

# Kayla G. Sprenger, Ph.D.

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## Education and Professional Positions

2024 – Present	Faculty Director for Engagement	<b>University of Colorado (CU) Boulder</b>   Chemical & Biological Eng
2020 – Present	Assistant Professor	<b>CU Boulder</b>   Chemical & Biological Engineering
2017 – 2020	Postdoctoral Associate	<b>MIT</b>   Institute for Medical Eng & Science
2014 – 2017	Ph.D.	<b>University of Washington (UW)</b>   Chemical Engineering (ChemE)
2012 – 2014	M.S.	<b>University of Washington</b>   ChemE
2008 – 2012	B.S.	<b>University of Washington</b>   ChemE

## Research Funding

### Development of PEG10 inhibitors in the fight against ALS-FTD

ACTIVE: DOD: Defense Health Program, Congressionally Directed Medical Research Programs (CDMRP), HT942524ALSRPTIA, AL240155, Amyotrophic Lateral Sclerosis Research Program (ALSRP) Therapeutic Idea Award (TIA), 2025 – 2027 \$600,000 total, ~\$20K direct/yr, co-PI.

### Coupled Multiscale Modeling and Diagnostics for Lithium-Sulfur Battery Design

ACTIVE: DOE: Office of Energy Efficiency and Renewable Energy (EERE), DE-FOA-0002892, 6/2024-5/2027, \$2,000,000 total, ~\$70K direct/yr, co-PI.

### REU Site: University of Colorado, Engineering Smart Biomaterials

ACTIVE: NSF: 2348856, 5/1/2024 – 4/30/2027, \$427,165 total, ~\$8.4K direct/yr, co-PI (thrust leader).

### Tunable Surface Coatings to Control Protein Dynamics and Attenuate the FBR

ACTIVE: NIH: 1R01AI177678-01A1, 2/5/2024 – 2/4/2029, \$2,765,149 total, ~\$57K direct/yr, co-PI.

### Research on Vaccine Development and Multi-fidelity Multi-objective Deep Symbolic Optimization, Lawrence Livermore National Laboratory (LLNL) Subcontract for Graduate Student Support

ACTIVE: Subcontract: B663859, 1/15/2024 – 7/31/2025, \$142,395 total, ~\$101K direct/18 mo, PI.

### Collaborative Research: DMREF: Accelerated Discovery of Sustainable Bioplastics: Automated, Tunable, Integrated Design, Processing and Modeling

ACTIVE: NSF: 2323979, 10/2023 – 09/2027, \$2,000,000 total, ~\$70K direct/yr, co-PI.

### Combining In Vitro and In Silico Models to Investigate Antiretroviral Drug Transport Across the Blood Brain Barrier for the Treatment of HIV-1 Infection in the Brain

ACTIVE: NIH: 1R21MH132159-01A1, 9/18/2023 – 9/17/2025, \$396,379 total, ~\$69K direct/yr, (multi-) PI.

### Employing Simulations & Experiments to Optimize Strategies for Co-activating Microglial Receptors to Treat AD

ACTIVE: CU Boulder: AB Nexus, 07/2023 – 06/2024 (NCE to 06/2025), \$100,000 total, ~\$41K direct/yr, PI.

### Mechanistic Studies of the Cathode-Electrolyte Interface - A Combined Experimental & Computational Approach

ACTIVE: DOE: Vehicles Technology Office, DE-LC-000L096, 5/2023–4/2026, \$2,250,000 total, ~\$70K direct/yr, co-PI.

### Characterizing Host-Virus Interactions in a New HIV Model Organism

ACTIVE: NIH: 1R01OD034046-01, 07/2022 – 06/2027, \$3,638,242 total, ~\$53K direct/yr, co-PI.

### Coupling Machine Learning with Agent-Based Modeling to Design a Universal Influenza Vaccine

ACTIVE: NIH: 1R21AI169364-01, 05/2022 – 04/2024 (NCE to 04/2025), \$411,905 total, ~\$138K direct/yr, PI.

### EFRI E3P: Hydrogenolysis for Upcycling of Polyesters and Mixed Plastics

ACTIVE: NSF: 2132033, 09/2021 – 08/2025, \$2,000,000 total, ~\$47K direct/yr, co-PI.

## Pericentrin Self-Assembly Regulates Intracellular Trafficking for Cilia Formation and Signaling

PAST: CU Boulder: AB Nexus, 07/2023 – 06/2024, \$125,000 total, \$0K direct/yr, co-PI.

## Combining Simulations & Experiments to Determine Protein/Ligand-Mediated Microglial Activation in Alzheimer's

PAST: CU Boulder: AB Nexus, 06/2021 – 05/2022, \$50,000 total, ~\$17.5K direct/yr, PI.

### Awards & Honors

2024	<b>Nominated</b>	Early Faculty Award   ACS Fall Meeting   PMSE & COMP Divisions
2024	<b>Selected Participant</b>	AIChE's Leadership Equity in Engineering (LEE) Program
2024	<b>Outstanding Junior Faculty Development Award</b>	Chemical & Biology Engineering Department   CU
2023	<b>Outstanding Partner Award</b>	Research and Innovation Office (RIO)   CU   <i>first time in the history of the award that it has been presented to a member of the faculty</i>
2023	<b>Outstanding Mentor Award</b>	Award for undergraduate research mentorship   CU Discovery Learning Apprenticeship (DLA) Program
2023	<b>35 Under 35 Award</b>	American Institute of Chemical Engineers (AIChE)
2023	<b>Nominated</b>	Outstanding Faculty Advisor Award   CU
2023	<b>Runner Up</b>	Kern Lipid Conference Roger Davis Award
2023	<b>Selected Participant</b>	ASEE DELTA Junior Faculty Institute
2022	<b>Nominated</b>	Outstanding Faculty Advisor Award   CU
2022	<b>Selected Participant</b>	Early Career Reviewer (ECR) Program, NIH
2022	<b>Fellow</b>	Research Impact Fellowship Program   CU   <i>chosen by dept chair/college dean</i>
2022	<b>Selected Participant</b>	US Frontiers of Engineering (FOE) Program   National Academy of Engineering
2022	<b>Grant Awardee</b>	National Center for Faculty Development & Diversity Faculty Success Program <i>Awarded by CU Boulder Office of Faculty Affairs</i>
2020	<b>Selected Participant</b>	NSF Mathematical & Physical Sciences (MPS) Workshop for New Investigators
2018	<b>Selected Participant</b>	MIT Rising Stars in Chemical Engineering Workshop
2018	<b>Selected Participant</b>	MIT/JHU Rising Stars in Biomedical Workshop
2018	<b>Best Speaker</b>	Distinguished Young Scholars Seminar (DYSS) series   UW ChemE
2017	<b>Graduate Research Award</b>	UW College of Engineering
2017	<b>Husky 100 Award</b>	UW
2016	<b>Oral Presentation Award</b>	2 <sup>nd</sup> place   Graduate Student Symposium   UW ChemE
2016	<b>Graduate Student Award</b>	Computational Molecular Science & Engineering Forum (CoMSEF)   AIChE
2016	<b>Oral Presentation Award</b>	2 <sup>nd</sup> place   Biomaterials: Graduate Student Award Session   AIChE
2016	<b>Research Excellence Award</b>	Chemical Computing Group   American Chemical Society (ACS)
2015	<b>Poster Presentation Award</b>	Foundations of Molecular Modeling & Simulation Conference <i>Sponsored by the Physical Chemistry Chemical Physics (PCCP) journal</i>
2015	<b>Conference Presentation Award</b>	Foundations of Molecular Modeling & Simulation Conference <i>Sponsored by CoMSEF</i>
2015	<b>Graduate Student Fellowship</b>	Foundations of Molecular Modeling & Simulation Conference <i>Sponsored by the National Science Foundation</i>
2015	<b>Outstanding Female Graduate Award</b>	Society of Women Engineers   UW
2014	<b>Scholarship</b>	Suzanne Brainard Women in Science and Engineering   UW
2014	<b>Oral Presentation Award</b>	Thermophysical Properties of Biological Systems Division   AIChE
2013	<b>Poster Presentation Award</b>	Catalysis and Reaction Engineering Division   AIChE

### Publications (39 total | 13 co-/first author, 11 co-/corr author, h-index of 14, 979 citations via [Google Scholar](#))

\* # Authors contributed equally; graduate trainees are in **red**, undergrad trainees are in **blue**; drafts available upon request.

### Faculty Publications

1. Luis Kitsu Iglesias; Samuel D. Marks; Nikhil Rampal; Emma N. Antonio; **Rafael Ferreira de Menezes**; Liang Zhang; Daniel Olds; Stephen E. Weitzner; K. G. Sprenger; Liwen F. Wan, Michael F. Toney, Microstructure-Dependent Sodium Storage Mechanisms in Hard Carbon Anodes, *Submitted (Energy & Environmental Science ('23 IF 32.4))*.

2. Rhuiago Mendes de Oliveira, Layza Nunes de Sousa, Alynne Vieira Gregorio, **Rafael Ferreira de Menezes**, **K. G. Sprenger**, Luiz Guilherme Machado de Macedo, Fernando Pirani, Ricardo Gargano, The Interatomic Bond Between Cd and Noble Gas Atoms: The Nature of the Intermolecular Forces, the Stability of the Adducts, Their Spectroscopic and Thermodynamical Properties, *Submitted (Theoretical and Computational Chemistry)*.
3. **Emma E. Lietzke**, **David Saeb**, **Emma C. Aldrich**, Kimberley D. Bruce\*, **K. G. Sprenger\***, Synergistic reduction in interfacial flexibility of TREM2<sup>R47H</sup> and ApoE4 may underlie AD pathology, *In Revision at Alzheimers & Dementia: The Journal of the Alzheimer's Association* ('23 IF 13.0).
4. Guilherme Carlos Carvalho de Jesus, Ráilson da Conceição Vasconcelos, Lucas Bezerra do Vale, **Rafael Ferreira de Menezes**, **K. G. Sprenger**, Ricardo Gargano, Electronic and Magnetic Properties of Manganese Bromide Monolayers, *In Revision at Langmuir* ('23 IF 3.7).
5. Wenhan Ou, Samuel D. Marks, **Rafael Ferreira de Menezes**, Rong He, Zihan Zhang, **Ziyue Dong**, Collin Sindt, Jonathan Thuston, Chernoy Jaye, Bruce Cowie, Thomsen Lars, Zhenqing Zhuo, Wanli Yang, Robert Tenent, **K. G. Sprenger**, Michael F. Toney, Unveiling the Mechanism of Mn Dissolution through a Dynamic Cathode-Electrolyte Interphase on LiMn<sub>2</sub>O<sub>4</sub>, *Advanced Energy Materials* ('23 IF 27.8), (2024), DOI: 10.1002/aenm.202404652.
6. Monica B. Kirby, **Brian M. Petersen**, **Jonathan G. Faris**, Siobhan Kells, **K. G. Sprenger**, T. A. Whitehead, Retrospective human antibody development trajectories are sparse and permissive, *PNAS* ('23 IF 9.4), 122, e2412787122 (2024), DOI: [10.1073/pnas.2412787122](https://doi.org/10.1073/pnas.2412787122).
7. Ian R. Campbell, **Ziyue Dong**, Paul Grandgeorge, Andrew M. Jimenez, **Emily R. Rhodes**, Ella lee, Scott Edmundson, Chinmayee Subban, **K. G. Sprenger\***, Eleftheria Roumeli\*, Analogue materials to isolate mechanisms for self-bonding in biomatter plastics, *Matter (Cell Press; '23 IF 17.3)*, (2024), DOI: [10.1016/j.matt.2024.101941](https://doi.org/10.1016/j.matt.2024.101941). **Featured on American Physical Society (APS) Division of Polymer Physics (DPOLY) Annual Meeting Cover.**
8. **Jonathan G. Faris**, Mikel Landajuela, **Kayla G. Sprenger**, Daniel faissol, Felipe Leno da Silva, Computational Antigen Optimization through Symbolic Optimization and Affinity Maturation Simulation, *NeurIPS 2024 Workshop on AI for New Drug Modalities*, 2024, URL: <https://openreview.net/forum?id=0KAFbnTAdW>.
9. Rong He, Liam McDonough, Wenhan Ou, Samuel D. Marks, **Rafael Ferreira de Menezes**, Elizabeth Allan-Cole, Hongmei Luo, Michael F. Toney, **K. G. Sprenger**, Meng Zhou\*, Robert C. Tenent\*, In Situ Characterization of the Oxidation Behavior of Carbonate-Based Electrolytes for Li-Ion Batteries by Scanning Electrochemical Microscopy, *ACS Electrochemistry*, (2024), DOI: [10.1021/acselectrochem.4c00106](https://doi.org/10.1021/acselectrochem.4c00106).
10. **Ziyue Dong**, Erin Dunphy, **Aidan B. Wegner**, J. Will Medlin, Michael F. Toney\*, **K. G. Sprenger\***, An *in silico* investigation into polyester adsorption onto alumina towards an improved understanding of hydrogenolysis catalysts, *Langmuir* ('23 IF 3.7), *Invited Paper: 2025 Pioneers in Applied and Fundamental Interfacial Chemistry: Shaoyi Jiang*, 40, 52, 27416–27429 (2024), DOI: [10.1021/acs.langmuir.4c03679](https://doi.org/10.1021/acs.langmuir.4c03679). **Featured on Journal Cover.**
11. **David Saeb**, **Emma E. Lietzke**, **Daisy I. Fuchs**, **Emma C. Aldrich**, Kimberley D. Bruce, **K. G. Sprenger**, The flexible stalk region of sTREM2 modulates its interactions with phospholipids in the brain, *eLife* ('23 IF 6.4), 13:RP102269 (2024), DOI: [10.7554/eLife.102269.1](https://doi.org/10.7554/eLife.102269.1).
12. J. Xiao\*, N. Adelstein, Y. Bi1, W. Bian, J. Cabana, C. Cobb, Y. Cui, S. Dillon, M. Doeff, S. Islam, K. Leung, M. Li, F. Lin, J. Liu, H. Luo, A. Marschilok, Y. Meng, Y. Qi, R. Sahore, **K. G. Sprenger**, R. Tenent, M. Toney, W. Tong, L. Wan, C. Wang, B. Wu, Y. Xu, Assessing cathode-electrolyte interfaces in batteries, *Nature Energy* ('23 IF 49.8), 1-11 (2024), DOI: [10.1038/s41560-024-01639-y](https://doi.org/10.1038/s41560-024-01639-y).
13. **Emily R. Rhodes**<sup>#</sup>, Nicole B. Day<sup>#</sup>, **Emma C. Aldrich**, C. Wyatt Shields IV\*, **K.G. Sprenger\***, Enhanced macromolecular stabilization of cytokines in PLGA particles for improved bioactivity and delivery to tumor microenvironments, *Bioengineering & Translational Medicine* ('23 IF 7.8), e10722 (2024), DOI: [10.1002/btm2.10722](https://doi.org/10.1002/btm2.10722). **Featured on Journal Cover.**
14. **Daisy I. Fuchs**, **Lauren D. Serio**, **Sahana Balaji**, **K. G. Sprenger**, Investigating how HIV-1 Antiretrovirals Differentially Behave as Substrates and Inhibitors of P-glycoprotein via Molecular Dynamics Simulations, *Computational and Structural Biotechnology Journal* ('23 IF 4.4), 23, 2669–2679 (2024), DOI: [10.1016/j.csbj.2024.06.025](https://doi.org/10.1016/j.csbj.2024.06.025).
15. **Jonathan G. Faris**, Conor F. Hayes, Andre R. Goncalves, **K. G. Sprenger**, Daniel Faissol, Brenden K. Petersen, Mikel Landajuela, Felipe Leno da Silva, Pareto Front Training for Multi-Objective Symbolic Optimization,

*The Sixteenth Workshop on Adaptive and Learning Agents (ALA), at the International Conference on Autonomous Agents and Multiagent Systems (AAMAS)*, 2024, URL: <https://openreview.net/forum?id=e0gswuNjcb>.

16. E.Z.L. Zhong-Johnson, **Ziyue Dong**, Christopher Canova, Francesco Destro, Marina Cañellas, Mikaila C. Hoffman, Jeanne Maréchal, Timothy M. Johnson, Gabriela S. Schlau-Cohen, Maria Fátima Lucas, Richard D. Braatz, **K. G. Sprenger**, Christopher A. Voigt, Anthony J. Sinskey, Analysis of Poly(ethylene terephthalate) Degradation Kinetics of Evolved IsPETase Variants Using a Surface Crowding Model, *Journal of Biological Chemistry* ('23 IF 4.0), 300, 3, 105783 (2024), DOI: [10.1016/j.jbc.2024.105783](https://doi.org/10.1016/j.jbc.2024.105783).
17. **Emily R. Rhodes**, **Jonathan G. Faris**, **Brian M. Petersen**, **K. G. Sprenger**, Common Framework Mutations Impact Antibody Interfacial Dynamics and Flexibility, *Frontiers in Immunology* ('23 IF 5.7), 14, 1120582 (2023), DOI: [10.3389/fimmu.2023.1120582](https://doi.org/10.3389/fimmu.2023.1120582).
18. **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* ('23 IF 5.7), 13, 1029167 (2022), DOI: [10.3389/fimmu.2022.1029167](https://doi.org/10.3389/fimmu.2022.1029167).
19. Dean Oldham, Hong Wang, Juliet Mullen, **Emma E. 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* ('23 IF 2.8), 9, 926631 (2022), DOI: [10.3389/fcvm.2022.926631](https://doi.org/10.3389/fcvm.2022.926631).
20. 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* ('23 IF 3.8), 18, e1009391 (2022), DOI: [10.1371/journal.pcbi.1009391](https://doi.org/10.1371/journal.pcbi.1009391).
21. **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* ('23 IF 5.7), 12, 728694 (2021), DOI: [10.3389/fimmu.2021.728694](https://doi.org/10.3389/fimmu.2021.728694).
22. Irene Francino Urdaniz<sup>#</sup>, Paul J. Steiner<sup>#</sup>, Monica B. Kirby<sup>#</sup>, 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* ('23 IF 7.5), 36, 109627 (2021), DOI: [10.1016/j.celrep.2021.109627](https://doi.org/10.1016/j.celrep.2021.109627).

#### Postdoctoral Publications

23. Arup Chakraborty and **K. G. Sprenger**, Eliciting Potent Antibodies Against Highly Mutable Pathogens by Vaccination, *Physical Biology*, 18, 13-15 (2021), DOI: [10.1088/1478-3975/abde8d](https://doi.org/10.1088/1478-3975/abde8d).
24. **K. G. Sprenger\***, Joy Louveau\*, Pranav Murugan, Arup Chakraborty, Optimizing Immunization Protocols to Elicit Broadly Neutralizing Antibodies, *PNAS*, 117, 20077-20087 (2020), DOI: [10.1073/pnas.1919329117](https://doi.org/10.1073/pnas.1919329117).

#### Graduate Publications

25. **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*, 12, 10684–10688 (2021), DOI: [10.1021/acs.jpcllett.1c02757](https://doi.org/10.1021/acs.jpcllett.1c02757).
26. 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*, 142, 2355-2363 (2020), DOI: [10.1021/jacs.9b11617](https://doi.org/10.1021/jacs.9b11617).
27. 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).
28. 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*, 37, 8665-8674 (2018), DOI: [10.1021/acs.jpcb.8b05850](https://doi.org/10.1021/acs.jpcb.8b05850).
29. **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).



30. Arushi Prakash\*, K. G. Sprenger\*, Jim Pfaendtner, Essential Slow Degrees of Freedom in Protein-Surface Simulations: A Metadynamics Investigation, *Biochemical and Biophysical Research Communications*, 498, 274-281 (2018), DOI: [10.1016/j.bbrc.2017.07.066](https://doi.org/10.1016/j.bbrc.2017.07.066).
31. 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*, 121, 10793-10803 (2017), DOI: [10.1021/acs.jpcb.7b08435](https://doi.org/10.1021/acs.jpcb.7b08435).
32. 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*, 19, 17426-17433 (2017), DOI: [10.1039/C7CP03013D](https://doi.org/10.1039/C7CP03013D).
33. 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](https://doi.org/10.1116/1.4983154).
34. 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*, 236, 404-413 (2017), DOI: [10.1016/j.molliq.2017.04.027](https://doi.org/10.1016/j.molliq.2017.04.027).
35. 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](https://doi.org/10.1021/acs.langmuir.6b01296).
36. 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](https://doi.org/10.1016/bs.mie.2016.05.020).
37. 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).
38. 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*, 120, 3863-3872 (2016), DOI: [10.1021/acs.jpcb.6b01688](https://doi.org/10.1021/acs.jpcb.6b01688).
39. 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*, 119, 5882-5895 (2015), DOI: [10.1021/acs.jpcb.5b00689](https://doi.org/10.1021/acs.jpcb.5b00689).

## Invited Talks

1. TBD | Telluride Science Research Center (TSRC) Workshop “Molecular Engineering of Soft Matter: Spanning Small Molecules to Macromolecules” | Telluride, CO | May 2025.
2. TBD | NC State, Chemical & Biomolecular Engineering | Raleigh, NC | 28 Mar 2025.
3. TBD | Ohio University, Chemical & Biomolecular Engineering | Athens, OH | Spring 2025.
4. Leveraging Diverse Computational Tools and Approaches to Advance Molecular Understanding of Infectious and Neurological Diseases | *New Frontiers of Molecular Thermodynamics*, AIChE | San Diego, CA | Oct 2024.
5. Leveraging *In Silico* Approaches to Elucidate Molecular Interfaces for Sustainable Advancements in Bioplastics | *ACS Fall Meeting, Polymeric Materials: Science and Engineering (PMSE) & Computers in Chemistry (COMP) Division* | Denver, CO | Aug 2024.
6. Leveraging High-Performance Computing for Advancing Molecular Understanding of Infectious and Neurological Diseases | **Invited Keynote Speaker** | *Rocky Mountain Advanced Computing Consortium (RMACC) Symposium* | Boulder, CO | 21 May 2024.
7. Leveraging *In Silico* Approaches to Elucidate Molecular Interfaces for Sustainable Advancements in Bioplastics and Batteries | *Arizona State University, Chemical Engineering Department* | Tempe, AZ | 5 Apr 2024.
4. Moving the Needle: Employing Deep Learning to Push the Boundaries of Computational Vaccine Models | *University of Notre Dame, Chemical & Biomolecular Engineering Department* | Notre Dame, IN | 28 Nov 2023.

5. Design of vaccine components and protocols for inducing protective antibodies against HIV | *Biological Physics & Physical Biology (BPPB) seminar series* | Remote | 20 Oct 2023.
6. From Vaccines to Protein-Polymer Bioconjugates: A High-Throughput Computational Approach | *Colorado State University, Chemical and Biological Engineering Department* | Golden, CO | 5 Oct 2023.
7. From Vaccines to Protein-Polymer Bioconjugates: A High-Throughput Computational Approach | *Telluride Science Research Center (TSRC) Workshop on Molecular Engineering of Soft Matter* | Telluride, CO | 20 Jun 2023.
8. A High-Throughput Computational Approach for Designing Broadly-Neutralizing Antibodies Against Highly Mutable Pathogens | *InDevR* | Boulder, CO | 5 Jun 2023.
9. Moving the Needle: Employing Deep Learning to Push the Boundaries of Computational Vaccine Models | *Colorado School of Mines, Chemical and Biological Engineering Department* | Golden, CO | 21 Apr 2023.
10. A Holistic Computational Approach to Combatting HIV | *University of Colorado Boulder, BioFrontiers Institute* | 4 Dec 2022.
11. A Holistic Computational Approach to Combatting HIV | *AIChE Honorific Session: Arup Chakraborty's 60<sup>th</sup> Birthday* | Boston, MA | 9 Nov 2021.
12. A Seemingly Unstoppable Virus: Can Humanity Ever Overcome HIV? | *University of Colorado Boulder, College of Engineering & Applied Science Alumni Webinar* | Remote | 20 Oct 2021.
13. 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.
14. 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.
15. Design of vaccine components and protocols for inducing protective antibodies against HIV | *University of Louisville, Chemical Engineering Department* | Remote | 30 Oct 2020.
16. 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.
17. 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.**

## Teaching Experience

2023 – 2024	<b>Instructor</b>	BMEN 3010: Biotransport
2020 – 2024	<b>Co-Instructor</b>	CHEN 3210: Heat and Mass Transfer
2019	<b>Kaufman Teaching Certificate Program</b>	MIT Teaching and Learning Lab
2016	<b>Guest Lecturer on Molecular Simulations</b>	CHEM E 498: Special Topics   UW ChemE
2015	<b>Teaching Assistant</b>	CHEM E 435: Mass Transfer   UW ChemE
2014	<b>Guest Lecturer on ASPEN</b>	CHEM E 375: Computer Skills   UW ChemE
2014	<b>Guest Lecturer on Molecular Simulations</b>	CHEM E 525: Graduate Thermo   UW ChemE
2013	<b>Teaching Assistant</b>	CHEM E 437: ChemE Laboratory II   UW ChemE

## Mentoring Experience

### Current Graduate Students

2025 – Present	Ana Costa, Chemical Engineering Ph.D. Student
2024 – Present	Sahana Balaji, Biomedical Engineering M.S. Student
2024 – Present	Fahsai Nakarin, Biomedical Engineering Ph.D. Student (incoming M.S.)
2024 – Present	David Saeb, Chemical Engineering Ph.D. Student (incoming M.S.)
2023 – Present	Haley Teil, Biomedical Engineering Ph.D. Student
2023 – Present	Hannah Padgett, Biological Engineering Ph.D. Student
2022 – Present	Emma Aldrich, Biological Engineering Ph.D. Student   <i>Interdisciplinary Quantitative Biology Program</i>
2022 – Present	Rafael Ferreira de Menezes, Chemical Engineering Ph.D. Student   <i>Co-advised w/ Mike Toney, CU</i>

2021 – Present	Bailey Zinger, Biological Engineering Ph.D. Student   <i>Interdisciplinary Quantitative Biology Program</i>
2021 – Present	Emma Lietzke, Biological Engineering Ph.D. Student   <i>Co-advised w/ Kimberley Bruce, CU Anschutz</i>
2021 – Present	Travis Dong, Chemical Engineering Ph.D. Student   <i>Co-advised w/ Mike Toney, CU Boulder</i>
2020 – Present	Jonathan Faris, Biological Engineering Ph.D. Student
2020 – Present	Daisy Fuchs, Chemical Engineering Ph.D. Student

### Former Graduate Students

2020 – 2024	Emily Rhodes, Biological Engineering Ph.D.
2019 – 2024	Brian Petersen, Chemical Engineering Ph.D.   <i>Co-advised w/ Timothy Whitehead, CU Boulder</i>
2023 – 2024	David Saeb, ChBE Bachelor's-Accelerated M.S. (BAM) Program
2022 – 2023	Megan Makam, Biomedical Engineering M.S.

### Current Undergraduate Students

2024 – Present	Andrea Negulescu   Graduate Mentors: David Saeb and Hannah Padgette
2024 – Present	Andrew Hickman   Graduate Mentor: Rafael Ferreira de Menezes
2024 – Present	Aidan Magruder   Graduate Mentor: David Saeb   <i>Cher4U</i>
2024 – Present	Pedro Cintrón Baerga   Graduate Mentor: Travis Dong   <i>YSSRP (Best Poster Award)</i>
2024 – Present	Arianna McCarty   Graduate Mentor: N/A   <i>Senior Thesis, co-advised w/ Dr. Sarah Clark at CU Anschutz</i>
2024 – Present	Bethany Graylin   Graduate Mentor: Emma Lietzke
2024 – Present	Anna Broerman   Graduate Mentor: Hannah Padgette   <i>Cher4U, UROP, YSSRP, DLA</i>
2024 – Present	Lily Gayou   Graduate Mentor: Travis Dong   <i>UROP, DLA</i>
2024 – Present	Evan Wood   Graduate Mentor: David Saeb   <i>UROP, Senior Thesis</i>
2023 – Present	Julia Keefe   Graduate Mentor: Emma Aldrich   <i>DLA</i>

### Former Undergraduate Students

2023 – 2024	Krista Phommatha   Graduate Mentor: Emma Lietzke   <i>Senior Thesis, CEAS Research Award 2024</i>
2023 – 2024	Lauren Serio   Graduate Mentor: Daisy Fuchs   <i>DLA, BSI, CEAS Research Award 2024</i>
2022 – 2024	Aidan Wegner   Graduate Mentors: Jonathan Faris/Travis Dong   <i>DLA, UROP, BSI, Senior Thesis, CEAS Research Award 2024</i>
2022 – 2024	Jim Grady   Graduate Mentors: Jonathan Faris/Emily Rhodes   <i>Cher4U, DLA</i>
2022 – 2024	Sheridan Duncan   Graduate Mentor: Bailey Zinger
2022 – 2023	Nicola Wheeler   Graduate Mentor: Bailey Zinger
2022 – 2023	Abdulkadir Said   Graduate Mentor: Emily Rhodes
Summer 2022	Karson Chrispens   Graduate Mentor: Brian Petersen
2021 – 2023	David Saeb   Graduate Mentors: Emma Lietzke/Daisy Fuchs
2021 – 2023	Sahana Balaji   Graduate Mentor: Daisy Fuchs   <i>DLA, BSI</i>
2021 – 2023	Daniel Orbidan   Graduate Mentor: Jonathan Faris   <i>DLA, UROP</i>
2020 – 2023	Alex Pham   Graduate Mentor: N/A
2020 – 2022	Dan Heher   Graduate Mentor: N/A

### External Leadership/Service Activities

5/2025	<b>Programming Committee</b>	The Seventeenth Workshop on Adaptive and Learning Agents
3/2025	<b>Panel Member</b>	NSF
2024 – 2027	<b>Committee Member</b>	Area 1a Programming Committee   AIChE (3-year term)
2024	<b>Session Co-Chair</b>	System Biology: Cancer and Immunoengineering   Div 15D   AIChE
2024	<b>Session Co-Chair</b>	Recent Advances in Multiscale Methodologies   CoMSEF   AIChE
2024	<b>Session Co-Chair</b>	Biomolecular Simulations   FOMMS Conference   Sponsored by AIChE
2024	<b>Panel Member</b>	NIH
2024	<b>Panel Member</b>	NSF
2023 – 2024	<b>Panel Member</b>	NIH
2023	<b>Panel Member</b>	NSF
2023	<b>Symposium Co-organizer</b>	EU-US Frontiers of Engineering   Computational Era of Life Sciences
2023	<b>Session Chair</b>	Recent Advances in Multiscale Methodologies   CoMSEF   AIChE
2023	<b>Session Chair</b>	TSRC Workshop on Molecular Engineering of Soft Matter   Telluride, CO

2021 – 2023	<b>Session Co-Chair</b>	Cell and Tissue Engineering   AIChE
2021 – 2023	<b>Session Co-Chair</b>	CoMSEF Poster Session   AIChE
2022	<b>Panel Member</b>	NIH
2022	<b>Session Chair</b>	Recent Advances in Multiscale Methodologies   CoMSEF   AIChE
2022	<b>Session Chair</b>	Arup Chakraborty's 60 <sup>th</sup> Celebration Symposium   Boston, MA
2022	<b>Guest Editor</b>	eLife
2020 – 2022	<b>Liaison Director</b>	CoMSEF   AIChE
2020 – 2022	<b>Committee Member</b>	National Academies of Sciences, Engineering, & Medicine <i>Proposal Evaluation for Allocation of Supercomputing Time for the Study of Molecular Dynamics, 11<sup>th</sup>-13<sup>th</sup> Rounds</i>
2020 – 2021	<b>Reviewer</b>	NSF Graduate Research Fellowship Program
2021	<b>Session Co-Chair</b>	Recent Advances in Multiscale Methodologies   CoMSEF   AIChE
2021	<b>Session Co-Chair</b>	Protein Aggregation and Immunogenicity   ACS
2017 – Present	<b>Journal Reviewer</b>	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 & Eng, Journal of Chemical Information & Modeling, Langmuir, Biomolecules

### Internal Leadership/Service Activities at CU Boulder

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2025	<b>Committee Member</b>	IQ Biology Admissions Committee   ChBE Representative
2024	<b>Thrust Lead</b>	NSF REU Site Proposal: Team Biomolecular Biomaterials
2024	<b>Steering Committee</b>	T32 Biophysics Program
2024	<b>Interviewer</b>	IQ Biology Graduate Admissions
2024 – Present	<b>Faculty Director for Engagement</b>	ChBE Department
2023 – Present	<b>Committee Member</b>	Executive Committee   ChBE Department
2021 – Present	<b>Committee Member</b>	Leadership Committee   ChBE Department
2020 – Present	<b>Committee Member</b>	Engagement Committee   ChBE Department
2023	<b>Committee Member</b>	Chair Search Committee   ChBE Department
2022 – 2023	<b>Organizer</b>	Departmental Patten Seminar Series   ChBE Department
2022 – 2023	<b>Workshop Organizer/Presenter</b>	PI Academy, Time Management for new CU faculty members   CU Boulder
2021 – 2023	<b>Co-Organizer</b>	NSF GRFP/NDSEG Grad Student Workshop   ChBE Department
2022 – 2023	<b>Faculty Host/Participant</b>	RCR: Mentor/Trainee Issues   CU Boulder
2021 – 2022	<b>Reviewer</b>	Graduate Student Awards   ChBE Department
2020 – 2022	<b>Reviewer</b>	AB Nexus Seed Grants   CU Boulder/Anschutz
2022	<b>Committee Member</b>	CHEN/BIEN Quantitative Training/Curriculum Development   ChBE Department
2022	<b>Participant</b>	CHEN Recruitment Video (energy)   ChBE Department
2021	<b>Co-Organizer</b>	Departmental Patten Seminar Series   ChBE Department
2020 – 2021	<b>Committee Member</b>	Faculty Search Committee   ChBE Department

### Outreach Activities

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