

Kayla G. Sprenger

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Education

Assistant Professor, University of Colorado Boulder Department of Chemical and Biological Engineering (ChBE)	Aug. 2020 – Present
Postdoctoral Associate, Massachusetts Institute of Technology (MIT) Institute for Medical Engineering and Science (IMES) Chakraborty Laboratory for Computational Immunology	Aug. 2017 – Aug. 2020
Ph.D. in Chemical Engineering, University of Washington (UW) <i>Advisor: Jim Pfaendtner</i>	July. 2017
M.S. in Chemical Engineering, UW <i>Advisors: Fernando Resende and Jim Pfaendtner</i>	Apr. 2014
B.S. in Chemical Engineering, UW	Jun. 2012

Publications (*Authors contributed equally)

1. [K. G. Sprenger*](#), Simone Conti*, Victor Ovchinnikov, Arup K. Chakraborty, and Martin Karplus, **Multiscale affinity maturation simulations to elicit broadly neutralizing antibodies against HIV, in preparation** (draft available upon request).
2. Arup Chakraborty & [K.G. Sprenger](#), **Eliciting Potent Antibodies Against Highly Mutable Pathogens by Vaccination**, *Phys. Biol.*, *accepted*.
3. [K. G. Sprenger*](#), Joy Louveau*, Pranav Murugan, Arup Chakraborty, **Optimizing Immunization Protocols to Elicit Broadly Neutralizing Antibodies**, *PNAS*, (2020), DOI: [10.1073/pnas.1919329117](https://doi.org/10.1073/pnas.1919329117).
4. Brittney Hellner, Sarah Alamdari, Harley Pyles, Shuai Zhang, Arushi Prakash, [K. G. Sprenger](#), Jim J. De Yoreo, David Baker, Jim Pfaendtner, Francois Baneyx, **Sequence-Structure-Binding Relationships Reveal Adhesion Behavior of the Car9 Solid-Binding Peptide: An Integrated Experimental and Simulation Study**, *JACS*, 142, 2355-2363 (2019), DOI: [10.1021/jacs.9b11617](https://doi.org/10.1021/jacs.9b11617).
5. Coco M. Mao, Janani Sampath, [K. G. Sprenger](#), Gary Drobny, Jim Pfaendtner, **Molecular Driving Forces in Peptide Adsorption to Metal Oxide Surfaces**, *Langmuir*, 35, 5911-5920 (2019), DOI: [10.1021/acs.langmuir.8b01392](https://doi.org/10.1021/acs.langmuir.8b01392).
6. Karl R. Oleson*, [K. G. Sprenger*](#), Jim Pfaendtner, Daniel T. Schwartz, **Inhibition of the Exoglucanase CEL7A by a Douglas-fir Condensed Tanning**, *JPCB*, 37, 8665-8674 (2018), DOI: [10.1021/acs.jpcc.8b05850](https://doi.org/10.1021/acs.jpcc.8b05850).
7. [K. G. Sprenger*](#), Arushi Prakash*, Gary Drobny, Jim Pfaendtner, **Investigating the Role of Phosphorylation in the Binding of Silaffin Peptide R5 to Silica with Molecular Dynamics Simulations**, *Langmuir*, 34, 1199-1207 (2018), DOI: [10.1021/acs.langmuir.7b02868](https://doi.org/10.1021/acs.langmuir.7b02868).
8. Arushi Prakash*, [K. G. Sprenger*](#), Jim Pfaendtner, **Essential Slow Degrees of Freedom in Protein-Surface Simulations: A Metadynamics Investigation**, *BBRC*, 498, 274-281 (2018), DOI: [10.1016/j.bbrc.2017.07.066](https://doi.org/10.1016/j.bbrc.2017.07.066).

9. Samantha R. Summers, [K. G. Sprenger](#), Michael F. Summers, Jim Pfaendtner, Jan Marchant, Joel L. Kaar, **Mechanism of Competitive Inhibition and Destabilization of *Acidothermus Cellulolyticus* Endoglucanase 1 by Ionic Liquids**, *J. Phys. Chem. B*, 121, 10793-10803 (2017), DOI: [10.1021/acs.jpcc.7b08435](#).
10. [K. G. Sprenger](#), Joseph Plaks, Joel L. Kaar, Jim Pfaendtner, **Elucidating Sequence and Solvent Specific Design Targets to Protect and Stabilize Enzymes for Biocatalysis in Ionic Liquids**, *Phys. Chem. Chem. Phys*, 19, 17426-17433 (2017), DOI: [10.1039/C7CP03013D](#).
11. Josh K. Smith*, [K. G. Sprenger*](#), Rick Liao, Elizabeth Nance, Jim Pfaendtner, **Determining Dominant Driving Forces Affecting Controlled Protein Release from Polymeric Nanoparticles**, *Biointerphases*, 12, 02D412 (2017), DOI: [10.1116/1.4983154](#).
12. Kovas Palunas*, [K. G. Sprenger*](#), Tobias Weidner, Jim Pfaendtner, **Effect of an Ionic Liquid/Air Interface on the Structure and Dynamics of Amphiphilic Peptides**, *J. ML*. 236, 404-413 (2017), DOI: [10.1016/j.molliq.2017.04.027](#).
13. [K. G. Sprenger](#), Jim Pfaendtner, **Strong Electrostatic Interactions Lead to Entropically Favorable Binding of Peptides on Surfaces**, *Langmuir*, 32, 5690-5701 (2016), DOI: [10.1021/acs.langmuir.6b01296](#).
14. [K. G. Sprenger](#), Jim Pfaendtner, **Using Molecular Simulation to Study Biocatalysis in Ionic Liquids**, *Methods in Enzymology*. S.I.: Elsevier, 577(16), 420-437 (2016), DOI: [10.1016/bs.mie.2016.05.020](#).
15. [K. G. Sprenger](#), Yi He, and Jim Pfaendtner. **Probing How Defects in Self-assembled Monolayers Affect Peptide Adsorption with Molecular Simulation**, *Foundations of Molecular Modeling and Simulation*. S.I.: Springer, 21-35, (2016), DOI: [10.1007/978-981-10-1128-3_2](#).
16. [K. G. Sprenger](#), Alaksh Choudhury, Joel L. Kaar, Jim Pfaendtner, **The Lytic Polysaccharide Monooxygenases ScLPMO10B and ScLPMO10C Are Stable in Ionic Liquids as Determined by Molecular Simulation**, *J. Phys. Chem. B*. 120, 3863-3872 (2016), DOI: [10.1021/acs.jpcc.6b01688](#).
17. [K. G. Sprenger](#), Vance Jaeger, Jim Pfaendtner, **The General AMBER Force Field (GAFF) can Accurately Predict Thermodynamic and Transport Properties of Many Ionic Liquids**, *J. Phys. Chem. B*. 119, 5882-5895 (2015), DOI: [10.1021/acs.jpcc.5b00689](#).

Achievements and Awards

NSF MPS Workshop for New Investigators, Selected Attendee	Nov. 2020
MIT Rising Stars in Chemical Engineering Workshop , Selected Attendee	Nov. 2018
MIT/JHU Rising Stars in Biomedical Workshop , Selected Attendee	Nov. 2018
1 st Place Oral Presentation Award , DYSS Series, UW ChemE	Aug. 2018
UW College of Engineering Student Research Award	Apr. 2017
Husky 100 Award , UW	Feb. 2017
2 nd Place Oral Presentation Award , ChemE Graduate Student Symposium, UW	Nov. 2016
AIChE CoMSEF Conference Presentation Award	Nov. 2016
2 nd Place Oral Presentation Award , Biomaterials Graduate Student Award, AIChE	Nov. 2016
ACS Chemical Computing Group Research Excellence Award	Nov. 2016
International HPC Summer School Travel Scholarship	Mar. 2016
UW ChemE Barbara Krieger-Brockett Travel Award	Nov. 2015
AIChE Women's Initiatives Committee (WIC) Travel Award	Sept. 2015
Graduate School's Fund for Excellence and Innovation Travel Award	Sept. 2015
PCCP Journal 1st Place Poster Prize at the FOMMS Conference	Jul. 2015
CoMSEF Conference Presentation Award at the FOMMS Conference	Jun. 2015
NSF FOMMS Graduate Student Fellowship	Apr. 2015
Suzanne Brainard Women in Science and Engineering Scholarship	2014 - 2015
UW Society of Women Engineers Outstanding Female Graduate Award	Jan. 2015

<u>Best Paper [Oral] Presentation</u> , Thermophysical Properties of Biological Systems Division, AIChE	Nov. 2014
<u>1st Place Poster Competition Prize</u> in Reaction Engineering, Catalysis and Reaction Engineering Division, AIChE Annual meeting	Nov. 2013
Graduate School's Fund for Excellence and Innovation (GSFEI) <u>Travel Award</u>	Oct. 2013

Invited Talks

1. Kayla Sprenger, Joy Louveau, Pranav Murugan, Charlie Wells, Brenden Petersen, Simone Conti, Victor Ovchinnikov, Martin Karplus, Arup Chakraborty, **Coupling machine learning with agent-based modeling to design vaccines against highly mutable pathogens**, *Women ExceLLing in COmputational Molecular Engineering (WELCOME) Seminar Series (2020)*.
2. Kayla Sprenger, Simone Conti, Victor Ovchinnikov, Martin Karplus, Arup Chakraborty, **Design of vaccine components and protocols for inducing protective antibodies against HIV**, *University of Louisville, Chemical Engineering Department (2020)*.
3. Kayla Sprenger, Simone Conti, Victor Ovchinnikov, Martin Karplus, Arup Chakraborty, **Design of components and protocols for inducing protective antibodies against HIV**, *Spotlights in Thermodynamics and Computational Molecular Science, AIChE (2019)*.

Selected Presentations

1. Kayla Sprenger, Joy Louveau, Pranav Murugan, Charlie Wells, Brenden Petersen, Daniel Faissol, Arup Chakraborty, **Machine learning-driven vaccine design against highly mutable pathogens**, *Oral Presentation, AIChE (2020)*.
4. Kayla Sprenger, Simone Conti, Martin Karplus, Arup Chakraborty, **Sequential vaccine administration of optimized HIV-like Ags elicits broadly-neutralizing antibodies of the VRC01 class *in silico***, *Oral Presentation, AIChE (2019)*.
5. Kayla Sprenger, Simone Conti, Martin Karplus, Arup Chakraborty, **Sequential vaccine administration of optimized HIV-like Ags elicits broadly-neutralizing antibodies of the VRC01 class *in silico***, *Oral Presentation, Ragon Institute of MGH, MIT, and Harvard (2018)*.
6. Kayla Sprenger, Simone Conti, Martin Karplus, Arup Chakraborty, **Sequential vaccine administration of optimized HIV-like Ags elicits broadly-neutralizing antibodies of the VRC01 class *in silico***, *Oral Presentation, MIT Interdepartmental Biophysics Retreat (2018)*.
7. Kayla Sprenger, Joy Louveau, Simone Conti, Martin Karplus, Arup Chakraborty, **Design of vaccine components and protocols for inducing protective antibodies against HIV**, *Invited Oral Presentation, UW Chemical Engineering Distinguished Young Scholars Seminar Series (2018). First place speaking prize.*
8. Kayla Sprenger, Tobias Weidner, Jim Pfaendtner, **Combining simulation and spectroscopy to determine the structure and orientation of a carbohydrate binding module (CBM) inspired model peptide on cellulose**, *Oral Presentation, ACS National Meeting (2017)*.
9. Kayla Sprenger, Samantha R. Summers, Jim Pfaendtner, Joel Kaar, **Understanding the structure and function of enzymes in ILs for improved biocatalysis**, *Poster Presentation, ACS (2017)*.
10. Kayla Sprenger, Tobias Weidner, Jim Pfaendtner, **Combining simulation and spectroscopy to determine the structure and orientation of a carbohydrate binding module (CBM) inspired model peptide on cellulose**, *Oral Presentation, AIChE (2016)*.
11. Kayla Sprenger, Samantha R. Summers, Jim Pfaendtner, Joel Kaar, **Understanding the structure and function of enzymes in ILs for improved biocatalysis**, *Poster Presentation, AIChE (2016)*.
12. Kayla Sprenger, Samantha R. Summers, Jim Pfaendtner, Joel Kaar, **Molecular simulations provide crucial insights into the mechanisms of biocatalysis in ionic liquids**, *Oral Presentation, UW Chemical Engineering Graduate Student Symposium (2016)*.

13. Kayla Sprenger, Yi He, Jim Pfaendtner, **Probing how defects in self-assembled monolayers affect protein adsorption with molecular simulation**, *Oral Presentation, AIChE* (2015).
14. Kayla Sprenger, Tobias Weidner, Jim Pfaendtner, **Combining spectroscopy experiments and molecular simulation to determine structural and mechanistic details of adsorbed biomolecules**, *Poster Presentation, AIChE* (2015).
15. Kayla Sprenger, Jim Pfaendtner, **Elucidating the role of ion concentration and peptide/surface charge on adsorption thermodynamics of model peptides on SAMs**, *Poster Presentation, ICBZM* (2015).
16. Kayla Sprenger, Tobias Weidner, Jim Pfaendtner, **Obtaining thermodynamic and structural information of surface-bound biomolecules from biased simulations**, *Poster Presentation, FOMMS* (2015).
17. Kayla Sprenger, Mike Deighan, Jim Pfaendtner, **Elucidating the role of ion concentration and peptide/surface charge on the adsorption thermodynamics of model peptides on self-assembled monolayers, with molecular simulation**, *Oral Presentation, AIChE* (2014).
18. Kayla Sprenger, Vance Jaeger, Jim Pfaendtner, **A molecular dynamics study assessing the accuracy of the generalized amber force field to predict the thermophysical properties of 19 ionic liquids**, *Poster Presentation, AIChE* (2014).
19. Kayla Sprenger, Mike Deighan, Jim Pfaendtner, **Elucidating the role of ion concentration and peptide/surface charge on the adsorption thermodynamics of model peptides on self-assembled monolayers, with molecular simulation**, *Poster Presentation, Graduate Student Symposium of UW Chemical Engineering, Seattle, WA* (2014).
20. Kayla Sprenger, Jim Pfaendtner, Fernando Resende, **Conversion of supercritical bioethanol into Hydrocarbons Over HZSM-5 Zeolite**, *e-Poster Oral Pres., AIChE, San Francisco, CA* (2013).
21. Kayla Sprenger, Jim Pfaendtner, Fernando Resende, **Conversion of supercritical bioethanol into Hydrocarbons Over HZSM-5 Zeolite**, *Poster Presentation, AIChE, San Francisco, CA* (2013).

Professional Affiliations and Service

Professional Affiliations: AIChE, ACS

AICHe CoMSEF Liaison Director	Nov. 2020 – Nov. 2022
Session Co-Chair, ACS National Meeting: <i>Protein Aggregation & Immunogenicity</i>	Aug. 2021
NSF Graduate Research Fellowship Program (GRFP) Reviewer	Dec. 2020
AB Nexus Seed Grant Reviewer, CU Boulder	Nov. 2020
National Academies of Sciences, Engineering, & Medicine Committee Member: <i>Proposal Evaluation for Allocation of Supercomputing Time for the Study of Molecular Dynamics, Eleventh Round</i>	Aug. 2020
Volunteer for Expanding Your Horizons (EYH)	Mar. 2015 – Jun. 2017
Volunteer for SWE Time to Invent (Co-Leader 2015-2016)	Oct. 2014 – Jun. 2017
Engineers Without Borders (EWB) Jamaica Biodiesel Team Member	Jun. 2011 – Aug. 2014
Reviewer for the following journals:	
○ eLife	
○ Cell Reports	
○ Scientific Reports	
○ The Journal of Physical Chemistry	
○ The Journal of Chemical Physics	
○ Physical Chemistry Chemical Physics	
○ Molecular Simulation/Journal of Experimental Nanoscience	
○ Biophysical Journal	
○ Process Biochemistry	
○ Applied Surface Science	
○ ACS Sustainable Chemistry & Engineering	
○ Journal of Chemical Information and Modeling	