Rees Chang

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Research Interests

I am interested in accelerating materials discovery with machine learning. My PhD has focused on developing approaches to few-shot materials property prediction and deep generative modeling of crystalline materials. I actively collaborate with computer scientists and materials scientists.

Education

2020– present	Ph.D. in Materials Science & Engineering, **University of Illinois at Urbana-Champaign** Advisor : Elif Ertekin — Building an active learning framework interfacing conditional generative modeling, uncertainty quantification, and materials simulation — Developing space group invariant deep generative models for crystals, co-advised by Ryan Adams (Princeton CS) — Creating deep learning frameworks for few-shot materials property prediction, co-advised by Yuxiong Wang (UIUC CS)
2016–2020	B.S. with Honors in Materials Science & Engineering, **Cornell University** Thesis Advisor : Julia Dshemuchadse

Awards

2024	Best Poster Nominee, Materials Research Society Fall Meeting MT04.09.21
2022	NSF Graduate Research Fellowship
2021	DIGI-MAT NSF Research Traineeship
2020	UIUC Hamer Fellowship
2017	Cornell Engineering Learning Initiatives Research Award

Research Experience

Aug 2019– May 2020	Undergraduate Researcher, **Cornell University** Advisor : Julia Dshemuchadse — Independent project using coarse-grained molecular dynamics and Random Embedding Bayesian optimization to accelerate discovery of self-assembling structures
Summer 2019	DOE SULI Intern at the Materials Project, **Lawrence Berkeley National Lab** Advisor : Anubhav Jain — Created high-throughput density functional theory calculation workflow using Compressed Sensing Lattice Dynamics to obtain phononic properties of materials — Contributed open-source code to pymatgen

Jan 2017– Jun 2019	Undergraduate Researcher, **Cornell University** Advisor : Tobias Hanrath — Developed a genetic algorithm to optimize nanostructure in an amorphous silicon thin film — Achieved 822% increase in light absorption as calculated with finite-difference time domain electromagnetic simulations
Summer 2018	Research and Development Intern, **NASA Goddard Space Flight Center** Mentor : Dr. Larry Hess — Designed, fabricated, patterned, and characterized multilayer thin film UV detectors with photolithographic and optical methods
Summer 2015, 2016	Research Assistant, **Columbia University** Advisor : Robert Farrauto — Synthesized and characterized new carbon dioxide adsorbents and methanation catalysts with gas flow reactors, Brunauer-Emmett-Teller analysis, and thermogravimetric analysis

Publications

2025	**Chang, R.**, Pak, A., Guerra, A., Zhan, N., Richardson, N., Ertekin, E., Adams, R.P. Space Group Equivariant Crystal Diffusion. *Under review.* (2025). Preprint
2025	**Chang, R.**, et al. Crystal Generative Modeling with Explicit Autoregressive Conditional Likelihoods and Nontrivial Space Group Stabilizers. AI4Mat workshop at ICLR (2025). Paper
2024	Zhu, Z., Park, J., Sahasrabuddhe, H., Ganose, A., **Chang, R.**, Lawson, J., Jain, A. A high-throughput framework for lattice dynamics. npj Comput Mater 10, 258 (2024). Paper
2022	**Chang, R.**, Wang, Y.X., Ertekin, E. Towards overcoming data scarcity in materials science : unifying models and datasets with a mixture of experts framework. npj Comput Mater 8, 242 (2022). Paper

Presentations

2023	A Crystal Generative Model Conditioned on Space Group Oral presentation at Materials Research Society Spring Meeting MD01.06 in San Francisco, CA.
2022	Overcoming Data Scarcity in Materials Science with Mixtures of Experts Oral presentation at Materials Research Society Spring Meeting in Honolulu, HI.

Teaching

UIUC

2022-2023	Undergraduate research mentoring — Mentored 2 undergraduates on independent research projects through the National Center for Supercomputing Applications' Students Pushing Innovation Program
2021	Engineers Volunteering in STEM Education — Virtually volunteered at Franklin Middle School to promote science and introduce materials science concepts

Cornell University

Fall 2019	Teaching Assistant for CS 4780 : Machine Learning for Intelligent Systems — Held weekly office hours and graded assignments for a supervised statistical ML course of over 600 students
Fall 2019	Volunteer Teaching Assistant in Environmental Science for the Cornell Prison Education Program — Led discussions and activities for 17 incarcerated students at Cayuga Correctional Facility
Fall 2017	Teaching Assistant in MSE 2610 : Mechanical Properties of Materials — Graded problem sets for a course of 80 sophomores and first-year graduate students

Selected Coursework

UIUC

— **Graduate** : Condensed Matter Physics, Quantum Mechanics, Mathematical Physics I and II, Statistical Mechanics, Atomic Structure and Bonding

Cornell University

— **Materials Science** : Computational Chemistry ; Computational Materials Science ; Materials Chemistry ; Electronic, Dielectric, and Magnetic Properties of Materials ; Mechanical Properties of Materials ; Kinetics and Phase Transformations ; Condensed Matter Thermodynamics

— **Computer Science** : Supervised Machine Learning, Unsupervised Machine Learning, Large-Scale Machine Learning, Numerical Linear Algebra, Bayesian Estimation, Networks, OOP and Data Structures

Skills

— **Proficient** : Python (PyTorch, Numpy, Pandas, pymatgen), Git, Bash, LaTeX

— **Experienced** : JAX, VASP, HOOMD-Blue, TensorFlow, BoTorch, Mongo, MATLAB, HTML/CSS, Mathematica, Java