

# HENGRUI ZHANG

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## 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.

**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

1. **Zhang, H.**, Huang, R., Chen, J., Rondinelli, J. & Chen, W. Do graph neural networks work for high-entropy alloys? arXiv:2408.16337; accepted by NeurIPS AI4Mat workshop (2024).
2. Chen, J., Ou, P., Chang, Y., **Zhang, H.**, *et al.* Adaptive catalyst discovery using multicriteria Bayesian optimization with representation learning. arXiv:2404.12445 (2024).
3. **Zhang, H.**, Lai, T., Chen, J., Manthiram, A., Rondinelli, J. & Chen, W. Learning molecular mixture property using chemistry-aware graph neural network. *PRX Energy* **3**, 023006 (2024).
4. Chang, Y., Benlolo, I., Bai, Y., Reimer, C., Zhou, D., **Zhang, H.**, *et al.* High-entropy alloy electrocatalysts screened using machine learning informed by quantum-inspired similarity analysis. *Matter* **7**, 4099–4113 (2024).
5. Chaney, L., van Beek, A., Downing, J., Zhang, J., **Zhang, H.**, *et al.* Bayesian optimization of environmentally sustainable graphene inks produced by wet jet milling. *Small* **20**, 2309579 (2024).
6. **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).
7. Chen, J., **Zhang, H.**, Wahl, C., *et al.* Automated crystal system identification from electron diffraction patterns using multiview opinion fusion machine learning. *PNAS* **120**, e2309240120 (2023).
8. **Zhang, H.**, Chen, W., Iyer, A., Apley, D. & Chen, W. Uncertainty-aware mixed-variable machine learning for materials design. *Scientific Reports* **12**, 19760 (2022).

9. Hui, J., Hu, Q., **Zhang, H.**, *et al.* High-throughput investigation of structural evolution upon solid-state in Cu–Cr–Co combinatorial multilayer thin-film. *Materials & Design* **215**, 110455 (2022).
10. **Zhang, H.** Demand-driven materials design (commissioned). *Journal of SJTU* **55**, 93 (2021).
11. Hui, J., **Zhang, H.**, Hu, Q., *et al.* Investigation of synchrotron X-ray induced oxidation of Ag–Cu thin-film. *Materials Letters* **272**, 127843 (2020).
12. 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).
13. **Zhang, H.** & Wang, B. *Supervised contrastive learning for electric motor bearing fault detection* in *International Conference on Electrical Machines* (2024).

## Selected Presentations

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- [Poster] “Graph representation of local environments for learning high-entropy alloy properties,” *NeurIPS AI for Materials Workshop*, Vancouver, BC, Canada (2024).
- [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] “Mitigating bias in materials data,” *SRC TechCon*, Austin, TX, 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

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

**Reviewer**, Journals: Neural Comput. Appl., MRS Adv., ISA Trans., J. Open Source Softw., MethodsX; Conferences: NeurIPS (top reviewer), ICLR, IDETC, AI4Mat workshop, ICEM

## Grant Writing

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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 content.

Proposal “Adaptive Sampling and High Throughput Data Analysis for Nanostructure Mega-Libraries” won NU Center for Nanocombinatorics fund (PIs: Wei Chen & Daniel Apley, Amount: \$140K), 2023.

## Honors & Awards

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Ryan Fellows Best Paper Prize	2024
Ryan Fellowship (Northwestern) [about]	2023
Predictive Science and Engineering Design Fellowship [about]	2021

Walter P. Murphy Fellowship (Northwestern)	2020
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

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

**Simulation:** ASE; DFT (VASP, GPAW, Quantum Espresso); MD (LAMMPS); KMC; FEA (Abaqus)

## References

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### Dr. James M. Rondinelli

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### Dr. Edward H. Sargent

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