

# HENGRUI ZHANG

Technological Institute – 2145 Sheridan Road – Evanston, IL 60208, USA  
☎ (847) 730-4352 • ✉ hrzhang@u.northwestern.edu • 🌐 hrzhang.me

## Education

**Northwestern University**, Evanston, IL, USA 9/2020–6/2025  
Ph.D., Mechanical Engineering, Topic: AI for materials design  
Committee: Wei Chen, James Rondinelli, Daniel Apley, Edward Sargent

**Shanghai Jiao Tong University**, Shanghai, China 9/2016–6/2020  
B.S. (Hons.), Materials Science & Engineering, Computer Science  
Visiting Student, University of Oxford (2018), Northwestern University (2019)

## Research Experiences

**Northwestern University - McCormick School of Engineering** 9/2021–Present  
Graduate Researcher, Advisors: Wei Chen & James Rondinelli  
○ Physics-based machine learning methods for crystal heterostructures and molecular mixtures.  
○ Co-design of microelectronic materials and devices using first-principles calculations and informatics.

**Mitsubishi Electric Research Labs**, Cambridge, MA, USA 6/2023–9/2023  
Research Intern, Host: Bingnan Wang  
○ Machine learning-based electric motor design and fault diagnosis.  
○ Paper to be presented at International Conference on Electrical Machines (ICEM) 2024.

**Shanghai Jiao Tong University - Materials Genome Initiative Center** 3/2018–6/2020  
Undergraduate Researcher, Advisor: Hong Wang  
○ Phase diagram construction using high-throughput experiments and machine learning.

## Publications & Manuscripts

1. **Zhang, H.**, Lai, T., Chen, J., Manthiram, A., Rondinelli, J. & Chen, W. Learning molecular mixture property using chemistry-aware graph neural network. *PRX Energy*. Accepted (2024).
2. Chaney, L., van Beek, A., Downing, J., Zhang, J., **Zhang, H.**, Hui, J., *et al.* Bayesian optimization of environmentally sustainable graphene inks produced by wet jet milling. *Small* **20**, 2309579 (2024).
3. **Zhang, H.**, Chen, W., Rondinelli, J. & Chen, W. ET-AL: Entropy-targeted active learning for bias mitigation in materials data. *Applied Physics Reviews* **10**, 021403 (2023).
4. Chen, J., **Zhang, H.**, Wahl, C., Liu, W., Mirkin, C., Dravid, V., *et al.* Automated crystal system identification from electron diffraction patterns using multiview opinion fusion machine learning. *Proceedings of the National Academy of Sciences* **120**, e2309240120 (2023).
5. **Zhang, H.**, Chen, W., Iyer, A., Apley, D. & Chen, W. Uncertainty-aware mixed-variable machine learning for materials design. *Scientific Reports* **12**, 19760 (2022).
6. Hui, J., Hu, Q., **Zhang, H.**, Zhao, J., Luo, Y., Ren, Y., *et al.* High-throughput investigation of structural evolution upon solid-state in Cu–Cr–Co combinatorial multilayer thin-film. *Materials & Design* **215**, 110455 (2022).
7. **Zhang, H.** Demand-driven materials design. *Journal of Shanghai Jiao Tong University* **55**, 93 (2021).
8. Hui, J., **Zhang, H.**, Hu, Q., Zhang, Z., Ren, Y., Zhang, L. & Wang, H. Investigation of synchrotron X-ray induced oxidation of Ag–Cu thin-film. *Materials Letters* **272**, 127843 (2020).

9. Hui, J., Ma, H., Wu, Z., Zhang, Z., Ren, Y., **Zhang, H.**, *et al.* High-throughput investigation of crystal-to-glass transformation of Ti–Ni–Cu ternary alloy. *Scientific Reports* **9**, 19932 (2019).
10. Chen, J., Ou, P., Chang, Y., **Zhang, H.**, Li, X., Sargent, E. & Chen, W. Adaptive catalyst discovery using multicriteria Bayesian optimization with representation learning. arXiv:2404.12445 (2024).
11. Chang, Y., Benlolo, I., Reimer, C., Zhou, D., **Zhang, H.**, Choubisa, H., *et al.* High-entropy alloy electrocatalysts screened using machine learning informed by quantum-inspired similarity analysis: computational prediction and experimental synthesis. Under review for *Matter* (2024).

## Selected Presentations

---

- [Oral] “MolSets: Molecular graph deep sets learning for mixture property modeling,” *APS March Meeting*, Minneapolis, MN, USA (2024).
- [Poster] “Mitigating bias in scientific data: a materials science case study,” *NeurIPS AI for Science Workshop*, New Orleans, LA, USA (2023).
- [Oral] “ET-AL: Entropy-targeted active learning for bias mitigation in materials data,” *MRS Spring Meeting*, San Francisco, CA, USA (2023).
- [Invited] “Adaptive discovery and mixed-variable optimization for next-generation synthesizable microelectronic materials,” *TMS Annual Meeting*, San Diego, CA, USA (2023).
- [Poster] “Autonomous phase diagram construction guided by active learning,” *Forum of Materials Genome Engineering* (best poster award), Mianyang, Sichuan, China (2020).

## Teaching & Services

---

**Teaching Assistant**, MSE 358: Materials Modeling and Simulation (Northwestern), 2023.

**Reviewer**, Journals: Neural Comput. Appl., MRS Adv., ISA Trans., J. Open Source Softw.; Conferences: NeurIPS AI4Mat, ICEM, IDETC

## Research Grants

---

Proposal “Accelerated Design, Discovery, and Deployment of Electronic Phase Transitions (ADEPT)” won **NSF DMREF** award (PIs: James Rondinelli & Wei Chen, Amount: \$798K), 2023.

- Conceived challenges and breakthroughs with PIs; drafted the AI/informatics-related contents.

## Honors & Awards

---

Ryan Fellowship (Northwestern) [about]	2023
Predictive Science and Engineering Design Fellowship [about]	2021
Zhiyuan Outstanding Student (Top 1% SJTU graduates)	2020
Fung Scholarship (Oxford) [about]	2018
China National Scholarship, Fan Hsu-chi Scholarship (SJTU)	2017, 2018

## Technical Skills

---

**Programming:** Python (proficient in PyTorch), MATLAB, R, C/C++, JavaScript

**Simulation:** Atomic Simulation Environment, VASP, GPAW, Quantum Espresso, LAMMPS, Abaqus