Sarah Alamdari

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github: https://github.com/sarahalamdari | **google scholar**: https://scholar.google.com/citations?user=AV7XVKMAAAAJhl=en

Experience

April 2022 - Present	**Data Scientist**, Microsoft Research, New England Lab, BioML Team
Jan 2022 - April 2022	**Postdoctoral Researcher**, Pfaendtner Research Group, University of Washington
Sept 2018 - Sept 2021	**NSF GRFP Fellow**, Pfaendtner Research Group, University of Washington
Sept 2017- Sept 2018	**NSF NRT Fellow**, DIRECT, University of Washington
Fall 2016	**Graduate Teaching Assistant**, Unit Ops I, University of Washington

Education

University of Washington

PhD Chemical Engineering

- Thesis: Discovery of Biomolecular Structure-Function Mechanisms with Computational Frameworks at the Nanoscale

University of Washington

MS Chemical Engineering

- Completed Data Science Option (DSO)

Arizona State University

BS Chemical Engineering

- Graduated Magna Cum Laude

Published Work

*First author contribution; * co-first author; $^{+}$ mentee*; ‡co-corresponding author

Journal Articles

17. **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. *(under review)*

16. **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. *(accepted)*

15. 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.

14. Strunge, K., Hoinkis, N., Lutz, H., **Alamdari, S.**, Roeters, S.J., Lu, H., Pfaendtner, J. and Weidner, T., 2022. Peptide Mimic of the Marine Sponge Protein Silicatein Fabricates Ultrathin Nanosheets of Silicon Dioxide and Titanium Dioxide. *Langmuir*, 2022.

13. 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., 2022. Hierarchical Self-Assembly Pathways of Peptoid Helices and Sheets. *Biomacromolecules*, 2022.

12. 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.

11. 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*)

9. 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.

8. **Alamdari, S.***, Roeters, S.J.*, Golbek, T.W., Schmüser, 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.

7. 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.

6. 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.

5. 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.

4. 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.

3. **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.

2. 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.

1. 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.

Teaching Experience

Win 2021	**CHEME 599 Fundamentals of Molecular Simulations (MOLSIM)**, Guest Lecturer	*UW*
Win 2021	**C-HACK Hackathon**, Tutorial Instructor	*UW*
Spr 2020	**Computational Chemistry Online Tutorial Series**, Guest Lecture	*UW*
Win 2020	**CHEME 599 MOLSIM**, Course Organizer/Lecturer	*UW*
Spr 2019	**CHEME 498, Topic: Molecular Simulation and Stat Mech**, Guest Lecture (3)	*UW*
Win 2019	**College Success in Engineering and Computer Science**, Guest Lecture	*Everett, CC*
Win 2019	**CHEME599 MOLSIM**, Guest Lecture	*UW*
Spr 2017	**CHEME 436, Chemical Engineering Unit Operations I**, Teaching Assistant	*UW*

Awards, Fellowships, & Grants

2022 **VITAL Future Faculty**, University at Buffalo

2021 **Chemical Engineering Faculty Lecture Award**, University of Washington
Chemical Computing Group Excellence Student Award, ACS COMP
Graduate and Postdoc Women's Fellowship, D.E. Shaw Research
NSF-RUA Postdoctoral Research Exchange, The California Alliance (*declined*)

2020 **Rising Star in Chemical Engineering**, MIT
Husky 100, University of Washington
ACES Graduate Student Symposium Top Speaker Award, University of Washington
Krieger-Brockett Travel Award, University of Washington
WIC Travel Award, AIChE
COMSEF Graduate Student Award, AIChE

2019 **NSF-AGEP Research Exchange**, The California Alliance

2018 **Graduate Research Fellowship Program (GRFP)**, NSF
National Research Traineeship (NRT), NSF
Hack Week US Army Research Office Travel Award , ECS
NSF Travel Award, FOMMS

2016 **ARCS Fellow**, University of Washington
Clean Energy Institute Recruitment Award, University of Washington

Presentations

Invited Talks

Exploration of the Peptoid Folding Landscape with Metadynamics. University at Buffalo CBE Seminar, Buffalo, NY. Spring 2022.

A Thermodynamic Basis for Peptoid Assembly into a Helix by A Chiral Sidechain. Broadbelt Group, Northwestern, Evanston, IL. Fall 2021.

Simulations of the Peptoid Folding Landscape with Metadynamics. UW ChemE Seminar, Seattle, WA. Fall 2021.

Exploration of the Peptoid Folding Landscape with Metadynamics. Molecular Foundry Lawrence Berkeley National Lab, virtual. Fall 2021.

Combining simulation and experiment to study protein structure at interfaces. Biophysics Society Student Networking Event, virtual. Spring 2021.

Biomolecular Assembly at Interfaces. ChE Future Faculty Seminar Series, virtual. Spring 2021

Capturing Protein Assembly at Interfaces. Women ExceLling in Computational Molecular Engineering (WELCOME), virtual. Fall 2020

Select Contributed Presentations

$^{+}$ *mentored undergraduate*

Alamdari, S. Pfaendtner, J. 2021. Exploration of the Secondary Structure Peptoid Folding Landscape with Metadynamics. AIChE Fall Meeting, Boston, MA.

Alamdari, S., J. Pfaendtner, 2021. Detailed exploration of peptoid folding thermodynamics with metadynamics, ACS Spring Meeting, virtual.

Alamdari, S., Roeters, S., Golbek T., Schmüser L., Weidner T., Pfaendtner J., 2020. Determination of Orientation and Conformation of Lysozyme at the Air-Water Interface Using an Integrated MD/SFG Approach, AIChE Fall, virtual.

Alamdari, S., Pfaendtner J, 2020. Hierarchical Assembly of Peptoids into Complex Nanostructures, AIChE Fall, virtual. (Poster)

Wang, X.$^{+}$, **Alamdari, S.**, Dollar O., Pfaendtner J., 2020. Stability of Peptoid Sheets and Tubes with Atomistic Molecular Dynamics Simulations, AIChE Fall, virtual. (Poster)

Alamdari, S., Pfaendtner J., 2020. Protein Assembly at Interfaces Through the Computational Microscope, UW Graduate Student Symposium, virtual.

Alamdari S., Gebhart R., Drobny G., Pfaendtner J., 2019. Using Enhanced Sampling Methods to Study the Behavior of Osteocalcin on Mineral Surfaces, AIChE, Orlando, FL.

Alamdari S., Pfaendtner J., 2019. Modeling Inhibition of Biocatalysts By Ionic Liquids Using Metadynamics, AIChE, Orlando, FL. (poster)

Alamdari, S., Pfaendtner J., 2019. A Physics-Based Approach to Elucidating the Structure and Function of Bone Proteins in the Presence of Implant Materials, SFU Frontiers in Biophysics, Vancouver, BC.

Alamdari, S., Pfaendtner J., 2018. Understanding the Role of Ionic Liquids in the Enzyme Catalyzed Breakdown of Cellulose Using Molecular Dynamics Simulations, AIChE, Pittsburgh, PA.

Alamdari, S., Pfaendtner J., 2018. Probing Enzyme Catalyzed Hydrolysis of Cellulose in Ionic Liquids Using Enhanced Sampling Techniques, AIChE, Pittsburgh, PA. (poster)

Alamdari, S., Pfaendtner J., 2018. Using Hybrid Molecular Dynamics Simulations to Understand the Role of Ionic Liquids on Enzyme Catalyzed Reactions, FOMMS, Delavan, WI. (Poster)

Alamdari, S., Pfaendtner J., 2018. Hybrid Molecular Dynamics Simulations to Guide the Rational Design of Biofuel System, Research Computing Club Shop Talks, Seattle, WA.

Alamdari, S., Pfaendtner J., 2017 Using Supercomputers to Study the Behavior of Biomolecules at Interfaces, UW Lightning Strikes: Successes in Research Computing, Seattle, WA.

Mentorship

Microsoft Research

2022-2023 **Nitya Thakkar**, MSR Intern/Undergrad, Brown University *(PhD Stanford)*

Pfaendtner Research Group

2021 **Samentha Dumervil**, COMSEF Scholar/Undergrad, Howard *(MS UC Berkley)*
2020-2021 **Zhaozuan (Mike) Huang**, Undergrad, UW
2019-2021 **Xiaoquan (Selina) Wang**, Undergrad, UW *(PhD University of Michigan)*
2020 **Joshua Alvarado**, UW CEI CEBR REU/ Student, San Joaquin Delta CC *(BS at UCSB)*
2019-2020 **Emily Rhodes**, Undergrad, UW *(PhD CU Boulder)*
2019-2020 **Miwa Ito**, Undergrad, UW *(deferred PhD)*
2018-2019 **Nikita Grover**, Undergrad, UW *(MS Indiana University)*

Científico Latino

2020 **Daniela M. Rivera Mirabal**, Cientifico Latino Mentee *(GRFP Awardee)*
2020 **Hosea A. Santiago Cruz**, Cientifico Latino Mentee *(GRFP Awardee)*

Outreach & Professional Development

Outreach

COMSEF Scholars REU Program

Co-organizer *2020 - Curr*

- 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 professional development

UW Global Renewables Infrastructure Development Club

Outreach Leader Officer *2020 - 2021*

- Recruit students, manage social media, seek out financial partnerships to fund solar panel installations in Guatemala and Puerto Rico

UW Hyak Governance Board

Student Representative Officer *2020 - 2021*

- Serve as the liaison between Hyak governance board and research computing club

UW Research Computing Club

President *2019 - 2020*

- 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)"

Científico Latino

GRFP Reviewer and GMIS Mentor *2019 - 2020*

- Mentor 1-3 undergraduate underrepresented minority students per year applying for GRFP fellowships and graduate school

UW Research Computing Club

Research Coordinator Officer *2018 - 2019*

- 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

UW WChE "Introduce a Girl" Series

Organizing Volunteer *2016 - 2019*

- Developed outreach activities, and helped organize/coordinate "Introduce a Girl.." series events

Techbridge Girls ACE and Global Connections High School

Role Model *2016 - 2019*

- 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 Role Model Spotlight in 2017

Grant Writing Experience

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*

Invited Panel Speaker

2022 **6th Annual Industry Event**, UW WChE
2022 **Grad School Panel for Undergrad Research Interns**, Microsoft Research
2022 **Applying to Graduate Fellowships**, UW ACES
2021 **Demystifying Graduate School in Engineering**, UW WiSE
2020 **Delineating biophysical landscape with comp and exp efforts**, Biophysical Society
2019 **GRFP Application Workshop**, UW College of Engineering

Service

Reviewer: (**1**) Process Biochemistry, (**2**) Physical Chemistry Chemical Physics
Professional Memberships: (**1**) ACS, (**2**) AIChE, (**3**) BPS, (**4**) WChE
Moderator, UW Summer Undergraduate Research Symposium
Panel Reviewer, UW Distinguished Young Seminar Series (DYSS)