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 structure representation and machine learning for complex materials systems.
- 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.

Northwestern University - Mechanical Engineering 7/2019–9/2019
Visiting Scholar, Advisor: Wei Chen
- Statistical representation of microstructures and MaterialsMine data platform development.

University of Oxford - Department of Materials 7/2018–9/2018
Visiting Scholar, Advisors: Peter Wilshaw & Sebastian Bonilla
- Physics-based modeling and simulation for the charge transport in Si solar cell surface and interfaces.

Publications

1. **Zhang, H.**, Huang, R., Chen, J., Rondinelli, J. & Chen, W. Graph representation of local environments for learning high-entropy alloy properties. *Machine Learning: Science and Technology.* In press (2025).
2. **Zhang, H.**, Georgescu, A., Yerramilli, S., Karpovich, C., Apley, D., Olivetti, E., Rondinelli, J. & Chen, W. Emerging microelectronic materials by design: Navigating combinatorial design space with scarce and dispersed data. arXiv:2412.17283 (2024).
3. Chen, J., Ou, P., Chang, Y., **Zhang, H.**, *et al.* Adaptive catalyst discovery using multicriteria Bayesian optimization with representation learning. arXiv:2404.12445 (2024).
4. **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).
5. 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).

6. 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).
7. **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).
8. 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).
9. **Zhang, H.**, Chen, W., Iyer, A., Apley, D. & Chen, W. Uncertainty-aware mixed-variable machine learning for materials design. *Scientific Reports* **12,** 19760 (2022).
10. 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).
11. **Zhang, H.** Demand-driven materials design (commissioned). *Journal of SJTU* **55,** 93 (2021).
12. 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).
13. 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).
14. **Zhang, H.** & Wang, B. *Supervised contrastive learning for electric motor bearing fault detection* in *International Conference on Electrical Machines* (2024).

Selected Presentations

- **[Oral]** "Investigating insulator–metal transitions in Ti_2O_3/$MnTiO_3$ superlattices," *MRS Spring Meeting*, Seattle, WA, USA (2025).
- **[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," *Semiconductor Research Corporation*, 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).

Grant Writing

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.

Teaching & Services

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

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

Co-organizer, Northwestern Institute on Complex Systems (NICO) Reading Group, 2022–23.

Volunteer, Baxter Symposium for Science Education, 2024.

Honors & Awards

MRS Graduate Student Award	2025
Ryan Fellows Best Paper Prize	2024
Ryan Fellowship (Northwestern) [about]	2023–25
Predictive Science and Engineering Design Fellowship [about]	2021–22
Walter P. Murphy Fellowship (Northwestern)	2020–21
Zhiyuan Outstanding Student (Top 1% SJTU graduates)	2020
Fung Scholarship (Oxford) [about]	2018
China National Scholarship, Fan Hsu-chi Scholarship (SJTU)	2017–19

Technical Skills

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

Simulation: ASE; DFT (VASP, GPAW, QE); MD (LAMMPS); KMC; FEA (Abaqus)

References

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Dr. Edward H. Sargent
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