPS, ASE, pymatgen

PUBLICATIONS[†]Equal contribution

- **Li, T.[†]**; Han, G.[†]; Xu, X.; Lee, J.; Qiu, G.; Sequeira, S.; Ajith, A.; Oses, C. The search for high-entropy fuel-cell catalysts using disorder descriptors. *Nano Futures* **9**, 045001 (2025).
- **Li, T.[†]**; Han, G.[†]; *et al.* Designing ultra-complex structurally disordered materials via machine learning interatomic potentials (in preparation).
- **Li, T.**; Han, G.; Xu, X.; Hu, J.; Oses, C. A Debye–Waller temperature for computed diffraction references (in preparation).
- Tseng, S.-Y.[†]; Han, G.[†]; **Li, T.**; Xu, X.; Hu, J.; Qiu, G.; Oses, C. Structural benchmarks overlook density-of-states errors in machine-learned interatomic potentials. *APL Mach. Learn.* **4**, 036117 (2026).
- Xu, X.; Han, G.; **Li, T.**; *et al.* Stabilizing iodine in pyrochlore: toward new nuclear waste forms. *Precis. Chem.* **4**, 1211–1224 (2026).
- Qiu, G.; **Li, T.**; Xu, X.; *et al.* High entropy powering green energy: hydrogen, batteries, electronics, and catalysis. *npj Comput. Mater.* **11**, 145 (2025).
- Oses, C.; **Li, T.**; Xu, X.; Han, G.; Qiu, G.; Owens, J. R. Beyond the four core effects: revisiting thermoelectrics with a high-entropy design. *Mater. Horiz.* **12**, 5946–5956 (2025).
- Chen, J.[†]; Yang, H.[†]; **Li, T.**; *et al.* The effects of reversibility of H₂–H₃ phase transition on Ni-rich layered oxide cathode for high-energy lithium-ion batteries. *Front. Chem.* **7**, 500 (2019).
- Hu, J.; Peiris, M. D. H. C.; Singh, S.; **Li, T.**; Xu, X.; Mukhopadhyaya, A.; Maranets, T.; Tseng, S.-Y.; Oses, C. From training data to molecular-dynamics deployment: transfer of machine-learning interatomic potentials in a refractory high-entropy alloy. Under review at *Mach. Learn.: Eng.* (2026).
- Hu, J.[†]; Tseng, S.-Y.[†]; Brownrigg, M.[†]; Bector, P.; Han, G.; **Li, T.**; *et al.* CHAOS: a first-principles database for high-entropy oxide discovery (under review).
- Singh, S.[†]; Peiris, M. D. H. C.[†]; Hu, J.[†]; **Li, T.**; *et al.* From optical constants to fusion mirrors: source-resolved optical screening of protective mirror architectures (under review).
- Hu, J.[†]; Kane, K.[†]; Bregman, A.[†]; King, K. A.; Rao, K. K.; He, M.-R.; Spada, J.; **Li, T.**; *et al.* Iron-driven phase allocation amplifies hydrogen production in poly-cation oxides (under review).

SERVICE, TEACHING & TALKS

Peer review: *Nature Communications*; *International Journal of Applied Glass Science* (co-reviewed with advisor)

Teaching Assistant: Gateway Computing: Python (EN.500.113, Spring 2024, ~40 students); Introduction to Computational Materials Modeling (EN.510.466/666, Fall 2023)

Talks: Data-Driven Materials Modeling Workshop, JHU (talk, [recording](#), 2024); ARPA-E Energy Innovation Summit (poster, 2025); ARPA-E Annual Fission Meeting (poster, 2024)