

# Anika Friedman

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## EDUCATION

### **Pursuing PhD Biological Engineering**

UNIVERSITY OF COLORADO BOULDER

Boulder, CO | August 2020 - Present

### **BS. Engineering Physics with Minor in Mathematics**

OHIO UNIVERSITY HONORS TUTORIAL COLLEGE

Athens, OH | August 2015 - May 2019

### **BS. Neuroscience**

OHIO UNIVERSITY HONORS TUTORIAL COLLEGE

Athens, OH | August 2015 - May 2019

## WORK EXPERIENCE

### **UNIVERSITY OF COLORADO BOULDER | GRADUATE ASSISTANT**

Boulder, CO | January 2021 – Present

- Planning and execution of 6 distinct research projects
- Writing manuscripts and assisting in grant writing
- Presenting research at conferences in the form of posters and oral presentations
- TA for bioseparations course, involving grading homework and running office hours
- Advanced TA for biology for engineers, involving teaching 2 lectures, writing homework assignments, grading homework and exams, and holding office hours

### **OHIO UNIVERSITY | RESEARCH ASSISTANT**

Athens, OH | April 2016 - August 2019

- Self-lead research creating and using mathematical modelling of neurofilament transport in the axon of neurons.
- Modelling of axon signaling in neuron networks

### **OHIO UNIVERSITY | TEACHING ASSISTANT**

Athens, OH | August 2016 - May 2018

- instructed 20 students through labs highlighting fundamental physics principles including: gravity, force balancing, radiation, etc.
- Evaluating student performance and grading lab reports

## ACTIVE PROJECTS

### **Ketoacyl Synthases + Reductases**

Using molecular dynamics (MD) simulations to elude the mechanism by which the ketoacyl synthase FabF elongates acyl chains for fatty acid synthesis and FabG performs reduction reactions on acyl products.

### **Free Energy Enhanced Sampling Methods** ([GitHub](#))

My research group has been developing a enhanced sampling method termed mutlti-topology ensemble of expanded ensemble. This method aims to target systems the computation of binding free energy for complex and flexible systems like protein-peptide and protein-protein binding interfaces by performing iterative relative free energy transformations which can engage in conformational exchanges.

### **SH2 Domain Binding** ([Github](#))

Using molecular dynamics (MD) simulations in combination with machine learning to determine the manner by which SH2 domains can exhibit simultaneous binding specificity as well as promiscuity between peptide targets. This project aims to implement a combination ML-MD pipline built off of exsisting ML protein structure prediction tools like AlphaFold and ESMFold for the simulation of protein-peptide complexes to efficiently sample complexes with increased conformational flexibility.

### **Protein Force Field Development** ([Webpage](#))

I collaborate with a large group of researchers with the goal of creating a unified protein and small molecule force field. My role is primarily in benchmarking force field candidates to determine their ability to accurately reproduce protein structure. I am also involved in improving force field training through the augmentation of the qutum chemical database used to train the force field.

## PUBLICATIONS

- Alison C. Leonard, **Anika J. Friedman**, Rachel Chayer, Brian M. Petersen, Janty Woojuh, Zenan Xing, Sean R. Cutler, Joel L. Kaar, Michael R. Shirts, and Timothy A. Whitehead. "Rationalizing Diverse Binding Mechanisms to the Same Protein Fold: Insights for Ligand Recognition and Biosensor Design." *ACS Chemical Biology*, 2024, 19, 8. <https://doi.org/10.1021/acscchembio.4c00243>.
- Kenichiro Takaba, **Anika J. Friedman**, Chapin E. Cavender, Pavan Kumar Behara, Iván Pulido, Michael M. Henry, Hugo MacDermott-Opeskin, et al. "Machine-Learned Molecular Mechanics Force Fields from Large-Scale Quantum Chemical Data." *Chemical Science*, Advance Article, 2024. <https://doi.org/10.1039/D4SC00690A>.
- Anika J. Friedman**, Hannah M. Padgett, Levi Kramer<sup>1</sup>, Evan T. Liechty, Gregory W. Donovan, Jerome M. Fox, and Michael R. Shirts "Selectivity of terpenoids within the conserved PTP enzyme family" *Journal of Physical Chemistry B* 2023, 127, 39, 8305–8316. <https://doi.org/10.1021/acs.jpcb.3c03791>
- Evan T. Liechty, Andrew Hren, Gregory Donovan, Levi Kramer, **Anika J. Friedman**, Michael R. Shirts, and Jerome M. Fox "Analysis of Neutral Mutational Drift in an Allosteric Enzyme" *Protein Science*, 2023, 32, 8. <https://doi.org/10.1002/pro.4719>
- Anika J. Friedman**, Evan T. Liechty, Levi Kramer, Ankur Sarkar, Jerome M. Fox, and Michael R. Shirts "Allosteric Inhibition of PTP1B by a Nonpolar Terpenoid." *Journal of Physical Chemistry B* 2022, 126, 42, 8427–8438 <https://doi.org/10.1021/acs.jpcb.2c05423>
- Rawan Nowier, **Anika Friedman**, Anthony Brown, and Peter Jung "The Role of Neurofilament Transport in the Radial Growth of Myelinated Axons" *Molecular Biology of the Cell*, 36, 6 2023. <https://doi.org/10.1091/mbc.E22-12-0565>

## PUBLICATIONS IN PROGRESS

- Anika J. Friedman**, Wei-Tse Hsu, and Michael R. Shirts "Multiple Topology Replica Exchange of Expanded Ensembles (MT-REXEE) for Multidimensional Alchemical Calculations" arxiv, 2024
- Sam Andrzejewski\*, **Anika J. Friedman**\*, Kathryn Mains, Annette Thompson, Michael R. Shirts, and Jerome M. Fox "Protein-protein interfacial stability controls substrate specificity in a novel  $\beta$ -ketoacyl-ACP reductase" *in progress*
- Anika J. Friedman** and Michael Shirts "Improved Conformational Sampling of Protein-Protein Complexes in Alchemical Free Energy Simulations Using MT-REXEE" *in progress*

## LEADERSHIP AND VOLUNTEER EXPERIENCE

### HEAD AND FOUNDER CU COMPUTATIONAL SUPERGROUP |

August 2023 - Present |

- Create, maintain, and run Slack
- Facilitate communication between computational researchers in different lab groups and departments

### CU STUDENT ORGANIZATION ALLOCATION COMMITTEE |

October 2021 – May 2023 |

- Evaluated funding applications from student organizations from CU. student organizations at weekly meetings
- Distributed student fee dollars efficiently, promoting enrichment, education, and inclusiveness across the CU Boulder community.

### DENVER PUBLIC SCHOOLS COACH MENTORING PROGRAM |

August 2021 – May 2022 |

- Mentored and empowered female high school students interested in engineering as a future career path.

### SECRETARY OF SOCIETY FOR PHYSICS STUDENTS |

May 2018- May 2019 |

- Attend weekly meetings and take minutes.

### TREASURER OF SOCIETY OF WOMAN ENGINEERS |

May 2016- May 2017 |

- Maintained budget for events and activities held throughout the year including the year-end engineering picnic attended by 500+ students
- Assisted in planing of career development and outreach events for middle to high school aged girls