

Summary

- My broader research interests lie at the intersection of **biology, deep learning, and molecular simulation**. I am motivated to design models to learn the fundamental driving forces in biological systems, with the goal of expediting rational and efficient design of new bioinspired technologies, ultimately accelerating advancements in human health.
- I have broad expertise in machine learning and computational research areas including **generative models** (diffusion), protein **language models** (BERT, MLM, autoregressive), protein **sequence-function models** (regression), and enhanced sampling **molecular simulations**.
- Technical Skills: Machine learning (Pytorch, Tensorflow, Scipy), high performance computing (Slurm and Azure, CPU- and GPU- parallelization), coding (Python, BASH), software (GROMACS, AMBER, PLUMED, Gaussian, Packmol VMD, Github)

Experience

- Dec 2023 – Present** Senior Applied Scientist, Biomedical ML Group, *Microsoft Research*
- Apr 2022 – Dec 2023** Data Scientist (Contract), Biomedical ML Group, *Microsoft Research*
- Jan 2022 – Apr 2022** Postdoctoral Researcher, Pfaendtner Research Group, *University of Washington*

Education

- 2021** PhD Chemical Engineering, *University of Washington*
- Thesis: Discovery of Biomolecular Structure-Function Mechanisms with Computational Frameworks at the Nanoscale (Advisor: Jim Pfaendtner)
 - Completed *Data Science Option* certification
- 2016** BS Chemical Engineering, *Arizona State University*
- Graduated *Magna Cum Laude*

Journal Publications

*First author contribution; * co-first authors; + mentee; ‡ co-corresponding authors*

Microsoft Research

1. **Alamdari, S.**, Thakkar, N.⁺, van den Berg, R., Lu, A. X., Fusi, N., Amini, A. P. and Yang, K. K. Generation of protein sequences and evolutionary alignments via discrete diffusion models. *bioRxiv*, **2023**. (*In review*)
2. Wu, K. E., Yang, K. K., van den Berg, R., **Alamdari, S.**, Zou, J. Y., Lu, A. X., and Amini, A. P. Protein structure generation via folding diffusion. *Nature Communications*. **2024**. (*In press*)

University of Washington

3. **Alamdari, S.** and Pfaendtner J., Origins of Conformational Heterogeneity in Peptoid Helices Formed by Chiral N-1-Phenylethyl Side Chains. *Journal of Physical Chemistry B*, **2023**.
4. **Alamdari, S.**, Torkelson, K., Wang, X.⁺, Chen, C. L., Ferguson, A. L. and Pfaendtner J., Thermodynamic Basis for Stabilization of Helical Peptoids by Chiral Sidechains. *Journal of Physical Chemistry B*, **2023**.

5. Zhao, M., Zhang, S., Zheng, R., **Alamdari, S.**, Mundy, C. J., Pfaendtner, J., Pozzo, L. D., Chen C. L., DeYoreo, J. and Ferguson A. L., Computational and Experimental Determination of the Properties, Structure, and Stability of Peptoid Nanosheets and Nanotubes. *Biomacromolecules*, **2023**.
6. Strunge, K., Hoinkis, N., Lutz, H., **Alamdari, S.**, Roeters, S. J., Lu, H., Pfaendtner, J. and Weidner, T., Peptide Mimic of the Marine Sponge Protein Silicatein Fabricates Ultrathin Nanosheets of Silicon Dioxide and Titanium Dioxide. *Langmuir*, **2022**.
7. Zhao, M., Lachowski, K. J., Zhang, S., **Alamdari, S.**, Sampath, J., Mu, P., Mundy, C. J., Pfaendtner, J., De Yoreo, J. J., Chen, C. L. and Pozzo, L. D., Hierarchical Self-Assembly Pathways of Peptoid Helices and Sheets. *Biomacromolecules*, **2022**.
8. Roeters, S. J.*, Golbek, T. W.*, Bregnhøj, M.*, Drace, T., **Alamdari, S.**, Roseboom, W., Kramer, G., Šantl-Temkiv, T., Finster, K., Pfaendtner, J. and Woutersen, S., Ice-nucleating proteins are activated by low temperatures to control the structure of interfacial water. *Nature Communications*, **2021**.
9. Summers, S. R.*, **Alamdari, S.***, Kraft, C. J., Brunecky, R., Pfaendtner, J. and Kaar, J. L., Substitution of distal and active site residues reduces product inhibition of E1 from *Acidothermus Cellulolyticus*. *Protein Engineering, Design and Selection*, **2021**.
10. **Alamdari, S.***, Sampath, J.*, Prakash, A., Gibson, L. D. and Pfaendtner, J., Efficient Sampling of High-Dimensional Free Energy Landscapes: A Review of Parallel Bias Metadynamics. *Foundations of Molecular Modeling and Simulation*, **2021**. (Book Chapter)
11. Thompson, N. L., Cohen, T. A., **Alamdari, S.**, Hsu, C. W., Williamson, G.A. and Holmberg, V. C., DiffCapAnalyzer: A Python Package for Quantitative Analysis of Total Differential Capacity Data. *Journal of Open Source Software*, **2020**.
12. **Alamdari, S.***, Roeters, S. J.*, Golbek, T. W., Schmäser, L., Weidner, T.† and Pfaendtner, J.†, Orientation and conformation of proteins at the air–water interface determined from integrative molecular dynamics simulations and sum frequency generation spectroscopy. *Langmuir*, **2020**.
13. Sampath, J.*, **Alamdari, S.***, and Pfaendtner, J., Closing the gap between modeling and experiments in the self-assembly of biomolecules at interfaces and in solution. *Chemistry of Materials*, **2020**.
14. Zhao, M., Sampath, J., **Alamdari, S.**, Shen, G., Chen, C. L., Mundy, C. J., Pfaendtner, J. and Ferguson, A.L., MARTINI-compatible coarse-grained model for the mesoscale simulation of peptoids. *The Journal of Physical Chemistry B*, **2020**.
15. Summers, S., Kraft, C., **Alamdari, S.**, Pfaendtner, J. and Kaar, J. L., Enhanced activity and stability of *Acidothermus cellulolyticus* endoglucanase 1 in ionic liquids via engineering active site residues and non-native disulfide bridges. *ACS Sustainable Chemistry and Engineering*, **2020**.
16. Hellner, B., **Alamdari, S.**, Pyles, H., Zhang, S., Prakash, A., Sprenger, K. G., De Yoreo, J. J., Baker, D., Pfaendtner, J.† and Baneyx, F.†, Sequence–structure–binding relationships reveal adhesion behavior of the Car9 solid-binding peptide: an integrated experimental and simulation study. *Journal of the American Chemical Society*, **2020**.
17. **Alamdari, S.** and Pfaendtner, J., Impact of glutamate carboxylation in the adsorption of the α -1 domain of osteocalcin to hydroxyapatite and titania. *Molecular systems design and engineering*, **2020**.
18. Verreault, D., **Alamdari, S.**, Roeters, S. J., Pandey, R., Pfaendtner, J. and Weidner, T., Ice-binding site of surface-bound type III antifreeze protein partially decoupled from water. *Physical Chemistry Chemical Physics*, **2018**.

Arizona State University

19. Wang, G., Robert, C., Suslu, A., Chen, B., Yang, S., **Alamdari, S.**, Gerber, I. C., Amand, T., Marie, X., Tongay, S.[‡] and Urbaszek, B.[‡], Spin-orbit engineering in transition metal dichalcogenide alloy monolayers. *Nature communications*, **2015**.

Conference and Workshop Papers

The presenting author is denoted.

1. Alamdari, S., Thakkar, N., van den Berg, R., Lu, A. X., Fusi, N., Amini, A. P. and Yang, K. K. Protein generation with evolutionary diffusion. *NeurIPS Generative AI and Biology (GenBio) Workshop*. (New Orleans, LA). **2023**. (poster)
2. Alamdari, S., Thakkar, N., van den Berg, R., Lu, A. X., Fusi, N., Amini, A. P. and Yang, K. K. Protein generation with evolutionary diffusion. *NeurIPS Machine Learning in Structural Biology (MLSB) Workshop*. (New Orleans, LA) **2023**. (contributed spotlight talk)
3. Alamdari, S., Thakkar, N., van den Berg, R., Lu, A. X., Fusi, N., Amini, A. P. and Yang, K. K. Protein generation with evolutionary diffusion. *MoML @ Koch Institute, MIT*. (Cambridge, MA) **2023**. (poster)

Invited Talks

- 2024** Discrete diffusion models for controllable protein generation. *Molecular ML Reading Group, Rosetta Commons (virtual)*
- 2023** Discrete diffusion models for controllable protein generation. *ML Ideas, Microsoft Research (Cambridge, MA)*
- 2023** An introduction to diffusion models. *Models, Inference & Algorithms (MIA) Initiative Seminar Series at the Broad Institute (Cambridge, MA)*
- 2023** Sequence-first generative approaches for protein design. *AstraZeneca Journal Club. (virtual)*
- 2023** Protein sequence generation with evolutionary diffusion. *Google Research. (Cambridge, MA)*
- 2022** Exploration of the Peptoid Folding Landscape with Metadynamics. *University at Buffalo CBE Seminar. (Buffalo, NY)*
- 2021** A Thermodynamic Basis for Peptoid Assembly into a Helix by A Chiral Sidechain. *Broadbelt Group, Northwestern. (Evanston, IL)*
- 2021** Simulations of the Peptoid Folding Landscape with Metadynamics. *UW ChemE Seminar. (Seattle, WA)*
- 2021** Exploration of the Peptoid Folding Landscape with Metadynamics. *Molecular Foundry Lawrence Berkeley National Lab. (virtual)*
- 2021** Combining simulation and experiment to study protein structure at interfaces. *Biophysics Society Student Networking Event. (virtual)*
- 2021** Biomolecular Assembly at Interfaces. *ChE Future Faculty Seminar Series. (virtual)*
- 2020** Capturing Protein Assembly at Interfaces. *Women ExcelLing in Computational Molecular Engineering – WELCOME. (virtual)*

Awards, Fellowships, and Grants

- 2022** VITAL Future Faculty, *University at Buffalo*
- 2021** Chemical Engineering Faculty Lecture Award, *University of Washington*
- 2021** Chemical Computing Group Excellence Student Award, *ACS COMP*

2021	Graduate and Postdoc Women's Fellowship, <i>D.E. Shaw Research</i>
2021	NSF-RUA Postdoctoral Research Exchange, <i>The California Alliance (declined)</i>
2020	Rising Star in Chemical Engineering, <i>MIT</i>
2020	Husky 100, <i>University of Washington</i>
2020	ACES Graduate Student Symposium Top Speaker Award, <i>University of Washington</i>
2020	Krieger-Brockett Travel Award, <i>University of Washington</i>
2020	WIC Travel Award, <i>AChE</i>
2020	COMSEF Graduate Student Award, <i>AChE</i>
2019	NSF-AGEP Research Exchange, <i>The California Alliance</i>
2018	Graduate Research Fellowship Program (GRFP), <i>NSF</i>
2018	National Research Traineeship (NRT), <i>NSF</i>
2018	Hack Week US Army Research Office Travel Award , <i>ECS</i>
2018	NSF Travel Award, <i>FOMMS</i>
2016	ARCS Fellow, <i>University of Washington</i>
2016	Clean Energy Institute Recruitment Award, <i>University of Washington</i>

Teaching Experience

2021 Winter	CHEME 599 Fundamentals of Molecular Simulations (MOLSIM), Guest Lecturer, <i>UW</i>
2021 Winter	C-HACK Hackathon, Tutorial Instructor, <i>UW</i>
2020 Spring	Computational Chemistry Online Tutorial Series, Guest Lecture, <i>UW</i>
2020 Winter	CHEME 599 MOLSIM, Course Organizer/Lecturer, <i>UW</i>
2019 Spring	CHEME 498, Topic: Molecular Simulation and Stat Mech, Guest Lecture (3x), <i>UW</i>
2019 Winter	CHEME599 MOLSIM, Guest Lecture, <i>UW</i>
2017 Spring	CHEME 436, Chemical Engineering Unit Operations I, Teaching Assistant, <i>UW</i>

Mentorship

2023	Sumaya Addish, COMSEF Scholar (<i>Undergrad at UW</i>)
2022-2023	Nitya Thakkar, MSR Intern (<i>Undergrad at Brown University, current: PhD Stanford</i>)
2021	Samentha Dumervil, COMSEF Scholar (<i>Undergrad at Howard, current: MS UC Berkley</i>)
2020-2021	Zhaozuan (Mike) Huang, UW Pfaendtner REU (<i>Undergrad at UW</i>)
2019-2021	Xiaoquan (Selina) Wang, UW Pfaendtner REU (<i>Undergrad at UW, current: PhD University of Michigan</i>)
2020	Daniela M. Rivera Mirabal, Científico Latino Mentee (<i>Undergrad at University of Puerto Rico-Mayaguez, current GRFP at UCSB</i>)
2020	Hosea A. Santiago Cruz, Científico Latino Mentee (<i>Undergrad at University of Puerto Rico-Mayaguez, current: GRFP at Carnegie Mellon</i>)
2020	Joshua Alvarado, UW CEI CEBR REU (<i>Student at San Joaquin Delta CC, current: BS at UCSB</i>)
2019-2020	Emily Rhodes, UW Pfaendtner REU (<i>Undergrad at UW, current: PhD CU Boulder</i>)
2019-2020	Miwa Ito, UW Pfaendtner REU (<i>Undergrad at UW; deferred PhD</i>)
2018-2019	Nikita Grover, UW Pfaendtner REU (<i>Undergrad at UW; MS Indiana University</i>)

Outreach and Professional Development

Invited Speaking Engagements

2023	STEM Careers: STEM 101, Guest Speaker, <i>Everett CC (virtual)</i>
2022	6th Annual Industry Event, <i>UW WChE (Seattle, WA)</i>
2022	Grad School Panel for Undergrad Research Interns, <i>Microsoft Research (virtual)</i>
2022	Applying to Graduate Fellowships, <i>UW ACES (Seattle, WA)</i>
2021	Demystifying Graduate School in Engineering, <i>UW WiSE (Seattle, WA)</i>
2020	Delineating biophysical landscape with comp and exp efforts, <i>Biophysical Society (virtual)</i>
2019	College Success in Engineering and Computer Science, Guest Lecture, <i>Everett CC (Everett, WA)</i>
2019	GRFP Application Workshop Q&A, <i>UW College of Engineering, (Seattle, WA)</i>

Leadership Roles

2020-2022	Co-organizer, COMSEF Scholars REU Program <ul style="list-style-type: none">• REU program aimed to increase DEI initiatives within COMSEF through investment in underserved undergraduate researchers and their allies across the field of computational research• Manage website, conduct outreach to nearly 100 HBCU and HSIs, create scoring rubrics, review applicant materials, and lead professional development workshops
2020-2021	Outreach Leader Officer, UW Global Renewables Infrastructure Development Club <ul style="list-style-type: none">• Recruit students, manage social media, seek out financial partnerships to fund solar panel installations in Guatemala and Puerto Rico
2020-2021	Student Representative Officer, UW Hyak Governance Board <ul style="list-style-type: none">• Serve as the liaison between Hyak governance board and research computing club
2019-2020	President, UW Research Computing Club <ul style="list-style-type: none">• Developed the club's first series of computational-focused outreach activities that was used for WChE's computational themed "Introduce a Girl to Computer Robotics and Data Science Day (CoRDS)"
2019-2020	GRFP Reviewer and GMIS Mentor, Científico Latino <ul style="list-style-type: none">• Mentor 1-3 undergraduate underrepresented students per year applying for GRFP fellowships and graduate school
2018-2019	Research Coordinator Officer, UW Research Computing Club <ul style="list-style-type: none">• Increased undergrad participation by 3x. This led to increased undergraduate research (leading to 1 conference paper), development of a Kaggle competition team, and an HPC competition travel team which was selected in a competitive application cycle to attend SC'19
2016-2019	Organizer, UW WChE "Introduce a Girl" Series <ul style="list-style-type: none">• Developed outreach activities, and helped organize/coordinate "Introduce a Girl.." series events
2016-2019	Role Model, Techbridge Girls ACE and Global Connections High School

- Mentorship program that serves underrepresented low-income middle and high school students. I worked with students to create, develop, and execute different STEM-centric projects over the course of a year (2-5hrs/month) to be presented at the end of year Maker Fair.
- Developed 3 “careers in STEM” days focused on Chemical Engineering, Clean Energy, and Data Science. *Featured as the nationwide Role Model Spotlight in 2017*

Grant Writing Experience

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| 2020 | Supporting Student Research Needs with HP Computing Resources, UW STF (Contributor) \$ 245,240 |
| 2019 | Cloud Credit Program Enabling Diversity in Computational Research, UW STF (Lead) \$ 60,000 |
| 2019 | Improving Access to High Performance, GPU-Based Resources, UW STF (Contributor) \$ 57,000 |

Professional Service

Journal Reviewer: (1) Process Biochemistry, (2) Physical Chemistry Chemical Physics, (3) Inorganic Chemistry, and (4) Journal of Physical Chemistry

Professional Memberships: (1) ACS, (2) AIChE, (3) BPS, (4) WChE

Moderator: UW Summer Undergraduate Research Symposium (2020)

Panel Reviewer: UW Distinguished Young Seminar Series (DYSS) (2020 and 2019)