Kirby Broderick

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About me

Accomplished research engineer specializing in computational materials design and machine learning applications in catalysis. Experienced in designing software engineering workflows to understand and predict experimental data. Proven track record in cutting-edge research and development. Brings a strong foundation in programming, and extensive skills in data analysis and computational modeling to drive technological advancements and solve complex problems.

Interests

Computational materials design, graph neural networks, materials design and discovery, high-performance computing, Density Functional Theory, design of experiments, data science

Education

Carnegie Mellon University — Pittsburgh, PA
PhD Chemical Engineering — *Aug 2019–Feb 2024*
Thesis:
*"*Bridging Computation and Experiment in Heterogeneous Catalysis with Applied Machine Learning*"*
Advisors*: John Kitchin, Zachary Ulissi*

Georgia Institute of Technology — Atlanta, GA
BS Chemical and Biomolecular Engineering — *Aug 2015–Apr 2019*

Experience

Software Research Engineer/Scientist
Intel Corporation; Hillsboro, OR — April 2024–present

- Developing new algorithms for inverse lithography and mask rule checking
- Supporting optical proximity correction software

Graduate Student Researcher
Carnegie Mellon University; Pittsburgh, PA — August 2019–February 2024

- Designed and developed protocols to combine machine learning and density functional theory for surface property prediction of heterogeneous catalysts for sustainable energy technology
- Worked with experimental chemists to design, predict, and understand experimental results

Undergraduate Student Researcher
Carnegie Mellon University; Pittsburgh, PA — August 2019–February 2024

- Developed data cleaning, image/signal processing, and data science workflows for analyzing *C elegans* videos for use with a high-throughput experimental setup for healthspan research

Skills

Software: Python, C++, MATLAB
Software packages: Pandas, Numpy, Pymatgen, ASE, OCP, Scikit-learn
Simulation and Modeling: VASP, ILT/OPC, DFT, Monte Carlo methods
HPC: Slurm, Dask-kubernetes

Projects

Ternary surface segregation simulations (code)
- Used graph neural networks in high throughput Monte Carlo simulations to predict dense experimental surface segregation trends across ternary transition metal alloys
- Trained and fine-tuned graph neural networks for reliability in Monte Carlo setting

Cleavage energy transfer learning (code)
- Designed and developed transfer learning protocols for predicting intermetallic cleavage energies across functionals, materials, and simulation settings
- Demonstrated applications of foundation models to out of domain tasks

High-throughput adsorption energy inference (code)
- Developed high throughput workflow to calculate adsorption energies at scale
- Helped develop and support dask-kubernetes back-end

Design of experiments for experimental hydrogen evolution reaction system
- Designed active learning loops for hydrogen evolution experiments
- Used signal processing and data science to predict and interpret experimental data

Publications and talks

Kirby Broderick, Robert Burnley, Andrew Gellman, John Kitchin (2024). "Surface Segregation Studies in Ternary Noble Metal Alloys: Comparing DFT and Machine Learning with Experimental Data". ChemPhysChem.

Kirby Broderick, Eric Lopato, Brook Wander, Stefan Bernhard, John Kitchin, Zachary Ulissi (2022). "Identifying Limitations in Screening High-Throughput Photocatalytic Bimetallic Nanoparticles with Machine-Learned Hydrogen Adsorptions". Applied Catalysis B: Environmental.

Brook Wander, **Kirby Broderick**, Zachary Ulissi (2022). "Catlas: an automated framework for catalyst discovery demonstrated for direct syngas conversion". Catalysis Science and Technology.

Kevin Tran, Willie Neiswanger, **Kirby Broderick**, Eric Xing, Jeff Schneider, and Zachary W. Ulissi (2021). "Computational catalyst discovery: Active classification through myopic multiscale sampling". Journal of Chemical Physics.

Yongmin Cho, Sol Ah Lee, Yee Lian Chew, **Kirby Broderick**, William Schafer, Hang Lu (2020). "Multimodal Stimulation in a Microfluidic Device Facilitates Studies of Interneurons in Sensory Integration in C. elegans". Small.

Talks

"The Sabatier Principle for Aqueous Photochemical Hydrogen Evolution over Bimetallic Nanoparticles", Poster presentation at AIChE 2021

"Simulating Closed-Loop Catalyst Discovery Processes Using an Experimental Band Gap Surrogate Model", Conference talk at AIChE 2022

Awards and Honors

- Phillips and Huang Family Graduate Fellowship in Energy 2023
- Omega Chi Epsilon at Georgia Tech

Hobbies

In my free time, I like to hike, read nonfiction, and cook. My favorite cuisines are Mexican, Chinese, and Indian, although I'll try just about any recipe.