

Christian Frech

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EDUCATION

University of Texas at Austin- PhD Candidate, Materials Science & Engineering
Cockrell School of Engineering Fellowship recipient
GPA: 3.8/4.00

Cohort of 2022
Austin, TX

Carnegie Mellon University- B.S. in Physics, Minor in Mathematics
GPA: 3.51/4.00

Class of 2022
Pittsburgh, PA

EXPERIENCE

Energy Storage & Materials Simulation Lab
PhD Candidate

August 2022-Present
Austin, TX

- Developed multiscale approach for simulating microstructure dynamics metal systems with defects and interfaces
 - o Programmed & maintained **parallelized** kinetic Monte Carlo **C++** package to leverage **HPC**
 - o Created battery design guidelines via maps relating lithium void dissolution times to solid electrolyte choice & lithium defect properties
 - o Calculated the influence of voids and solid electrolyte interfaces on the self-diffusivity of lithium using **Density Functional Theory (DFT)**
 - o Quantified the effect of stress on vacancy formation energy in lithium metal from first-principles approach
- Designed scheme for predicting decomposition reactions and associated toughening in various solid electrolytes
 - o Identified thermodynamically stable & dendrite-resistant solid electrolytes for long-lasting battery cells
 - o Created workflow for leveraging the materials databases to predict volume change & toughening against fracture from solid electrolyte decomposition with lithium & sodium
 - o Calculated energies of cutting-edge solid electrolyte compounds to construct phase diagrams via **DFT**

Marom Group- Computational Quantum Materials
Research Assistant

January 2021-May 2022
Pittsburgh, PA

- Calculated hundreds of solar cell compounds' energetic properties using **ORCA** and **FHI-Aims (DFT)**
- Optimized ridge regression (**SISSO**) and bayesian regression models (**PyTorch**) for efficiently predicting candidate materials for next-gen high-efficiency solar cells

Genetically Engineered Materials Science & Engineering Center
Research Intern

April 2020-August 2022
University of Washington

- Built a **GPU-optimized Python library** for energy state calculations in organic molecular systems
- Drafted manuscript for publication using Random Matrix Theory for feature generation in **Generative Adversarial Networks** for predicting protein folding

PUBLICATIONS & CONFERENCES

- 1) DFT-Informed kMC Simulations of Void Dynamics in Lithium Anodes"
C. Frech and D. Siegel. *MUSIC EFRC Conference, 2025*
 - Presented talk on using kMC to simulate lithium void shrinkage with defects & interfaces
- 2) "Screening of Solid Electrolyte Electrochemical Embrittlement and Fracture Resistance from First Principles"
C. Frech, S. Greene, C. Fincher, Y. Chiang, and D. Siegel. *In preparation.*
 - Quantified effect of decomposition on fracture toughness and identified long-lasting candidate solid electrolytes
- 3) "Investigating the Effect of Li Anode Microstructure on the Solid Electrolyte Interface via Atomistic Simulations"
C. Frech and D. Siegel. *In preparation.*
 - Simulated anode-electrolyte interface & developed design guidelines for degradation-resistant batteries through defect & interface engineering

SKILLS

- Programming: Python (Advanced), C++ (Intermediate), MPI Protocols (Intermediate), MatLab (Intermediate)
- Softwares: VASP (Advanced), LAMMPS (Intermediate), Ovito (Intermediate), VESTA (Intermediate)
- Language: Chinese (Intermediate), Spanish (B1)

ACTIVITIES AND INTERESTS

Carnegie Mellon Track & Field (NCAA Division III), Volunteer at Habitat for Humanity and San Antonio Food Bank