

Reid C. Van Lehn

Curriculum Vitae, January 2025

Room 3012, 1415 Engineering Drive, Madison WI, 53706-1607
(608) 263 9487 – vanlehn@wisc.edu – <http://vanlehngroup.che.wisc.edu/>

Professional Appointments

University of Wisconsin-Madison

<i>Hunt-Hougen Associate Professor in the Department of Chemical and Biological Engineering</i>	2022 – Present
<i>Associate Professor in the Department of Chemistry (By Courtesy)</i>	2023 – Present
<i>Conway Assistant Professor in the Department of Chemical and Biological Engineering</i>	2016 – 2022
<i>Faculty Trainer for Biophysics Graduate Program</i>	2016 – Present
<i>Faculty Trainer for Chemistry-Biology Interface Training Program</i>	2017 – Present
<i>Faculty Trainer for Biotechnology Training Program</i>	2018 – Present
<i>Co-Investigator, Great Lakes Bioenergy Research Center</i>	2018 – Present

Professional Preparation

California Institute of Technology <i>Postdoctoral Scholar in the Division of Chemistry and Chemical Engineering</i> Advisor: Thomas F. Miller III	2015 – 2016
Massachusetts Institute of Technology <i>Postdoctoral Associate in the Department of Materials Science and Engineering</i> Advisor: Alfredo Alexander-Katz	2014 – 2015
Massachusetts Institute of Technology <i>Ph.D. in Materials Science and Engineering, Minor in Teaching</i> Thesis: “Interactions of Environmentally-Responsive Nanoparticles with Synthetic and Biological Membranes” Advisor: Alfredo Alexander-Katz	2009 – 2014
Massachusetts Institute of Technology <i>B.S. in Materials Science and Engineering</i>	2005 – 2009

Honors and Awards

Benjamin Smith Reynolds Award for Excellence in Teaching from the UW-Madison College of Engineering	2024
Named the Hunt-Hougen Associate Professor in the Dept. of Chemical and Biological Engineering	2022
AIChE CoMSEF Young Investigator Award for Modeling & Simulation	2021
Named University of Wisconsin-Madison Vilas Associate	2021
NSF CAREER Award	2021
3M Non-Tenured Faculty Award	2020
Named the Conway Assistant Professor in the Department of Chemical and Biological Engineering	2019
Named the Jay and Cynthia Ihlenfeld Faculty Scholar in the College of Engineering	2016
Named to Forbes 30 Under 30 in Science List	2016
National Institutes of Health Ruth-Kirschstein F32 Postdoctoral Fellowship	2015
Materials Research Society Graduate Student Award, Gold Medal Winner	2013
John Wulff Award for Excellence in Teaching an Undergraduate Subject (awarded by MIT Dept. of Mat. Sci.)	2013
National Science Foundation Graduate Research Fellowship	2010
Robert Rose Presidential Fellowship (awarded by MIT Office of the Provost)	2009

Publications

* indicates corresponding author(s), ^ indicates equal contributions

As Independent Investigator at UW-Madison

1. Z Xu, K Sanchez-Rivera, C Granger, P Zhou, AC Munguia-Lopez, UM Ikegwu, S Avraamidou, VM Zavala, **RC Van Lehn**, E Bar-Ziv, S De Meester, GW Huber*. “Solvent-based plastic recycling technologies.” *Nature Chemical*

Engineering, in revision.

2. T Yan, C Granger, KL Sanchez-Rivera, P Zhou, S Grey, K Nelson, F Long, E Bar-Ziv, **RC Van Lehn**, S Avraamidou, GW Huber*. "Pigment Removal from Reverse-Printed Laminated Flexible Films by Solvent-Targeted Recovery and Precipitation." *Science Advances*, **in revision**.
3. B Park and **RC Van Lehn***. "Mechanistic and thermodynamic characterization of dynamic topology in an unassembled transmembrane protein." *ChemRxiv*, **preprint**; *Journal of Physical Chemistry B*, **in revision**.
4. DH Chang[^], JD Richardson[^], M Lee, DM Lynn*, SP Palecek*, **RC Van Lehn***. Machine Learning-Driven Discovery of Highly Selective Antifungal Peptides Containing Non-Canonical β -Amino Acids." *ChemRxiv*, **preprint**; *Chemical Science*, **in revision**.
5. KL Sanchez-Rivera, P Zhou, E Radkevich, A Sharma, E Bar-Ziv, **RC Van Lehn**, GW Huber*. "A solvent-targeted recovery and precipitation scheme for the recycling of up to ten polymers from post-industrial mixed plastic waste." *Waste Management*, **accepted**.
6. L Fuller, G Zhang, S Noh, **RC Van Lehn**, M Schreier*. "Electrolyte Anions Suppress Hydrogen Generation in Electrochemical CO Reduction on Cu." *Angewandte Chemie*, **accepted**.
7. CA Huang and **RC Van Lehn***. "Influence of branched ligand architectures on nanoparticle interactions with lipid bilayers." *Nanoscale*, **2025**, *17*, 1659-1672.
8. S Qin, S Omolabake, A Diaby, J Li, LD Gonzalez, CM Holland, VM Zavala, SS Stahl*, **RC Van Lehn***. "Identifying Green Solvent Mixtures for Bioproduct Separation Using Bayesian Experimental Design." *ACS Sustainable Chemistry & Engineering*, **2024**, *12* (52), 18634-18647.
9. AC Munguia-Lopez, P Zhou, UM Ikegwu, **RC Van Lehn**, and VM Zavala*. "A fast computational framework for the design of solvent-based plastic recycling processes." *LAPSE (FOCAPD 2024 Conference Proceedings)*, **2024**, 1612.
10. UM Ikegwu, VM Zavala, and **RC Van Lehn***. "Screening Green Solvents for Multilayer Plastic Films Separation." *LAPSE (FOCAPD 2024 Conference Proceedings)*, **2024**, 1605.
11. J Li and **RC Van Lehn***. "Effects of acid dissociation and ionic solutions on the aggregation of 2-pyrone-4,6-dicarboxylic acid." *ACS Omega*, **2024**, *9* (39), 40759-40768. PMC11447750.
12. JD Richardson and **RC Van Lehn***. "Free Energy Analysis of Peptide-Induced Pore Formation in Lipid Membranes by Bridging Atomistic and Coarse-Grained Simulations." *Journal of Physical Chemistry B*, **2024**, *128* (36), 8737-8752.
13. S Jiang, S Qin, **RC Van Lehn**, P Balaprakash, VM Zavala*. "Uncertainty quantification for molecular property predictions with graph neural architecture search." *Digital Discovery*, **2024**, *3*, 1534-1553.
14. KL Sanchez-Rivera, C Granger, H Appiah, K Nelson, S Grey, D Sun, JE Garcia, E Chen, Z Xu, TA Osswald, L-S Turng, A McDonald, **RC Van Lehn**, E Bar-Ziv, GW Huber*. "Cast film production with polyethylene recycled from a post-industrial printed multilayer film by solvent-targeted recovery and precipitation." *ACS Materials Letters*, **2024**, *6* (9), 4042-4050.
15. A Marzouq[^], L Morgenstein[^], CA Huang-Zhu[^], S Yudovich, A Atkins, A Grupi, **RC Van Lehn***, S Weiss*. "Long-chain lipids facilitate insertion of large nanoparticles into membranes of small unilamellar vesicles." *Langmuir*, **2024**, *40* (20), 10477-10485.
16. CL Bassini, G van Anders, U Banin, D Baranov, Q Chen, M Dijkstra, MS Dimitriyev, E Efati, J Faraudo, O Gang, N Gaston, R Golestanian, GI Guerrero-Garcia, M Gruenwald, A Haji-Akbari, M Ibanez, M Karg, T Kraus, B Lee, **RC Van Lehn**, RJ Macfarlane, BM Mognetti, A Nikoubashman, S Osat, OV Prezhdo, GM Rotskoff, L Saiz, A Shi, S Skrabalak, II Smalyukh, M Tagliazucchi, DV Talapin, AV Tkachenko, S Tretiak, D Vaknin, A Widmer-Cooper, GCL Wong, X Ye, S Zhou, E Rabani, M Engel, A Travesset*. "Nanocrystal Assemblies: Current Advances and Open Problems." *ACS Nano*, **2024**, *18* (23), 14791-14840.
17. J Li, **RC Van Lehn**, CT Maravelias*. "An Explainable Classification Framework for Determining and Understanding Extraction Suitability." *ACS Sustainable Chemistry & Engineering*, **2024**, *12* (14), 5436-5446.
18. E Bar-Ziv, S Kolapkar, GW Huber, **RC Van Lehn**. "A novel solvent-based recycling technology: From theory to pilot plant." *Technology Innovation for the Circular Economy: Recycling, Remanufacturing, Design, Systems Analysis and Logistics*, **2024**, 477-495.
19. CA Huang-Zhu[^], JK Sheavly[^], AK Chew, SJ Patel, **RC Van Lehn***. "Ligand Lipophilicity Determines Molecular Mechanisms of Nanoparticle Adsorption to Lipid Bilayers." *ACS Nano*, **2024**, *18* (8), 6424-6437.
20. X Cui, P Zhou, Z Xu, Q Liu, Y Nuli, J Wang, **RC Van Lehn**, J Yang*. "High-Voltage Li Metal Batteries Enabled by A

- Nonflammable Amphiphilic Electrolyte.” *Energy Storage Materials*, **2024**, 66, 103235.
21. JI Gold, JK Sheavly, N Bao, H Yu, JJ Schauer, VM Zavala, NL Abbott*, **RC Van Lehn***, M Mavrikakis*. “Combining First Principles Calculations and Classical Molecular Dynamics Simulations to Predict the Anchoring Behavior of Liquid Crystal Mixtures.” *ACS Nano*, **2023**, 17 (22), 22620-22631.
 22. F Wang, S Qin, C Acevedo-Velez, **RC Van Lehn**, VM Zavala*, DM Lynn*. “Decoding Optical Responses of Contact-Printed Arrays of Thermotropic Liquid Crystals Using Machine Learning: Detection and Reporting of Aqueous Amphiphiles with Enhanced Sensitivity and Selectivity.” *ACS Applied Materials and Interfaces*, **2023**, 15 (43), 50532-50545.
 23. S Jiang, N Bao, AD Smith, S Byndoor, **RC Van Lehn**, M Mavrikakis, NL Abbott, VM Zavala*. “Scalable Extraction of Information from Spatio-Temporal Patterns of Chemoresponsive Liquid Crystals Using Topological Descriptors.” *Journal of Physical Chemistry C*, **2023**, 127 (32), 16081-16098.
 24. P Zhou, J Yu, KL Sanchez-Rivera, GW Huber, **RC Van Lehn***. “Large-scale computational polymer solubility predictions and applications to dissolution-based plastic recycling.” *Green Chemistry*, **2023**, 25, 4002-4014.
 25. KL Sanchez-Rivera, A del Carmen Munguia-Lopez, P Zhou, VS Cecon, J Yu, K Nelson, D Miller, S Grey, Z Xu, E Bar-Ziv, KL Vorst, GW Curtzwiler, **RC Van Lehn**, VM Zavala, GW Huber*. “Recycling of a post-industrial printed multilayer plastic packaging film containing polyurethane inks by solvent-targeted recovery and precipitation.” *Resources, Conservation & Recycling*, **2023**, 197, 107086.
 26. AD Smith, S Runde, AK Chew, AS Kelkar, U Maheshwari, **RC Van Lehn**, VM Zavala*. “Topological analysis of molecular dynamics simulations using the Euler Characteristic.” *Journal of Chemical Theory and Computation*, **2023**, 19 (5), 1553-1567.
 27. S Qin, S Jiang, J Li, P Balaprakash, **RC Van Lehn**, VM Zavala*. “Capturing molecular interactions in graph neural networks: A case study in multi-component phase equilibrium.” *Digital Discovery*, **2023**, 2, 138-151.
 28. BC Dallin, AS Kelkar, **RC Van Lehn***. “Structural features of interfacial water predict the hydrophobicity of chemically heterogeneous surfaces.” *Chemical Science*, **2023**, 14, 1308-1319.
 29. CG Gahan, **RC Van Lehn**, HE Blackwell, DM Lynn*. Interactions of bacterial quorum sensing signals with model lipid membranes: Influence of membrane composition on membrane remodeling.” *Langmuir*, **2023**, 39 (1), 295-307.
 30. Z Sumer, **RC Van Lehn***. “Heuristic computational model for predicting lignin solubility in tailored organic solvents.” *ACS Sustainable Chemistry & Engineering*, **2023**, 11 (1), 187-198.
 31. RG Dastidar, MS Kim, P Zhou, Z Luo, C Shi, KJ Barnett, DJ McClelland, EYX Chen, **RC Van Lehn**, GW Huber*. Catalytic production of tetrahydropyran (THP): A biomass-derived, economically competitive solvent with demonstrated use in plastic dissolution.” *Green Chemistry*, **2022**, 24, 9101-9113.
Highlighted by editors as a Green Chemistry HOT manuscript in 2022.
 32. H Li, H Aguirre-Villegas, RD Allen, X Bai, CH Benson, GT Beckham, SL Bradshaw, JL Brown, MA Sanchez Castillo, VS Cecon, JB Curley, GW Curtzwiler, S Dong, S Gaddameedi, JE Garcia, I Hermans, MS Kim, J Ma, LO Mark, M Mavrikakis, OO Olafasakin, TA Osswald, KG Papanikolaou, H Radhakrishnan, KL Sanchez-Rivera, KN Tuma, **RC Van Lehn**, KL Vorst, MM Wright, J Wu, VM Zavala, P Zhou, GW Huber*. “Expanding plastics recycling technologies: Chemical aspects, technology status, and challenges.” *Green Chemistry*, **2022**, 24, 8899-9002.
 33. J Morstein*, A Capecchi[^], K Hinnah[^], B Park[^], J Petit-Jacques, **RC Van Lehn**, J-L Reymond, D Trauner. “Medium-chain lipid conjugation facilitates cell-permeability and bioactivity.” *Journal of the American Chemical Society*, **2022**, 144 (40), 18532-18544.
Highlighted in commentaries by Nature (<https://www.nature.com/articles/d41586-022-03282-7>) and Science (<https://www.science.org/content/blog-post/greasing-your-way-cells>)
 34. Z Sumer, **RC Van Lehn***. “Data-centric development of lignin structure – solubility relationships in deep eutectic solvents using molecular simulations.” *ACS Sustainable Chemistry & Engineering*, **2022**, 10 (31), 10144-10156.
 35. N Bao, S Jiang, AD Smith, JJ Schauer, M Mavrikakis, **RC Van Lehn**, VM Zavala*, NL Abbott*. “Sensing gas mixtures by analyzing the spatiotemporal optical responses of liquid crystals using 3D convolutional neural networks.” *ACS Sensors*, **2022**, 7 (9), 2545-2555.
 36. N Bao, JL Gold, JK Sheavly, JJ Schauer, VM Zavala, **RC Van Lehn**, M Mavrikakis, NL Abbott*. “Ordering transitions of liquid crystals triggered by metal oxide-catalyzed reactions of sulfur oxide species.” *Journal of the American Chemical Society*, **2022**, 144 (36), 16378-16388.

37. Z Shen, JH Dwyer, J Sun, KR Jenkins, MS Arnold, P Gopalan, **RC Van Lehn***. "A simple simulation-derived descriptor for the deposition of polymer-wrapped carbon nanotubes on functionalized substrates." *Soft Matter*, **2022**, *18*, 4653-4659.
38. J Li, CT Maravelias, **RC Van Lehn***. "Adaptive conformer sampling for property prediction using the Conductor-Like Screening Model for Real Solvents." *Industrial & Engineering Chemistry Research*, **2022**, *61* (25), 9025-9036.
39. AK Chew, JA Pedersen, **RC Van Lehn***. "Predicting the physicochemical properties and biological activities of monolayer-protected gold nanoparticles using simulation-derived descriptors." *ACS Nano*, **2022**, *16* (4), 6282-6292.
40. L Je, GW Huber, **RC Van Lehn**, VM Zavala*. "On the integration of molecular dynamics, data science, and experiments for studying solvent effects on catalysis." *Current Opinion in Chemical Engineering*, **2022**, *36*, 100796.
41. AS Kelkar, BC Dallin, **RC Van Lehn***. "Identifying nonadditive contributions to the hydrophobicity of chemically heterogeneous surfaces via dual-loop active learning." *Journal of Chemical Physics*, **2022**, *156*, 024701.
42. CG Gahan, **RC Van Lehn***, HE Blackwell*, DM Lynn*. "Interactions of bacterial quorum sensing signals with model lipid membranes: Influence of acyl tail structure on multi-scale response." *Langmuir*, **2021**, *37* (41), 12049-12058.
43. S Qin, T Jin, **RC Van Lehn***, VM Zavala*. "Predicting critical micelle concentrations for surfactants using graph convolutional neural networks." *J Phys Chem B*, **2021**, *125*, 10610-10620.
44. P Zhou, KL Sánchez-Rivera, GW Huber, **RC Van Lehn***. "Computational approach for rapidly predicting temperature-dependent polymer solubilities using molecular-scale models." *ChemSusChem*, **2021**, *14* (9), 4307-4316.
45. KL Sánchez-Rivera, P Zhou, MS Kim, LD González Chávez, S Grey, K Nelson, S-C Wang, I Hermans, VM Zavala, **RC Van Lehn**, GW Huber*. "Reducing Antisolvent Use in the STRAP Process by Enabling a Temperature-Controlled Polymer Dissolution and Precipitation for the Recycling of Multilayer Plastic Films." *ChemSusChem*, **2021**, *14* (9), 4317-4329.
46. CG Gahan, SJ Patel, LM Chen, DE Manson, ZJ Ehmer, HE Blackwell*, **RC Van Lehn***, DM Lynn*. "Bacterial quorum sensing signals promote large-scale remodeling of lipid membranes." *Langmuir*, **2021**, *35* (30), 9120-9136.
47. SJ Patel, **RC Van Lehn***. "Analysis of charged peptide loop-flipping across a lipid bilayer using the string method with swarms-of-trajectories." *Journal of Physical Chemistry B*, **2021**, *125* (22), 5862-5873.
48. CA Lochbaum[^], AK Chew[^], X Zhang, VM Rotello, **RC Van Lehn***, JA Pedersen*. "The lipophilicity of cationic ligands promotes irreversible adsorption of nanoparticles to lipid bilayers." *ACS Nano*, **2021**, *15*, 6562-6572.
49. AK Chew, BC Dallin, **RC Van Lehn***. "The interplay of ligand properties and core size dictates the hydrophobicity of monolayer-protected gold nanoparticles." *ACS Nano*, **2021**, *15* (3), 4534-4545.
50. BM Hoover, Z Shen, CG Gahan, DM Lynn, **RC Van Lehn**, RM Murphy*. "Membrane remodeling and simulation of aggregation following α -synuclein adsorption to phosphatidylserine vesicles." *Journal of Physical Chemistry B*, **2021**, *125* (6), 1582-1594.
51. T Jin, SJ Patel, **RC Van Lehn***. "Molecular simulations of lipid membrane partitioning and translocation by bacterial quorum sensing modulators." *PLoS ONE*, **2021**, *16* (2), e0246187.
52. TW Walker, N Frelka, Z Shen, AK Chew, J Bannick, S Grey, MS Kim, JA Dumesic, **RC Van Lehn**, GW Huber*. "Recycling of multilayer plastic packaging materials by solvent-targeted recovery and precipitation." *Science Advances*, **2020**, *6* (47), eaba7599.

Featured by UW-Madison and popular press: <https://news.wisc.edu/new-solvent-based-recycling-process-could-cut-down-on-millions-of-tons-of-plastic-waste/>

53. AK Chew, S Jiang, W Zhang, VM Zavala, **RC Van Lehn***. "Fast predictions of liquid-phase acid-catalyzed reaction rates using molecular dynamics simulations and convolutional neural networks." *Chemical Science*, **2020**, *11*, 12464-12476.
54. AS Kelkar, BC Dallin, **RC Van Lehn***. "Predicting hydrophobicity by learning spatiotemporal features of interfacial water structure: Combining molecular dynamics simulations with convolutional neural networks." *Journal of Physical Chemistry B*, **2020**, *124* (41), 9103-9114.
55. JK Sheavly, **RC Van Lehn***. "Bilayer-mediated assembly of cationic nanoparticles adsorbed to lipid bilayers: Insights from molecular simulations." *AIChE Journal*, **2020**, *66* (12), e16993.

Included as part of the 2020 Futures issue.

56. CG Gahan[^], SJ Patel[^], ME Boursier, KE Nyffeler, J Jennings, NL Abbott, HE Blackwell*, **RC Van Lehn***, DM Lynn*.

- “Gram-negative bacterial quorum sensing signals self-assemble in aqueous media to form micelles and vesicles: an integrated experimental and molecular dynamics study.” *Journal of Physical Chemistry B*, **2020**, 124 (18), 3616-3628.
57. TW Walker[^], AK Chew[^], **RC Van Lehn**, JA Dumesic, GW Huber*. “Rational design of mixed solvent systems for acid-catalyzed biomass conversion processes using a combined experimental, molecular dynamics and machine learning approach.” *Topics in Catalysis*, **2020**, 63, 649-663.
58. Z Shen, **RC Van Lehn***. “Solvent selection for the separation of lignin-derived monomers using the Conductor-like Screening Model for Real Solvents.” *Industrial & Engineering Chemical Research*, **2020**, 59 (16), 7755-7764.
- Highlighted by the Great Lakes Bioenergy Research Center: <https://www.glbrc.org/research/highlights/using-modeling-determine-best-solvents-lignin-product-separations>*
59. AK Chew[^], TW Walker[^], Z Shen, B Demir, L Witterman, J Euclide, GW Huber, JA Dumesic, **RC Van Lehn***. “Effect of mixed-solvent environments on the selectivity of acid-catalyzed reactions.” *ACS Catalysis*, **2020**, 10, 1679-1691.
60. JK Sheavly, JI Gold, M Mavrikakis, **RC Van Lehn***. “Molecular simulations of analyte partitioning and diffusion in liquid crystal sensors.” *Molecular Systems Design & Engineering*, **2020**, 5, 304-316.
- Invited contribution to the 2020 Emerging Investigators issue; highlighted by editors as HOT article.*
61. JH Dwyer, Z Shen, KR Jenkins, W Wei, MS Arnold, **RC Van Lehn***, P Gopalan*. “Solvent-mediated affinity of polymer-wrapped single-walled carbon nanotubes for chemically modified surfaces.” *Langmuir*, **2019**, 35, 12492.
62. BC Dallin, **RC Van Lehn***. “Spatially heterogeneous water properties at disordered surfaces decrease the hydrophobicity of nonpolar self-assembled monolayers.” *Journal of Physical Chemistry Letters*, **2019**, 10, 3991.
63. AK Chew, **RC Van Lehn***. “Quantifying the stability of the hydronium ion in organic solvents with molecular dynamics simulations.” *Frontiers in Chemistry*, **2019**, 7, 439.
- Included as part of “Rising Stars” collection*
64. JK Sheavly, JA Pedersen, **RC Van Lehn***. “Curvature-driven adsorption of cationic nanoparticles to phase boundaries in multicomponent lipid bilayers.” *Nanoscale*, **2019**, 11, 2767.
65. BC Dallin, H Yeon, AR Ostwalt, NL Abbott, **RC Van Lehn***. “Molecular order affects interfacial water structure and temperature-dependent hydrophobic interactions between nonpolar self-assembled monolayers.” *Langmuir*, **2019**, 35(6), 2078-2088.
66. AK Chew, **RC Van Lehn***. “Effect of core morphology on the structural asymmetry of alkanethiol monolayer-protected gold nanoparticles.” *Journal of Physical Chemistry C*, **2018**, 122(45), 26288-26297.
67. SJ Patel, **RC Van Lehn***. “Characterizing the molecular mechanisms for flipping charged peptide flanking loops across a lipid bilayer.” *Journal of Physical Chemistry B*, **2018**, 122(45), 10337-10348.
68. A Alexander-Katz, **RC Van Lehn***. “Perspective: Random copolymers that protect proteins.” *Science*, **2018**, 359, 1216-1217.
69. TW Walker[^], AK Chew[^], H Li, B Demir, ZC Zhang, GW Huber, **RC Van Lehn***, JA Dumesic*. “Universal kinetic solvent effects in acid-catalyzed reactions of biomass-derived oxygenates.” *Energy & Environmental Science*, **2018**, 11, 617-628.
- Highlighted by editors as a HOT manuscript in 2018.*
70. M Werner, T Auth, P Beales, JB Fleury, F Hook, H Kress, **RC Van Lehn**, M Muller, E Petrov, L Sarkisov, J-U Sommer, VA Baulin. “Nanomaterial interactions with biomembranes: Bridging the gap between soft matter models and biological context.” *Biointerphases*, **2018**, 13, 028501.
71. H Yeon, C Wang, **RC Van Lehn**, NL Abbott. “Influence of order within non-polar monolayers on hydrophobic interactions.” *Langmuir*, **2017**, 33, 4628-4637.
- Prior to UW-Madison*
72. **RC Van Lehn**, A Alexander-Katz. “Energy landscape for insertion of amphiphilic nanoparticles into lipid membranes: a computational study.” *PLoS One*, **2019**, 14(1), e0209492.
73. PU Atukorale, DS Yun, **RC Van Lehn**, RP Carney, A Bekdemir, PHJ Silva, A Alexander-Katz, F Stellacci, DJ Irvine. “A study of amphiphilic gold nanoparticle design characteristics and bilayer properties that govern interaction with membranes.” *Bioconjugate Chemistry*, **2018**, 29, 1131-1140.
74. MJM Niesen, CY Wang, **RC Van Lehn**, TF Miller III. “Structurally detailed coarse-grained model for Sec-facilitated

- co-translational protein translocation and membrane integration." *PLoS Computational Biology*, **2017**, *13*, e1005427.
75. **RC Van Lehn**, A Alexander-Katz. "Grafting charged species to membrane-embedded scaffolds dramatically increases the rate of bilayer translocation." *ACS Central Science* **2017**, *3*, 185.
 76. M Tahir, **RC Van Lehn**, SH Choi, A Alexander-Katz. "Solvent-exposed lipid tail protrusions depend on lipid membrane composition and curvature." *BBA Biomembranes* **2016**, *1858*, 1207.
 77. **RC Van Lehn**, B Zhang, TF Miller III. "Regulation of multispanning membrane protein topology by post-translational annealing." *eLife* **2015**, *4*, e08697.
- Highlighted with a commentary by Stephen White*
78. **RC Van Lehn**, A Alexander-Katz. "Pathway for insertion of amphiphilic nanoparticles into defect-free lipid bilayers from atomistic molecular dynamics simulations." *Soft Matter* **2015**, *11*, 3165.
 79. **RC Van Lehn**, A Alexander-Katz. "Membrane-embedded nanoparticles induce lipid rearrangements similar to those exhibited by biological membrane proteins." *The Journal of Physical Chemistry B* **2014**, *118*, 12586.
 80. **RC Van Lehn**[^], M Ricci[^], PHJ Silva, P Andreozzi, J Reguera, K Voitchovsky, F Stellacci, A Alexander-Katz. "Lipid tail protrusions mediate the insertion of nanoparticles into model cell membranes." *Nature Communications* **2014**, *5*, 4482.
 81. **RC Van Lehn**, A Alexander-Katz, "Fusion of ligand-coated nanoparticles with lipid bilayers: Effect of ligand flexibility." *Journal of Physical Chemistry A* **2014**, *118*, 5848.
 82. **RC Van Lehn**, A Alexander-Katz, "Free energy change for insertion of charged, monolayer-protected nanoparticles into lipid bilayers." *Soft Matter* **2014**, *10*, 648.
 83. **RC Van Lehn**, A Alexander-Katz, "Structure of mixed-monolayer-protected gold nanoparticles in aqueous salt solution from atomistic molecular dynamics simulations." *Journal of Physical Chemistry C* **2013**, *117*, 20104.
 84. **RC Van Lehn**, PU Atukorale, RP Carney, Y-S Yang, F Stellacci, DJ Irvine, A Alexander-Katz, "Effect of particle diameter and surface composition on the spontaneous fusion of monolayer-protected gold nanoparticles with lipid bilayers." *Nano Letters* **2013**, *13*, 4060.
 85. **RC Van Lehn**, A Alexander-Katz, "Ligand-mediated short-range attraction drives aggregation of charged monolayer-protected gold nanoparticles." *Langmuir* **2013**, *29*, 8788.
 86. **RC Van Lehn**, A Alexander-Katz, "Penetration of lipid bilayers by nanoparticles with environmentally-responsive surfaces: simulations and theory." *Soft Matter* **2011**, *7*, 11392.
 87. **RC Van Lehn**, A Alexander-Katz, "Lateral phase separation of mixed polymer brushes physisorbed on planar substrates." *Journal of Chemical Physics* **2011**, *135*, 141106.
 88. **RC Van Lehn**, CE Sing, H Chen, A Alexander-Katz. "Multidimensional targeting: using physical and chemical forces in unison." *Current Pharmaceutical Biotechnology* **2010**, *11*, 320.

Extramural Funding

Current

American Chemical Society Green Chemistry Institute – Pharmaceutical Roundtable Grant – Van Lehn (PI)
 "Data-Driven Replacement of Halogenated Solvents by Green Solvent Mixtures"
 10/1/2024-09/30/2025 Total (to Van Lehn): \$80,000

Cytiva – Huber (PI)
 "Assessing the Viability of STRAP Technology as an Effective and Economical End-of-Life Process for Select Cytiva Products"
 12/18/2023-12/17/2025 Total (to Van Lehn): \$123,520

DOE (BER) – GLBRC – Donohue (PI)
 "Molecular Modeling of Solvent Effects in Biomass Conversion"
 12/1/2023-11/30/2028 Total (to Van Lehn): \$129,077/yr

DOE (EERE) – BETO – Huber (PI)

“Multi-University Center on Chemical Upcycling of Waste Plastics (CUWP)”

6/1/2021-5/31/2026

Total (to Van Lehn): \$440,558

NIH (NIDDK) – R01 – Rotello (PI)

“Point of Care Diagnostics for Liver Disease using Fluorescent Nanosensors”

9/17/2024-9/16/2028

Total (to Van Lehn): \$231,481

NSF – DMR – Condensed Matter and Materials Theory – Van Lehn (PI)

“CAREER: Molecular and Data-Centric Modeling of Cell-Penetrating Nanoparticles”

3/15/2021-3/14/2025

Total (to Van Lehn): \$581,212

NSF – CBET – Condensed Matter and Materials Theory – Van Lehn (PI)

“Collaborative Research: Integrating Simulations, Experiments, and Machine Learning to Understand and Design Hydrophobic Interactions”

8/01/2023-7/31/2026

Total (to Van Lehn): \$296,970

NSF – CBET – Computation and Data-Enabled Science and Engineering – Van Lehn (PI)

“CDS&E: Combining Molecular Simulations and Topological Data Analysis to Predict Nanoparticle-Protein Interactions”

9/01/2024-8/31/2027

Total (to Van Lehn): \$193,056

Schmidt Sciences – Virtual Institutes for Future Feedstocks – Huber (PI)

“Converting Inconsistent and Heterogenous Biomass and Municipal Solid Wastes into Demineralized and Uniform Feedstocks for Thermal-Catalytic Processing to Low Carbon Fuels, Chemicals, and Materials”

5/01/2024-4/30/2029

Total (to Van Lehn): \$561,867

Completed

3M – Non-Tenured Faculty Award – Van Lehn (PI)

“Combining Physics-Based and Data-Centric Models for Soft Materials Design”

7/1/2020-6/30/2023

Total (to Van Lehn): \$45,000

Argonne National Laboratory – Van Lehn (PI)

“Design and Development of Machine-Learning-Based Methods for Molecular Property Prediction on Diverse Data Sets”

11/1/2020-10/31/2022

Total (to Van Lehn): \$72,356

NSF – MRSEC – Seed Project – Blackwell (PI), Van Lehn (co-PI)

“Synthetic Soft Matter Inspired by Behaviors of Bacterial Communities”

4/1/2019-3/30/2020

Total (to Van Lehn): \$39,270

NSF – MRSEC – Seed Project – Van Lehn (PI)

“Design Rules for the Self-Assembly, Transport, and Activity of Bio-inspired Amphiphiles”

4/1/2018-3/30/2019

Total (to Van Lehn): \$39,270

NSF – MCB – Molecular Biophysics - Van Lehn (PI)

“Molecular Mechanisms of Topological Rearrangements in Integral Membrane Proteins”

7/1/2018-6/31/2023

Total (to Van Lehn): \$319,733

NSF – BIGDATA – Zavala (PI)

“BIGDATA: IA: Collaborative Research: Data-Driven, Multi-Scale Design of Liquid Crystals for Wearable Sensors for Monitoring Human Exposure and Air Quality”

9/1/2018-8/31/2023

Total (to Van Lehn): \$569,973

Invited Conference Presentations and Seminars

1. Michigan State University Center for Research on Ingredient Safety Science Day, Lansing, MI, October 2, **2024**.
2. Association for Roll-to-Roll Converters USA Conference & Expo, Charlotte, NC, September 26, **2024**.
3. American Chemical Society Fall Meeting (Invited), Denver, CO, August 19, **2024**.

4. *Great Lakes Bioenergy Center (GLBRC) Annual Science Meeting (Invited)*, Lake Geneva, WI, May 13, **2024**.
5. *Center for the Chemical Upcycling of Waste Plastics (CUWP) Annual Meeting (Invited)*, Madison, WI, May 14, **2024**.
6. *FlexPack PLACE Conference (Invited)*, San Diego, CA, April 17, **2024**.
7. *American Chemical Society Spring Meeting, Panel Discussion on Technology Perspective for Implementing the Circular Economy for Polymers (Invited)*, New Orleans, LS, March 20, **2024**.
8. *PFAS: Impact on the Planet and Solutions for the Packaging Industry (Invited)*, Madison, WI, November 2, **2023**.
9. *American Chemical Society Fall Meeting (Invited)*, San Francisco, CA, August 15, **2023**.
10. *Center for the Chemical Upcycling of Waste Plastics (CUWP) Annual Meeting (Invited)*, Madison, WI, May 16, **2023**.
11. *Nanoparticle Assemblies: A New Form of Matter with Classical Structure and Quantum Function (Invited Participant)*, Kavli Institute of Theoretical Physics, attended from April 24 – May 12, **2023**.
12. *Lignin Community of Practice Presentation Series (Invited)*, Virtual, March 24, **2023**.
13. *Wisconsin Energy Institute Sustainable Energy Seminar Series (Invited)*, Madison, WI, March 20, **2023**.
14. *AATR/STMS Joint Seminar Series (Invited)*, Virtual, October 28, **2022**.
15. *Molecular Foundry User Meeting (Invited)*, Lawrence Berkeley National Laboratory, Virtual, August 19, **2022**.
16. *Computational Chemistry and Materials Science Summer Institute Seminar Series*, Lawrence Livermore National Laboratory, Virtual, August 8-9, **2022**.
17. *Center for the Chemical Upcycling of Waste Plastics (CUWP) Annual Meeting (Invited)*, Madison, WI, June 7, **2022**.
18. *Department Seminar, Purdue Davidson School of Chemical Engineering*, West Lafayette, IN, March 24, **2022**.
19. *Biosciences Division Seminar, Oak Ridge National Laboratory*, Virtual, January 31, **2022**.
20. *PacifiChem, Experimental and Computational Analysis of the Nano-Bio Interface for Sustainable Nanotechnology (Invited)*, Virtual, December 21, **2021**.
21. *American Institute of Chemical Engineers Annual Meeting, Computational Molecular Science and Engineering Forum Plenary Session (Invited)*, Boston, MA, November 10, **2021**.
22. *3M Non-Tenured Faculty Award Forum (Invited)*, Virtual, November 4, **2021**.
23. *Department Seminar, Northwestern University Department of Chemical and Biological Engineering*, Evanston, IL, October 14, **2021**.
24. *Computing in Engineering Forum (Invited)*, Madison, WI, September 22, **2021**.
25. *Center for the Chemical Upcycling of Waste Plastics (CUWP) Annual Meeting*, Virtual, June 9, **2021**.
26. *Princeton Institute for the Science and Technology of Materials (PRISM)/Princeton Center for Complex Materials (PCCM) Seminar, Princeton University*, Virtual, April 28, **2021**.
27. *Department Seminar, University of Notre Dame, Department of Chemical and Biomolecular Engineering*, Virtual, April 13, **2021**.
28. *ACS Spring (Invited), Session on Surface Chemistry and Solvation Effects on Catalysis in Confined Environments*, Virtual, April 5, **2021**.
29. *Department Seminar, University of Illinois Urbana-Champaign Chemical and Biomolecular Engineering*, Virtual, March 30, **2021**.
30. *Department Seminar, University of Maine Department of Chemical and Biomedical Engineering*, Virtual, March 19, **2021**.
31. *3M Non-Tenured Faculty Award Forum (Invited)*, Virtual, February 5, **2021**.
32. *American Chemical Society Fall Meeting*, Virtual, August 17-21, **2020**.
33. *Bioenergy Research Centers Workshop on AI and Machine Learning (Invited)*, Washington DC, MD, February 27, **2020**.
34. *Department Seminar, Vanderbilt University Department of Chemical and Biomolecular Engineering*, Nashville, TN, February 24, **2020**.
35. *American Institute of Chemical Engineers Annual Meeting, Topical Plenary: Topical Conference in Molecular and Materials Data Science (Invited)*, Orlando, FL, November 11, **2019**.
36. *American Institute of Chemical Engineers Annual Meeting, Session on Spotlights in Thermodynamics and Computational Molecular Science (Invited)*, Orlando, FL, November 11, **2019**.
37. *Computing in Engineering Forum (Invited)*, Madison, WI, September 10-11, **2019**.
38. *Midwest Thermodynamics and Statistical Mechanics Meeting (Invited)*, Urbana, IL, June 2-4, **2019**.
39. *Materials Research Society Spring Meeting, Symposium on Nanomaterial Synthesis, Characterizations and Applications*, Phoenix, AZ, April 22-26, **2019**.
40. *American Chemical Society Spring Meeting, Symposium on Nanomaterials (Invited)*, Orlando, FL, March 31-April 4, **2019**.
41. *American Institute of Chemical Engineers Annual Meeting, Symposium on Modeling of Lipid Membranes and Membrane Proteins*, Pittsburgh, PA, October 28 - November 2, **2018**.
42. *Foundations of Molecular Modeling and Simulation*, Delavan, WI, July 15-19, **2018**.
43. *Midwest Thermodynamics & Statistical Mechanics Conference*, Pittsburgh, PA, June 10-12, **2018**.
44. *American Chemical Society Spring Meeting, Symposium on Understanding the Complexity of the Nano/Bio Interface with Experiments & Computations*, New Orleans, LA, March 18-23, **2018**.

45. *American Institute of Chemical Engineers Annual Meeting, Symposia on Modeling of Biomaterials, Protein Structure, Function, and Stability, and Modeling of Lipid Membranes and Membrane Proteins*, Minneapolis, MN, October 26- November 3, **2017**.
46. *9th Sino-US Joint Conference of Chemical Engineering (Invited)*, Beijing, China, October 15-19, **2017**.
47. *Department Seminar, University of Wisconsin-Madison Department of Chemistry*, Madison, WI, September 26, **2017**.
48. *Department Seminar, University of Wisconsin-Madison Department of Materials Science and Engineering*, Madison, WI, September 7, **2017**.
49. *American Chemical Society Colloids & Surface Science Symposium*, New York, NY, July 9-12, **2017**.
50. *Midwest Thermodynamics and Statistical Mechanics Meeting*, Notre Dame, IN, June 4-6, **2017**.
51. *Materials Research Society Spring Meeting, Symposium on Computer-based Modeling and Experiment for the Design of Soft Materials*, Phoenix, AZ, April 20-21, **2017**.
52. *QBio Fall Seminar Series*, University of Wisconsin-Madison, Madison, WI, December 7, **2016**.
53. *Materials Research Society Fall Meeting, Symposium on Spatiotemporally and Morphologically-Controlled Biomaterials for Medical Applications*, Boston, MA, November 26-December 1, **2016**.
54. *American Institute of Chemical Engineers Annual Meeting, Symposium on Nanostructured, Biomimetic, and Biohybrid Materials and Devices*, San Francisco, CA, November 14-18, **2016**.
55. *San Francisco Bay Area Nanotechnology Council Annual Fall Symposium*, Santa Clara, CA, November 15, **2016**.
56. *Workshop on Biomaterials and their Interactions with Biological and Model Membranes*, Salou, Spain, September 30 – October 2, **2016**.
57. *American Chemical Society Spring Meeting, COMP Symposium on Structure, Dynamics, & Reactivity at Complex Interfaces with Relevance in Renewable Energy & Environmental Applications*, San Diego, CA, March 13-17, **2016**.
58. *Materials Research Society Fall Meeting, Symposium on Modeling and Theory-Driven Design of Soft Materials*, Boston, MA, November 29-December 4, **2015**.
59. *American Institute of Chemical Engineers Annual Meeting, Symposium on Protein Structure, Function, and Stability*, Salt Lake City, UT, November 8-13, **2015**.
60. *American Institute of Chemical Engineers Annual Meeting, Symposium on Biomolecules at Biomaterial Interfaces*, Salt Lake City, UT, November 8-13, **2015**.
61. *Materials Research Society Fall Meeting, Symposium on Medical Applications of Noble Metal Nanoparticles*, Boston, MA, November 29-December 4, **2014**.
62. *Materials Research Society Spring Meeting, Symposium on Biomaterials for Biomolecule Delivery and Understanding Cell-Niche Interactions*, San Francisco, CA, April 21-25, **2014**.
63. *American Physical Society March Meeting, DBIO Symposium on Assembly and Function of Biomimetic and Bioinspired Materials*, Denver, CO, March 3-7, **2014**.
64. *Materials Research Society Fall Meeting, Symposium on Modeling and Theory-Driven Design of Soft Materials*, Boston, MA, December 1-6, **2013**.
65. *American Physical Society March Meeting, DBIO Focus Session on Structure and Dynamics of Biomembranes*, Baltimore, MD, March 18-22, **2013**.
66. *American Physical Society March Meeting, FIAP Symposium on Bionanotechnology*, Dallas, TX, March 21-25, **2011**.

Patents

1. George Huber, Kevin Sánchez-Rivera, **Reid Van Lehn**, Theodore Walker, Panzheng Zhou. Provisional patent application. RECYCLING OF PLASTICS BY SOLVENT-TARGETED RECOVERY AND PRECIPITATION (STRAP). Filed November 18, 2022 by the Wisconsin Alumni Research Foundation.
2. Charles Granger, Tianwei Yan, Kevin Sánchez-Rivera, George Huber, **Reid Van Lehn**, Ezra Bar Ziv, Fei Long, Panzheng Zhou. Provisional patent application. A SOLVENT-BASED PLASTIC RECYCLING METHOD TO REMOVE COLORED COMPONENTS AND PRODUCE UNCOLORED RESINS. Filed May 15, 2024 by the Wisconsin Alumni Research Foundation.

Teaching

Instructor, Chemical Engineering Materials, CBE 440, UW-Madison	<i>Spring 2025</i>
Instructor (Colleague Coverage), Advanced Chem. Engineering Thermodynamics, CBE 710, UW-Madison	<i>Fall 2024</i>
Instructor, Thermodynamics of Mixtures, CBE 311, UW-Madison	<i>Fall 2024</i>
Instructor, Thermodynamics of Mixtures, CBE 311, UW-Madison	<i>Spring 2024</i>
Instructor, Introduction to Graduate School, CBE 562, UW-Madison	<i>Fall 2023</i>
Instructor, Chemical Engineering Materials, CBE 440, UW-Madison	<i>Fall 2023</i>
Instructor, Introduction to Colloid and Surface Science, CBE 547, UW-Madison	<i>Spring 2023</i>
Instructor, Soft Materials, CBE 562, UW-Madison	<i>Fall 2022</i>

Instructor, Thermodynamics of Mixtures, CBE 311, UW-Madison	Spring 2022
Instructor, Thermodynamics of Mixtures, CBE 311, UW-Madison	Fall 2021
Instructor, Introduction to Colloid and Surface Science, CBE 547, UW-Madison	Spring 2021
Instructor, Soft Materials, CBE 562, UW-Madison	Fall 2020
Instructor, Advanced Chemical Engineering Thermodynamics, CBE 710, UW-Madison	Fall 2019
Instructor, Introduction to Colloid and Surface Science, CBE 547, UW-Madison	Spring 2019
Instructor, Advanced Chemical Engineering Thermodynamics, CBE 710, UW-Madison	Fall 2018
Instructor, Thermodynamics of Mixtures, CBE 311, UW-Madison	Spring 2018
Instructor, Advanced Chemical Engineering Thermodynamics, CBE 710, UW-Madison	Fall 2017
Instructor, Thermodynamics of Mixtures, CBE 311, UW-Madison	Spring 2017
Instructor, Advanced Chemical Engineering Thermodynamics, CBE 710, UW-Madison	Fall 2016
Guest Lecturer, Selected Topics in Macromolecular and Biophysical Chemistry, Chem 872, UW-Madison	Fall 2016
Participant in UW-Madison Instructor-Learning Environment and Pedagogics Program	Summer 2016
Teaching Assistant and Recitation Instructor, Introduction to Solid State Chemistry, 3.091, MIT	Fall 2012
Teaching Assistant and Recitation Instructor, Polymer Physics, 3.063, MIT	Spring 2012
Teaching Assistant and Recitation Instructor, Polymer Physics, 3.063, MIT	Spring 2011

Mentorship

Current Graduate Student Researchers

Yuhui Huang, Chemical and Biological Engineering, UW-Madison	Fall 2024 – Present
Yicheng Li, Chemical and Biological Engineering, UW-Madison <i>Co-advised with Prof. Victor Zavala</i>	Fall 2024 – Present
Letian Wang, Chemical and Biological Engineering, UW-Madison	Fall 2024 – Present
Ali Altamimi, Chemistry, UW-Madison	Fall 2023 – Present
Jung Min Lee, Chemical and Biological Engineering, UW-Madison	Fall 2023 – Present
Changsu Kim, Chemical and Biological Engineering, UW-Madison	Fall 2023 – Present
Srija Chakraborty, Chemical and Biological Engineering, UW-Madison	Fall 2022 – Present
Ugochukwu Ikegwu, Chemical and Biological Engineering, UW-Madison <i>Co-advised with Prof. Victor Zavala</i>	Fall 2022 – Present
Carlos Huang-Zhu, Chemical and Biological Engineering, UW-Madison	Fall 2021 – Present
Byunguk Park, Biophysics Training Program, UW-Madison	Fall 2021 – Present
Joshua Richardson, Chemical and Biological Engineering, UW-Madison	Fall 2021 – Present
Lisa Je, Chemical and Biological Engineering, UW-Madison <i>Co-advised with Prof. Victor Zavala</i>	Summer 2021 – Present
Panzheng Zhou, Chemical and Biological Engineering, UW-Madison	Fall 2019 – Present

Former Ph.D. Students

Dr. Benginur Demir, Chemical and Biological Engineering, UW-Madison <i>Co-advised with Prof. James Dumesic</i> <u>Thesis</u> : “Kinetics of Catalytic Upgrading Reactions of Biomass-derived and Model Oxygenates”	Fall 2019 – Summer 2020
Dr. Alex Chew, Chemical and Biological Engineering, UW-Madison <u>Thesis</u> : “Molecular Dynamics and Machine Learning for Reaction and Nanomaterial Design”	Fall 2016 – Summer 2021
Dr. Bradley Dallin, Chemical and Biological Engineering, UW-Madison <u>Thesis</u> : “Understanding Modulations to Hydrophobicity by Spatially Heterogeneous Interfaces”	Fall 2016 – Summer 2021
Dr. Samarhaben Patel, Chemical and Biological Engineering, UW-Madison <u>Thesis</u> : “Molecular Simulations to Characterize the Assembly and Transport of Biomolecules in Solution and at Lipid Interfaces”	Fall 2016 – Summer 2021
Dr. Shiyi (Amy) Qin, Chemical and Biological Engineering, UW-Madison <i>Co-advised with Prof. Victor Zavala</i> <u>Thesis</u> : “Machine Learning Methods for Chemical Property Prediction, Sensing, and Design”	Fall 2019 – Summer 2024
Dr. Jonathan Sheavly, Chemical and Biological Engineering, UW-Madison <u>Thesis</u> : “Multiscale Modeling of Responsive Soft Material Interfaces”	Fall 2017 – Summer 2022

Former M.S. Students

Atharva Kelkar, Chemical and Biological Engineering, UW-Madison <u>Thesis</u> : “Machine Learning and Molecular Dynamics Methods to Study the Hydrophobicity of Self-Assembled Monolayers”	Fall 2018 – Summer 2021
---	-------------------------

Current Postdoctoral Researchers

Dr. Juriti Rajbangshi, Chemical and Biological Engineering, UW-Madison

Summer 2022 – Present

Former Postdoctoral Researchers

Dr. Alvaro Posada-Borbón, Chemical and Biological Engineering, UW-Madison

Fall 2021 – Summer 2023

Co-advised with Prof. Manos Mavrikakis and Prof. Victor Zavala

Dr. Jianping Li, Chemical and Biological Engineering, UW-Madison

Summer 2020 – Summer 2023

Co-advised with Prof. Christos Maravelias

Dr. Zeynep Sümer, Chemical and Biological Engineering, UW-Madison

Spring 2021 – Summer 2022

Dr. Zhizhang Shen, Chemical and Biological Engineering, UW-Madison

Fall 2018 – Fall 2020

Undergraduate Researchers / Summer Interns

Sara Bender, UW-Madison undergraduate

Fall 2023 – Spring 2024

Taskina Jui, REU student

Summer 2023

Nicole Babineau, REU student

Summer 2022

Natalia Ramos Acevedo, REU student

Summer 2022

Steven Yeo, UW-Madison undergraduate

Fall 2021 – Spring 2023

Dane Christiansen, Undergraduate Research Scholars student

Fall 2021 – Spring 2022

Elizabeth Griffin, REU student

Summer 2021

Mariela R. Rodriguez-Otero, REU student

Summer 2021

Luis Roberto Padilla, REU student

Summer 2021

Kourtney Reed, REU student

Summer 2021

Devesh Shah, UW-Madison Master's student (CS)

Summer 2021

Vedaant Tambi, UW-Madison undergraduate (CS)

Spring 2020 – Spring 2021

Wei He, UW-Madison undergraduate

Spring 2020 – Fall 2020

Isabella Wegner, UW-Madison undergraduate

Summer 2019

Herry Jin, UW-Madison undergraduate

Spring 2019 – Summer 2020

Ricardo Mathison, UW-Madison undergraduate

Fall 2018 – Spring 2019

Zhiwen Zhang, UW-Madison undergraduate

Fall 2018 – Spring 2019

Alexis Oswalt, REU student (Nanotechnology)

Summer 2018

Jack Euclide, UW-Madison undergraduate

Spring 2018 – Summer 2018

Geyao Gu, REU student (Theoretical Chemistry)

Summer 2017

Bret Wolter, UW-Madison undergraduate

Summer 2017 – Fall 2018

Seth Winger, UW-Madison undergraduate

Summer 2017 – Fall 2018

Sakura Kawano, UW-Madison undergraduate

Fall 2016 – Spring 2018

Collin Davda, Caltech undergraduate

Summer 2015 – Spring 2016

Sang Hyun Choi, MIT undergraduate

Fall 2013 – Spring 2014

Paul Jones, MIT-Imperial College exchange student

Summer 2013

Maxwell Plaut, MIT undergraduate

Fall 2012

Karthik Chellamuthu, Research Science Institute high school student

Summer 2012

Tiffany Tang, MIT undergraduate

Fall 2011 – Spring 2012

Alec Garza-Gallindo, MIT undergraduate

Fall 2011 – Spring 2012

Qian Lin, MIT undergraduate

Fall 2010 – Spring 2011

Eriko Iwatate, Center for Materials Science and Engineering REU Intern

Summer 2010

Academic Service and Synergistic Activities

Manuscript Review Service:

ACS Catalysis, ACS Chemical Neuroscience, ACS Macro Letters, ACS Nano, ACS Sustainable Chemistry & Engineering, Advanced Healthcare Materials, BBA Biomembranes, Chemical Science, Current Opinion in Chemical Engineering, Environmental Science: Nano, Journal of Chemical Physics, Journal of Chemical Theory and Computation, The Journal of Physical Chemistry, Journal of Physical Chemistry Letters, Langmuir, Nanoscale, Nanoscale Horizons, Nature Computational Science, Physical Chemistry Chemical Physics, Physical Review E, Physical Review Letters, PLoS ONE, Science Advances, Scientific Reports, Soft Matter, and Surface Science.

Proposal Review Service:

UW 2020 Physical Sciences Division (2018), NSF Chemistry of Life Processes (2018), ACS Petroleum Research Fund (2018-2019), DOE BES Condensed Phase and Interfacial Molecular Sciences (2019), NSF Panelist (2020, 2021, 2022), NSF Condensed Matter and Materials Theory (2020, 2021, 2022, 2023, 2024), Graduate Women in Science Fellowship Program (2021), NSF DMREF (2021), NSF Nanoscale Interactions (2022)

Conference Organization:

- Session chair and organizer for *American Institute of Chemical Engineers Annual Meeting, Symposia on Modeling of Lipid Membranes and Membrane Proteins*, San Diego CA, October 27-November 1, **2024**.
- Session chair and organizer for *American Institute of Chemical Engineers Annual Meeting, Symposia on Modeling of Lipid Membranes and Membrane Proteins*, Orlando, FL, November 5-November 10, **2023**.
- Session chair and organizer for *American Institute of Chemical Engineers Annual Meeting, Symposia on Modeling of Lipid Membranes and Membrane Proteins*, Phoenix, AZ, November 13-November 18, **2022**.
- Session chair and organizer for *American Institute of Chemical Engineers Annual Meeting, Symposia on Modeling of Lipid Membranes and Membrane Proteins*, Boston, MA, November 5-November 11, **2021**.
- Theme organizer for *2021 Computing in Engineering Forum* at UW-Madison, September 21-22, **2021**.
- Organizer of *2021 Midwest Thermodynamics and Statistical Mechanics* conference, June 14-June 16, **2021**.
- Session chair and organizer for *American Institute of Chemical Engineers Annual Meeting, Symposia on Modeling of Lipid Membranes and Membrane Proteins*, Virtual Meeting, November 16-November 20, **2020**.
- Session chair and organizer for *American Institute of Chemical Engineers Annual Meeting, Symposia on Data-Driven Design and Modeling of Biomaterials, and Modeling of Lipid Membranes and Membrane Proteins*, Orlando, FL, November 10-November 15, **2019**.
- Session chair and organizer for *American Institute of Chemical Engineers Annual Meeting, Symposia on Thermodynamics of Biomolecular Folding and Assembly, Modeling of Lipid Membranes and Membrane Proteins, and Modeling of Biomaterials*, Pittsburgh, PA, October 29-November 2, **2018**.
- Session chair for *Materials Research Society Spring Meeting, Symposium on Computer-based Modeling and Experiment for the Design of Soft Materials*, Phoenix, AZ, April 20-21, **2017**.
- Session chair for *American Chemical Society Spring Meeting, COMP Symposium on Structure, Dynamics, & Reactivity at Complex Interfaces with Relevance in Renewable Energy & Environmental Applications*, San Diego, CA, March 13-17, **2016**.

Leadership:

- Programming Cmte for AIChE Thermodynamics and Transport Processes (Area 1A) *Spring 2025 - Present*
- Selected for College of Engineering Faculty Leadership Development Series *Fall 2023-Spring 2024*
- Topic Area 5 leader for Center for the Chemical Upcycling of Waste Plastics *Fall 2020-Present*
- Executive Board member for Center for the Chemical Upcycling of Waste Plastics *Fall 2020-Present*
- Liaison Director for AIChE Computational Molecular Sciences and Engineering Forum *Fall 2021-Fall 2023*

Service to the Community:

- Reviewer for ACS COMP Chemical Computing Group graduate student award for Fall 2020
- Judge for Bionanotechnology Graduate Student awards at AIChE Fall Conference 2017
- Judge for Polymer Graduate Student awards at AIChE Fall Conference 2017

Memberships and Affiliations:

American Chemical Society, American Institute for Chemical Engineers, Materials Research Society, Biophysical Society

Outreach:

- Mentored high-school teacher as part of Research Experiences for Teachers program (**2023**)
- Mentored 10 Research Experiences for Undergraduate students and presented in seminar series (**2017-2024**)
- Speaker at “Wednesday Nite at the Lab” on “New Recycling Technologies to Combat Plastic Pollution (**2021**)
- Volunteer at UW-Madison Engineering Expo, Wisconsin Science Festival (**2017-2022**)
- Speaker at Institute of Chemical Education “Fun with Engineering” Summer Camp (**2017**)
- Speaker at Midwest Undergraduate Computational Chemistry Consortium Conference (**2016**)
- Speaker at Opportunities in Engineering Conference (**2016, 2021**)

Departmental Service:

- Director of Graduate Studies *Summer 2024 - Present*
- Chair of Graduate Program Committee *Summer 2024 - Present*
- Member of Faculty Search Committee *Summer 2024 - Present*
- Member of Mentoring Committee for Prof. Styliana Avraamidou *Fall 2023 - Present*
- Member of Mentoring Committee for Prof. Rose Cersonsky *Spring 2023 - Present*
- Member of Mentoring Committee for Prof. Whitney Loo *Spring 2023 - Present*
- Member of Salary Committee *Fall 2022 - Present*

- Member of Graduate Program Committee *Summer 2021 – Present*
- CBE Strategic Planning Committee *Fall 2020, 2024-Present*
- Chair of Graduate Admissions Committee *Summer 2021 – Summer 2024*
- CBE Seminar Chair *Spring 2019 – Summer 2021*
- AIChE Student Chapter Advisor *Fall 2018 – Summer 2021*
- AIChE Reception Chair *Fall 2017 – Summer 2021*
- Member of Graduate Admissions Committee *Fall 2016 – Summer 2021*
- Member of Kramer Lectureship Committee *Fall 2016 – Spring 2021*
- CBE Faculty Senator *Fall 2016 – Fall 2020*

College Service:

- Panelist for WiscProf Workshop *Spring 2022*
- Panelist for NSF CAREER Broader Impacts Workshop *Spring 2021*
- Panelist for NSF Graduate Research Fellowship Engineering Panel *Fall 2020*
- Selection committee for COE University and Academic Staff Distinguished Service Award *Fall 2020*

University Service:

- Member of the Office of the VCGRE Research Committee *Fall 2022 – Present*

Press Coverage:

- Featured in Spectrum News1, <https://spectrumnews1.com/wi/madison/news/2020/12/27/wisconsin-researchers-lead-efforts-to-improve-plastic-recycling> *December 27, 2020*
- Interviewed on Perpetual Notion Machine, <https://www.wortfm.org/complex-plastic-recycling-in-post-industrial-waste/> *December 10, 2020*
- Interviewed on Larry Meiller Show, <https://www.wpr.org/listen/1728281> *November 30, 2020*
- Featured on Channel 3000 News, <https://www.channel3000.com/revolutionizing-recycling-uw-madison-research-team-works-to-find-better-ways-to-reuse-plastics/> *January 30, 2020*