Hengrui Zhang

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Education

Northwestern University, Evanston, IL, USA 2020–2025
Ph.D., Mechanical Engineering, Advisors: Wei Chen & James Rondinelli
Thesis: Data-centric design of combinatorial materials systems.

Shanghai Jiao Tong University, Shanghai, China 2016–2020
B.S. (Hons.), Materials Science & Engineering, Computer Science, Advisor: Hong Wang
Thesis: Autonomous phase diagram construction guided by active learning.

Visiting Student, **University of Oxford** (2018), **Northwestern University** (2019)

Professional Experiences

Northwestern University - McCormick School of Engineering 2021–2025
Graduate Researcher, Teaching Assistant: AI for materials design.

Mitsubishi Electric Research Labs, Cambridge, MA, USA Summer 2023
Research Intern: ML-based electric machine design and diagnosis.

Selected Publications [full list]

1. **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. *Accounts of Materials Research* **6,** 730–741 (2025).
2. **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* **6,** 025005 (2025).
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).

Selected Presentations

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

- **[Poster]** "Do graph neural networks work for high entropy alloys?" *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]** "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).

Grant Writing

- "Accelerated design, discovery, and deployment of electronic phase transitions (ADEPT)" won **NSF DMREF** award (PIs: James Rondinelli & Wei Chen, Amount: $798K), 2023.
- "Adaptive sampling and high-throughput data analysis for nanostructure mega-libraries" funded by NU Center for Nanocombinatorics (PIs: Wei Chen & Daniel Apley, Amount: $140K), 2023.

Services & Outreach

Reviewer, [Journals] EPJ B, 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; All Scout Nano Day, 2025.

Honors & Awards

MRS Graduate Student Silver Award [about]	2025
Management for PhDs Certificate (Northwestern Kellogg)	2024
Ryan Fellowship (Northwestern) [about]	2023–25
Predictive Science and Engineering Design Certificate [about]	2021–22
Walter P. Murphy Fellowship (Northwestern)	2020–21
Zhiyuan Outstanding Student (Top 1% SJTU graduates)	2020
Fung Scholarship (SJTU–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)