

Kayla G. Sprenger, Ph.D.

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[Faculty Webpage](#), [Group Webpage](#)
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Education

2020 – Present	Assistant Professor	University of Colorado (CU) Boulder Chemical & Biological Engineering
2017 – 2020	Postdoctoral Associate	Massachusetts Institute of Technology Institute for Medical & Science
2014 – 2017	Ph.D.	University of Washington (UW) Chemical Engineering (ChemE)
2012 – 2014	M.S.	University of Washington Chemical Engineering
2008 – 2012	B.S.	University of Washington Chemical Engineering

Research Funding

Mechanistic Studies of the Cathode-Electrolyte Interface - A Combined Experimental & Computational Approach
DOE Vehicles Technology Office, 10/22-9/25, \$2,250,000, co-PI.

Characterizing Host-Virus Interactions in a New HIV Model Organism
NIH: 1R01OD034046-01, 07/22-06/27, \$3,638,242, co-PI.

Coupling Machine Learning with Agent-Based Modeling to Design a Universal Flu Vaccine
NIH: 1R21AI169364-01, 05/2022 – 04/2024, \$411,905, PI.

EFRI E3P: Hydrogenolysis for upcycling of polyesters and mixed plastics
NSF: 2132033, 09/2021 – 08/2025, \$2,000,000, co-PI.

Combining simulations and experiments to determine protein/ligand-mediated microglial activation in Alzheimer's Disease
CU Boulder: AB Nexus, 06/2021 – 05/2022, \$50,000, PI.

Awards & Honors

2022	Selected Participant	Early Career Reviewer (ECR) Program, NIH
2022	Fellow	Research Impact Fellowship (RIF) Program CU Boulder <i>Personally chosen by department chair and college dean</i>
2022	Nominated	Outstanding Faculty Advisor Award CU Boulder
2022	Selected Participant	US Frontiers of Engineering Program National Academy of Engineering
2022	Grant Awardee	National Center for Faculty Development & Diversity Faculty Success Program <i>Awarded by CU Boulder Office of Faculty Affairs</i>
2020	Selected Participant	NSF Mathematical & Physical Sciences (MPS) Workshop for New Investigators
2018	Selected Participant	MIT Rising Stars in Chemical Engineering Workshop
2018	Selected Participant	MIT/JHU Rising Stars in Biomedical Workshop
2018	Best Speaker	Distinguished Young Scholars Seminar (DYSS) series UW ChemE
2017	Graduate Research Award	UW College of Engineering
2017	Husky 100 Award	UW
2016	Oral Presentation Award	2 nd place Graduate Student Symposium UW ChemE
2016	Graduate Student Award	Computational Molecular Science & Engineering Forum (CoMSEF) AIChE
2016	Oral Presentation Award	2 nd place Biomaterials: Graduate Student Award Session AIChE
2016	Research Excellence Award	Chemical Computing Group American Chemical Society (ACS)
2015	Poster Presentation Award	Foundations of Molecular Modeling & Simulation Conference <i>Sponsored by the Physical Chemistry Chemical Physics (PCCP) journal</i>
2015	Conference Presentation Award	Foundations of Molecular Modeling & Simulation Conference <i>Sponsored by CoMSEF</i>

2015	Graduate Student Fellowship	Foundations of Molecular Modeling & Simulation Conference <i>Sponsored by the National Science Foundation</i>
2015	Outstanding Female Graduate Award	Society of Women Engineers UW
2014	Scholarship	Suzanne Brainard Women in Science and Engineering UW
2014	Oral Presentation Award	Thermophysical Properties of Biological Systems Division AIChE
2013	Poster Presentation Award	Catalysis and Reaction Engineering Division AIChE

Publications (23 total | 13 co-/first author, 4 co-/corresponding author, h-index 12, 579 citations via [Google Scholar](#))

*Authors contributed equally; graduate trainees are underlined

Faculty Publications

1. Emily R. Rhodes, Jonathan G. Faris, Brian M. Petersen, **K. G. Sprenger**, Common Framework Mutations Impact Antibody Interfacial Dynamics and Flexibility, *In Press at Frontiers in Immunology (2022 IF 7.561)*, (2023), DOI: [10.3389/fimmu.2023.1120582](https://doi.org/10.3389/fimmu.2023.1120582).
2. Jonathan G. Faris, Daniel Orbidan, Charles Wells, Brenden K. Petersen*, **K. G. Sprenger***, Moving the Needle: Employing Deep Reinforcement Learning to Push the Boundaries of Coarse-Grained Vaccine Models, *Frontiers in Immunology (2022 IF 7.561)*, 13, 1029167 (2022), DOI: [10.3389/fimmu.2022.1029167](https://doi.org/10.3389/fimmu.2022.1029167).
3. Dean Oldham, Hong Wang, Juliet Mullen, Emma Lietzke, **K. G. Sprenger**, Philip Reigan, Robert H Eckel, Kimberley D Bruce, Using synthetic ApoC-II peptides and nAngptl4 fragments to measure lipoprotein lipase activity in radiometric and fluorescent assays, *Frontiers in Cardiovascular Medicine (2021 IF 6.050)*, 9, 926631 (2022), DOI: [10.3389/fcvm.2022.926631](https://doi.org/10.3389/fcvm.2022.926631).
4. Simone Conti, Victor Ovchinnikov, Jonathan G. Faris, Arup K. Chakraborty, Martin Karplus*, **K.G. Sprenger***. Multiscale affinity maturation simulations to elicit broadly neutralizing antibodies against HIV, *PLoS Computational Biology (2021 IF 4.779)*, 18, e1009391 (2022), DOI: [10.1371/journal.pcbi.1009391](https://doi.org/10.1371/journal.pcbi.1009391).
5. Brian M. Petersen, Sophia A. Ulmer, Emily R. Rhodes, **K. G. Sprenger***, Timothy A. Whitehead*. Regulatory approved monoclonal antibodies contain framework mutations predicted from human antibody repertoires, *Frontiers in Immunology (2022 IF 7.561)*, 12, 728694 (2021), DOI: [10.3389/fimmu.2021.728694](https://doi.org/10.3389/fimmu.2021.728694).
6. Irene Francino Urdaniz[#], Paul J. Steiner[#], Monica B. Kirby[#], Fangzhu Zhao, Cyrus M. Haas, Shawn Barman, Emily R. Rhodes, Linghang Peng, **K. G. Sprenger**, Joseph G. Jardine, Timothy A. Whitehead, One-shot identification of SARS-CoV-2 S RBD escape mutants using yeast screening, *Cell Reports (2021 IF 9.995)*, 36, 109627 (2021), DOI: [10.1016/j.celrep.2021.109627](https://doi.org/10.1016/j.celrep.2021.109627).

Postdoctoral Publications

7. Arup Chakraborty & **K. G. Sprenger**, Eliciting Potent Antibodies Against Highly Mutable Pathogens by Vaccination, *Physical Biology (2020 IF 2.583)*, 18, 13-15 (2021), DOI: [10.1088/1478-3975/abde8d](https://doi.org/10.1088/1478-3975/abde8d).
8. **K. G. Sprenger***, Joy Louveau*, Pranav Murugan, Arup Chakraborty, Optimizing Immunization Protocols to Elicit Broadly Neutralizing Antibodies, *Proceedings of the National Academy of Sciences (2021 IF 12.78)*, 117, 20077-20087 (2020), DOI: [10.1073/pnas.1919329117](https://doi.org/10.1073/pnas.1919329117).

Graduate Publications

9. **K. G. Sprenger**, Sergio Mauri, Steven Roeters, Rolf Mertig, Yoshiharu Nishiyama, Jim Pfaendtner*, Tobias Weidner*. Direct Evidence for Alignment of Cellulase Enzymes on Cellulose Surfaces, *The Journal of Physical Chemistry Letters (2022 IF 6.475)* 12, 10684–10688 (2021), DOI: [10.1021/acs.jpcllett.1c02757](https://doi.org/10.1021/acs.jpcllett.1c02757).
10. 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, *Journal of the American Chemical Society (IF 2021 16.38)*, 142, 2355-2363 (2020), DOI: [10.1021/jacs.9b11617](https://doi.org/10.1021/jacs.9b11617).
11. Coco M. Mao, Janani Sampath, **K. G. Sprenger**, Gary Drobny, Jim Pfaendtner, Molecular Driving Forces in Peptide Adsorption to Metal Oxide Surfaces, *Langmuir (2021 IF 4.331)*, 35, 5911-5920 (2019), DOI: [10.1021/acs.langmuir.8b01392](https://doi.org/10.1021/acs.langmuir.8b01392).

12. Karl R. Oleson*, **K. G. Sprenger***, Jim Pfaendtner, Daniel T. Schwartz, Inhibition of the Exoglucanase CEL7A by a Douglas-fir Condensed Tanning, *The Journal of Physical Chemistry B* (2020 IF 2.781), 37, 8665-8674 (2018), DOI: [10.1021/acs.jpccb.8b05850](https://doi.org/10.1021/acs.jpccb.8b05850).
13. **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* (2021 IF 4.331), 34, 1199-1207 (2018), DOI: [10.1021/acs.langmuir.7b02868](https://doi.org/10.1021/acs.langmuir.7b02868).
14. Arushi Prakash*, **K. G. Sprenger***, Jim Pfaendtner, Essential Slow Degrees of Freedom in Protein-Surface Simulations: A Metadynamics Investigation, *Biochemical and Biophysical Research Communications* (2022 IF 3.575), 498, 274-281 (2018), DOI: [10.1016/j.bbrc.2017.07.066](https://doi.org/10.1016/j.bbrc.2017.07.066).
15. 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, *The Journal of Physical Chemistry B* (2020 IF 2.781), 121, 10793-10803 (2017), DOI: [10.1021/acs.jpccb.7b08435](https://doi.org/10.1021/acs.jpccb.7b08435).
16. **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, *Physical Chemistry Chemical Physics* (2020 IF 3.676), 19, 17426-17433 (2017), DOI: [10.1039/C7CP03013D](https://doi.org/10.1039/C7CP03013D).
17. Josh K. Smith*, **K. G. Sprenger***, Rick Liao, Elizabeth Nance, Jim Pfaendtner, Determining Dominant Driving Forces Affecting Controlled Protein Release from Polymeric Nanoparticles, *Biointerphases* (2021 IF 1.916), 12, 02D412 (2017), DOI: [10.1116/1.4983154](https://doi.org/10.1116/1.4983154).
18. Kovas Palunas*, **K. G. Sprenger***, Tobias Weidner, Jim Pfaendtner, Effect of an Ionic Liquid/Air Interface on the Structure and Dynamics of Amphiphilic Peptides, *Journal of Molecular Liquids* (2022 IF 6.165), 236, 404-413 (2017), DOI: [10.1016/j.molliq.2017.04.027](https://doi.org/10.1016/j.molliq.2017.04.027).
19. **K. G. Sprenger**, Jim Pfaendtner, Strong Electrostatic Interactions Lead to Entropically Favorable Binding of Peptides on Surfaces, *Langmuir* (2021 IF 4.331), 32, 5690-5701 (2016), DOI: [10.1021/acs.langmuir.6b01296](https://doi.org/10.1021/acs.langmuir.6b01296).
20. **K. G. Sprenger**, Jim Pfaendtner, Using Molecular Simulation to Study Biocatalysis in Ionic Liquids, *Methods in Enzymology* (2021 IF 1.682). S.I.: Elsevier, 577(16), 420-437 (2016), DOI: [10.1016/bs.mie.2016.05.020](https://doi.org/10.1016/bs.mie.2016.05.020).
21. **K. G. Sprenger**, Yi He, and Jim Pfaendtner. Probing How Defects in Self-assembled Monolayers Affect Peptide Adsorption with Molecular Simulation, In: Snurr, R., Adjiman, C., Kofke, D. (eds) Foundations of Molecular Modeling & Simulation. *Molecular Modeling and Simulation*. Springer, Singapore (2016), DOI: [10.1007/978-981-10-1128-3_2](https://doi.org/10.1007/978-981-10-1128-3_2).
22. **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, *The Journal of Physical Chemistry B* (2020 IF 2.781), 120, 3863-3872 (2016), DOI: [10.1021/acs.jpccb.6b01688](https://doi.org/10.1021/acs.jpccb.6b01688).
23. **K. G. Sprenger**, Vance Jaeger, Jim Pfaendtner, The General AMBER Force Field (GAFF) can Accurately Predict Thermodynamic and Transport Properties of Many Ionic Liquids, *The Journal of Physical Chemistry B* (2020 IF 2.781), 119, 5882-5895 (2015), DOI: [10.1021/acs.jpccb.5b00689](https://doi.org/10.1021/acs.jpccb.5b00689).

Invited Talks

1. A Holistic Computational Approach to Combatting HIV | *University of Colorado Boulder, BioFrontiers Institute* | 4 Dec 2022.
2. A Holistic Computational Approach to Combatting HIV | *AIChE Honorific Session: Arup Chakraborty's 60th Birthday* | Boston, MA | 9 Nov 2021.
3. A Seemingly Unstoppable Virus: Can Humanity Ever Overcome HIV? | *University of Colorado Boulder, College of Engineering & Applied Science Alumni Webinar* | Remote | 20 Oct 2021.
4. Coupling machine learning with agent-based modeling to design vaccines against highly mutable pathogens | *University of Kentucky, Department of Chemical and Materials Engineering* | Remote | 28 Apr 2021.
5. Coupling machine learning with agent-based modeling to design vaccines against highly mutable pathogens | *Women Excelling in Computational Molecular Engineering (WELCOMe) Virtual Seminar Series* | Remote | 13 Jan 2021.

- Design of vaccine components and protocols for inducing protective antibodies against HIV | *University of Louisville, Chemical Engineering Department* | Remote | 30 Oct 2020.
- Design of vaccine components and protocols for inducing protective antibodies against HIV | *Spotlights in Thermodynamics and Computational Molecular Science, AIChE* | Orlando, FL | 11 Nov 2019.
- Design of vaccine components and protocols for inducing protective antibodies against HIV | *UW ChemE Distinguished Young Scholars Seminar Series* | Seattle, WA | 13 Aug 2018 | **Awarded Best Speaker prize.**

Selected Presentations (out of 14 total)

- Machine learning-driven vaccine design against highly mutable pathogens | *Oral Presentation, AIChE* | 2020.
- 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.
- 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.
- 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.
- 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.
- Probing how defects in self-assembled monolayers affect protein adsorption with molecular simulation | *Oral Presentation, AIChE* | 2015.
- 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.

Teaching Experience

2023	Instructor	CHEN 4898: Biomolecular Simulations
2020 – 2022	Co-Instructor	CHEN 3210: Heat and Mass Transfer
2019	Kaufman Teaching Certificate Program	MIT Teaching and Learning Lab
2016	Guest Lecturer on Molecular Simulations	CHEM E 498: Special Topics UW ChemE
2015	Teaching Assistant	CHEM E 435: Mass Transfer UW ChemE
2014	Guest Lecturer on ASPEN	CHEM E 375: Computer Skills UW ChemE
2014	Guest Lecturer on Molecular Simulations	CHEM E 525: Graduate Thermo UW ChemE
2013	Teaching Assistant	CHEM E 437: ChemE Laboratory II UW ChemE

Mentoring Experience

Current Graduate Students

2023	Emma Aldrich, Biological Engineering/Interdisciplinary Quantitative Biology Ph.D. Student
2022 – Present	Rafael Ferreira de Menezes, Chemical Engineering Ph.D. Student <i>Co-advised with Dr. Mike Toney, CU Boulder</i>
2022 – Present	Bailey Zinger, Biological Engineering/ Interdisciplinary Quantitative Biology Ph.D. Student
2022 – Present	Emma Lietzke, Biological Engineering Ph.D. Student <i>Co-advised with Dr. Kimberley Bruce, CU Denver, Anschutz Medical Campus</i>
2022 – Present	Travis Dong, Chemical Engineering Ph.D. Student <i>Co-advised with Dr. Mike Toney, CU Boulder</i>
2021 – Present	Jonathan Faris, Biological Engineering Ph.D. Student
2021 – Present	Emily Rhodes, Biological Engineering Ph.D. Student
2021 – Present	Daisy Fuchs, Chemical Engineering Ph.D. Student
2020 – Present	Brian Petersen, Chemical Engineering Ph.D. Student <i>Co-advised with Dr. Timothy Whitehead, CU Boulder</i>

Former Graduate Students

2022 Megan Makam, Biomedical Engineering M.S.

Current Undergraduate Students

2023 – Present Lauren Serio
2022 – Present Nicola Wheeler
2022 – Present Aidan Wegner
2022 – Present Jim Grady
2022 – Present Abdulkadir Said
2021 – Present Daniel Orbidan
2021 – Present Sahana Balaji
2021 – Present David Saeb
2020 – Present Alex Pham

External Leadership/Service Activities

2022 **Panel Member** NIH Vaccines Against Infectious Diseases (VID; formerly VMD)
2022 **Session Chair** Recent Advances in Multiscale Methodologies | CoMSEF | AIChE
2022 **Session Chair** Arup Chakraborty's 60th Celebration Symposium | Boston, MA
2022 **Guest Editor** eLife
2021 – 2022 **Session Co-Chair** Cell and Tissue Engineering | AIChE
2021 – 2022 **Session Co-Chair** CoMSEF Poster Session | AIChE
2020 – 2022 **Liaison Director** CoMSEF | AIChE
2020 – 2022 **Committee Member** National Academies of Sciences, Engineering, & Medicine
Proposal Evaluation for Allocation of Supercomputing Time for the Study of Molecular Dynamics, 11th-13th Rounds
2020 – 2021 **Reviewer** NSF Graduate Research Fellowship Program
2021 **Session Co-Chair** Recent Advances in Multiscale Methodologies | CoMSEF | AIChE
2021 **Session Co-Chair** Protein Aggregation and Immunogenicity | ACS
2017 – Present **Journal Reviewer** Nature Communications, Chem Catalysis, eLife, Cell Reports, Scientific Reports, Nanomaterials, Viruses, Vaccines, The Journal of Physical Chemistry, The Journal of Chemical Physics, Physical Chemistry Chemical Physics, Chemical Physics Letters, Molecular Simulation/Journal of Experimental Nanoscience, Biophysical Journal, AIChE Journal, Process Biochemistry, Applied Surface Science, ACS Sustainable Chemistry & Engineering, Journal of Chemical Information & Modeling, Langmuir, Biomolecules

Internal Leadership/Service Activities at CU Boulder

2022 – Present **Organizer** Departmental Patten Seminar Series | ChBE Department
2021 – Present **Committee Member** Leadership Team | ChBE Department
2020 – Present **Committee Member** Diversity, Equity, and Inclusion Committee | ChBE Department
2021 – 2022 **Reviewer** Graduate Student Awards | ChBE Department
2021 – 2022 **Co-Organizer** NSF GRFP/NDSEG Grad Student Workshop | ChBE Department
2020 – 2022 **Reviewer** AB Nexus Seed Grants | CU Boulder/Anschutz
2022 **Committee Member** CHEN/BIEN Quantitative Training/Curriculum Development | ChBE Department
2022 **Workshop Organizer/Presenter** PI Academy, Time Management for new CU faculty members | CU Boulder
2022 **Faculty Host/Participant** RCR: Mentor/Trainee Issues | CU Boulder
2022 **Participant** CHEN Recruitment Video (energy) | ChBE Department
2021 **Co-Organizer** Departmental Patten Seminar Series | ChBE Department
2020 – 2021 **Committee Member** Faculty Search Committee | ChBE Department

Outreach Activities

2015 – 2017	Volunteer	Expanding Your Horizons (EYH)
2014 – 2017	Volunteer	Society of Women Engineers (SWE) Time to Invent Program <i>Co-Director from 2015-2016</i>
2011 – 2014	Team Member	Engineers Without Borders (EWB) Jamaica Biodiesel Team