Xinzhe Dai

AI for Science | Computational Materials Science
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EDUCATION

Cornell University **Ithaca, NY | Sep 2024 – Present**
Ph.D. Student, Materials Science and Engineering | GPA: 3.97 Advisor: Prof. Jingjie Yeo

University of Chinese Academy of Sciences (UCAS) **Beijing, China | Sep 2019 – Jun 2024**
B.S. in Physics, School of Physical Sciences | GPA: 3.85

RESEARCH EXPERIENCE

Cornell University – Research Assistant **Sep 2024 – Present**
Sibley School of Mechanical and Aerospace Engineering | Advisor: Prof. Jingjie Yeo
Deformation-Guided Transport of Anisotropic Particles in Polymer Networks

- Developed large-scale dissipative particle dynamics simulations in LAMMPS to study anomalous transport through mechanically deformed polymer networks.
- Mapped anisotropic diffusivity across particle aspect ratio, size ratio, and network stretch; analyzed orientational correlations to characterize translation-rotation coupling and investigate non-monotonic transport trends.
- Built an automated Python workflow to generate non-overlapping polymer-particle configurations and used enhanced sampling to compute potentials of mean force for particle passage through polymer cross-links.
- Developing a memory-kernel-based reduced representation to characterize non-Markovian dynamics and dynamical coupling.

University of California, Berkeley – Visiting Student **Jun 2023 – May 2024**
Department of Materials Science and Engineering | Advisor: Prof. Gerbrand Ceder
CHGGen: Crystal Inpainting with Diffusion and Foundation Potentials

- Adapted an SE(3)-equivariant diffusion model for crystal inpainting, implementing score-based denoising to generate intercalation structures conditioned on host frameworks.
- Implemented a resampling algorithm to overcome the locality bias of GNNs, increasing the fraction of generated structures with higher crystallographic symmetry.
- Integrated foundation potentials (CHGNet) for structure relaxation and stability screening, identifying low-energy candidate structures in Li-Si and Zn-P-S systems.

Benchmarking Universal Machine-Learning Interatomic Potentials Against NequIP

- Investigated the effects of dataset size and symmetry constraints on the performance of universal machine learning interatomic potentials, using NequIP as a benchmark.

Massachusetts Institute of Technology – Research Intern **May 2022 – Jul 2022**
Department of Materials Science and Engineering | Advisor: Prof. Rodrigo Freitas
Data-Centric Crystal Structure Identification with Graph Neural Networks

- Applied graph convolutional neural networks to classify local crystalline environments in atomistic simulations, achieving 2-5x lower error rate than baseline methods.
- Engineered physics-informed features to achieve 3x faster inference than the original GNN pipeline.

University of Chinese Academy of Sciences – Research Intern **Oct 2021 – Aug 2024**
School of Physical Sciences | Advisor: Prof. Wu Zhou
DeepSTEM: Deep Learning for Atomic-Scale Imaging and Spectroscopy

- Implemented a rotation-invariant variational autoencoder (r-VAE) for unsupervised feature discovery in amorphous carbon, disentangling latent variables associated with topological descriptors, such as ring sizes and atom counts per ring.
- Combined a supervised U-Net denoiser with physical Z-contrast power-law models to achieve high-precision chemical characterization of single atoms from low-dose images.
- Engineered a statistical pipeline for EELS spectral denoising, enhancing the signal-to-noise ratio to enable atomic-scale isotope mapping.

University of Chinese Academy of Sciences – Research Intern **Mar 2021 – Oct 2021**
School of Physical Sciences | Advisor: Prof. Qian Liu
Machine Learning and Simulation for Radiation Detection

- Implemented a 9-layer CNN for neutron-gamma pulse-shape discrimination, achieving 99.85% accuracy with performance comparable to traditional methods.
- Developed and evaluated reconstruction algorithms for cosmic-ray muon imaging using Geant4 simulation data.

SELECTED PUBLICATIONS

- **Inpainting crystal structure generations with score-based denoising.** *ICML AI for Science Workshop, 2024.* **Dai, X.**, Zhong, P., Deng, B., Chen, Y., Ceder, G.
- **Crystal structure prediction with host-guided inpainting generation and foundation potentials.** *Materials Horizons, 2025.* Zhong, P., **Dai, X.**, Deng, B., Ceder, G., Persson, K. A.
- **Mechano-diffusion of particles in hydrogels.** *Extreme Mechanics Letters, 2026.* Ma, J., Wong, T., Yu, Z., **Dai, X.**, Ye, C., Yeo, J., Lin, S.
- **Low-dose imaging denoising with one pair of noisy images.** *Optics Express, 2023.* Yang, D., Lv, W., Zhang, J., Chen, H., Sun, X., Lv, S., **Dai, X.**, Luo, R., Zhou, W., Qiu, J., Shi, Y.

TECHNICAL SKILLS

Programming and tools: Python (NumPy, SciPy, pandas), C/C++, Linux/Bash, Git, LaTeX
Machine learning: PyTorch, PyTorch Lightning, graph neural networks (e3nn, CHGNet, NequIP), diffusion/score-based models, variational autoencoders, U-Net, scikit-learn
Scientific simulation: LAMMPS (atomistic/mesoscale simulation), enhanced sampling, OVITO, VESTA, Materials Studio (CASTEP), Gaussian
Languages: English (proficient), Mandarin (native)

HONORS AND AWARDS

UCAS Academic Scholarship 2022, 2021, 2020
UCAS Overseas Graduate Studies Fellowship 2022