

Reid C. Van Lehn

Curriculum Vitae, October 2022

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Professional Appointments

University of Wisconsin-Madison

<i>Hunt-Hougen Associate Professor in the Department of Chemical and Biological Engineering</i>	2022 – 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	2015 – 2016
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Postdoctoral Scholar in the Division of Chemistry and Chemical Engineering
Advisor: Thomas F. Miller III

Massachusetts Institute of Technology	2014 – 2015
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Postdoctoral Associate in the Department of Materials Science and Engineering
Advisor: Alfredo Alexander-Katz

Massachusetts Institute of Technology	2009 – 2014
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Ph.D. in Materials Science and Engineering, Minor in Teaching
Thesis: "Interactions of Environmentally-Responsive Nanoparticles with Synthetic and Biological Membranes"
Advisor: Alfredo Alexander-Katz

Massachusetts Institute of Technology	2005 – 2009
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B.S. in Materials Science and Engineering

Honors and Awards

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. 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*, **submitted**.

2. CG Gahan, **RC Van Lehn**, HE Blackwell, and DM Lynn*. Interactions of bacterial quorum sensing signals with model lipid membranes: Influence of membrane composition on membrane remodeling." *Langmuir*, **submitted**.
3. AD Smith, S Runde, AK Chew, AS Kelkar, U Maheshwari, **RC Van Lehn**, and VM Zavala*. "Topological Analysis of Molecular Dynamics Simulations using the Euler Characteristic." *Journal of Chemical Theory and Computation*, **in revision**.
4. S Qin, S Jiang, J Li, P Balaprakash, **RC Van Lehn**, and VM Zavala*. "Capturing molecular interactions in graph neural networks: A case study in multi-component phase equilibrium." *Digital Discovery*, **in revision**.
5. BC Dallin, AS Kelkar, and **RC Van Lehn***. "Generalized features of interfacial water structure predict the hydrophobicity of chemically heterogeneous surfaces." *Chemical Science*, **in revision**. Preprint available: <https://doi.org/10.33774/chemrxiv-2021-1w1nc>.
6. Z Sumer and **RC Van Lehn***. "Heuristic computational model for predicting lignin solubility in tailored organic solvents." *ACS Sustainable Chemistry & Engineering*, **in revision**.
7. J Morstein*, A Capecci[^], 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*, **accepted**.
8. 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, and GW Huber*. "Expanding plastics recycling technologies: Chemical aspects, technology status, and challenges." *Green Chemistry*, **accepted**.
9. Z Sumer and **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.
10. N Bao, S Jiang, AD Smith, JJ Schauer, M Mavrikakis, **RC Van Lehn**, VM Zavala*, and NL Abbott*. "Sensing gas mixtures by analyzing the spatiotemporal optical responses of liquid crystals using 3D convolutional neural networks." *ACS Sensors*, **accepted**.
11. N Bao, JL Gold, JK Sheavly, JJ Schauer, VM Zavala, **RC Van Lehn**, M Mavrikakis, and NL Abbott*. "Ordering transitions of liquid crystals triggered by metal oxide-catalyzed reactions of sulfur oxide species." *Journal of the American Chemical Society*, **accepted**.
12. Z Shen, JH Dwyer, J Sun, KR Jinkins, MS Arnold, P Gopalan, and **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.
13. J Li, CT Maravelias, and **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.
14. 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.
15. L Je, GW Huber, **RC Van Lehn**, and 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.
16. AS Kelkar, BC Dallin, and **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.
17. CG Gahan, **RC Van Lehn***, HE Blackwell*, and 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.
18. S Qin, T Jin, **RC Van Lehn***, and VM Zavala*. "Predicting critical micelle concentrations for surfactants using graph convolutional neural networks." *J Phys Chem B*, **2021**, *125*, 10610-10620.
19. P Zhou, KL Sánchez-Rivera, GW Huber, and **RC Van Lehn***. "Computational approach for rapidly predicting temperature-dependent polymer solubilities using molecular-scale models." *ChemSusChem*, **2021**, *14* (9), 4307-4316.
20. KL Sánchez-Rivera, P Zhou, MS Kim, LD González Chávez, S Grey, K Nelson, S-C Wang, I Hermans, VM Zavala, **RC Van Lehn**, and 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.

21. CG Gahan, SJ Patel, LM Chen, DE Manson, ZJ Ehmer, HE Blackwell*, **RC Van Lehn***, and DM Lynn*. "Bacterial quorum sensing signals promote large-scale remodeling of lipid membranes." *Langmuir*, **2021**, 35 (30), 9120-9136.
22. SJ Patel and **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.
23. CA Lochbaum[^], AK Chew[^], X Zhang, VM Rotello, **RC Van Lehn***, and JA Pedersen*. "The lipophilicity of cationic ligands promotes irreversible adsorption of nanoparticles to lipid bilayers." *ACS Nano*, **2021**, 15, 6562-6572.
24. AK Chew, BC Dallin, and **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.
25. BM Hoover, Z Shen, CG Gahan, DM Lynn, **RC Van Lehn**, and 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.
26. T. Jin, SJ Patel, and **RC Van Lehn***. "Molecular simulations of lipid membrane partitioning and translocation by bacterial quorum sensing modulators." *PLoS ONE*, **2021**, 16 (2), e0246187.
27. TW Walker, N Frelka, Z Shen, AK Chew, J Bannick, S Grey, MS Kim, JA Dumesic, **RC Van Lehn**, and 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/>

28. AK Chew, S Jiang, W Zhang, VM Zavala, and **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.
29. AS Kelkar, BC Dallin, and **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.
30. JK Sheavly and **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.

31. CG Gahan[^], SJ Patel[^], ME Boursier, KE Nyffeler, J Jennings, NL Abbott, HE Blackwell*, **RC Van Lehn***, and 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.
32. TW Walker[^], AK Chew[^], **RC Van Lehn**, JA Dumesic, and 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.
33. Z Shen and **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>

34. AK Chew[^], TW Walker[^], Z Shen, B Demir, L Witteman, J Euclide, GW Huber, JA Dumesic, and **RC Van Lehn***. "Effect of mixed-solvent environments on the selectivity of acid-catalyzed reactions." *ACS Catalysis*, **2020**, 10, 1679-1691.
35. JK Sheavly, JI Gold, M Mavrikakis, and **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.

36. JH Dwyer, Z Shen, KR Jenkins, W Wei, MS Arnold, **RC Van Lehn***, and P Gopalan*. "Solvent-mediated affinity of polymer-wrapped single-walled carbon nanotubes for chemically modified surfaces." *Langmuir*, **2019**, 35, 12492.
37. BC Dallin and **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.

38. AK Chew and **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

39. JK Sheavly, JA Pedersen, and **RC Van Lehn***. "Curvature-driven adsorption of cationic nanoparticles to phase boundaries in multicomponent lipid bilayers." *Nanoscale*, **2019**, *11*, 2767.
40. BC Dallin, H Yeon, AR Ostwalt, NL Abbott, and **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.
41. AK Chew and **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.
42. SJ Patel and **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.
43. A Alexander-Katz and **RC Van Lehn***. "Perspective: Random copolymers that protect proteins." *Science*, **2018**, *359*, 1216-1217.
44. TW Walker[^], AK Chew[^], H Li, B Demir, ZC Zhang, GW Huber, **RC Van Lehn***, and 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.

45. M Werner, T Auth, P Beales, JB Fleury, F Hook, H Kress, **RC Van Lehn**, M Muller, E Petrov, L Sarkisov, J-U Sommer, and VA Baulin. "Nanomaterial interactions with biomembranes: Bridging the gap between soft matter models and biological context." *Biointerphases*, **2018**, *13*, 028501.
46. H Yeon, C Wang, **RC Van Lehn**, and NL Abbott. "Influence of order within non-polar monolayers on hydrophobic interactions." *Langmuir*, **2017**, *33*, 4628-4637.

Prior to UW-Madison

47. **RC Van Lehn** and A Alexander-Katz. "Energy landscape for insertion of amphiphilic nanoparticles into lipid membranes: a computational study." *PLoS One*, **2019**, *14*(1), e0209492.
48. PU Atukorale, DS Yun, **RC Van Lehn**, RP Carney, A Bekdemir, PHJ Silva, A Alexander-Katz, F Stellacci, and DJ Irvine. "A study of amphiphilic gold nanoparticle design characteristics and bilayer properties that govern interaction with membranes." *Bioconjugate Chemistry*, **2018**, *29*, 1131-1140.
49. MJM Niesen, CY Wang, **RC Van Lehn**, and TF Miller III. "Structurally detailed coarse-grained model for Sec-facilitated co-translational protein translocation and membrane integration." *PLoS Computational Biology*, **2017**, *13*, e1005427.
50. **RC Van Lehn** and A Alexander-Katz. "Grafting charged species to membrane-embedded scaffolds dramatically increases the rate of bilayer translocation." *ACS Central Science* **2017**, *3*, 185.
51. M Tahir, **RC Van Lehn**, SH Choi, and A Alexander-Katz. "Solvent-exposed lipid tail protrusions depend on lipid membrane composition and curvature." *BBA Biomembranes* **2016**, *1858*, 1207.
52. **RC Van Lehn**, B Zhang, and TF Miller III. "Regulation of multispinning membrane protein topology by post-translational annealing." *eLife* **2015**, *4*, e08697.

Highlighted with a commentary by Stephen White

53. **RC Van Lehn** and A Alexander-Katz. "Pathway for insertion of amphiphilic nanoparticles into defect-free lipid bilayers from atomistic molecular dynamics simulations." *Soft Matter* **2015**, *11*, 3165.
54. **RC Van Lehn** and 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.
55. **RC Van Lehn**[^], M Ricci[^], PHJ Silva, P Andreozzi, J Reguera, K Voitchovsky, F Stellacci, and A Alexander-Katz. "Lipid tail protrusions mediate the insertion of nanoparticles into model cell membranes." *Nature Communications* **2014**, *5*, 4482.
56. **RC Van Lehn** and A Alexander-Katz, "Fusion of ligand-coated nanoparticles with lipid bilayers: Effect of ligand

- flexibility.” *Journal of Physical Chemistry A* **2014**, 118, 5848.
57. **RC Van Lehn** and A Alexander-Katz, “Free energy change for insertion of charged, monolayer-protected nanoparticles into lipid bilayers.” *Soft Matter* **2014**, 10, 648.
 58. **RC Van Lehn** and 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.
 59. **RC Van Lehn**, PU Atukorale, RP Carney, Y-S Yang, F Stellacci, DJ Irvine, and 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.
 60. **RC Van Lehn** and A Alexander-Katz, “Ligand-mediated short-range attraction drives aggregation of charged monolayer-protected gold nanoparticles.” *Langmuir* **2013**, 29, 8788.
 61. **RC Van Lehn** and A Alexander-Katz, “Penetration of lipid bilayers by nanoparticles with environmentally-responsive surfaces: simulations and theory.” *Soft Matter* **2011**, 7, 11392.
 62. **RC Van Lehn** and A Alexander-Katz, “Lateral phase separation of mixed polymer brushes physisorbed on planar substrates.” *Journal of Chemical Physics* **2011**, 135, 141106.
 63. **RC Van Lehn**, CE Sing, H Chen, and A Alexander-Katz. “Multidimensional targeting: using physical and chemical forces in unison.” *Current Pharmaceutical Biotechnology* **2010**, 11, 320.

Funding

Current

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 Direct (to Van Lehn): \$50,939 Total (to Van Lehn): \$72,356

This project develops machine-learning techniques that treat molecular structure as graphs to predict molecular properties. We are developing methods to discover high-performing neural network architectures automatically and utilizing them to predict experimental outcomes (reaction rates and interfacial hydrophobicity) based on large data sets generated from molecular dynamics simulations.

DOE (BER) – GLBRC – Donohue (PI)

“Molecular Modeling of Solvent Effects in Biomass Conversion”

12/1/2019-11/30/2022 Direct (to Van Lehn): \$129,077 Total (to Van Lehn): \$129,077

The DOE-funded Great Lakes Bioenergy Research Center (GLBRC) supports one-year Emerging Opportunity Projects designed to integrate PIs within existing GLBRC teams. This project supports the development of computational methods for separating bioproducts from fermentation broths and further modeling the effect of mixed-solvent environments on lignin deconstruction.

DOE (EERE) – BETO – Huber (PI)

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

6/1/2021-5/31/2026 Direct (to Van Lehn): \$305,247 Total (to Van Lehn): \$440,558

This project is a center dedicated to the upcycling of post-industrial waste plastics. The center is divided into six teams: Van Lehn is the Lead of Team 5, which is dedicated to the development of a solvent-mediated process for the recycling of multilayer plastic films. We are developing computational tools to rapidly predict polymer solubility for different film components to enable the targeted recovery of film components as pure resins.

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 Direct (to Van Lehn): \$411,400 Total (to Van Lehn): \$581,212

This project focuses on developing computational methods to understand and predict the penetration of functionalized nanoparticles into cells for applications in targeted drug delivery and biosensing. The proposal will

also develop a series of simulation modules for use in educational and outreach initiatives in collaboration with UW-Madison experts.

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

“Molecular Mechanisms of Topological Rearrangements in Integral Membrane Proteins”

7/1/2018-6/31/2023 Direct (to Van Lehn): \$237,035 Total (to Van Lehn): \$319,733

This project uses molecular dynamics simulations to understand the molecular mechanisms by which integral membrane protein topology can rearrange during or after protein folding. We are developing and applying enhanced sampling methods to characterize the pathways and quantify corresponding free energy barriers associated with translocating hydrophilic loops across the lipid bilayer and relating these quantities to protein sequence features.

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 Direct (to Van Lehn): \$392,623 Total (to Van Lehn): \$569,973

This project combines experiments, machine-learning techniques, density functional theory calculations, and molecular dynamics simulation (Van Lehn contribution) to design new chemoresponsive liquid crystal sensors for monitoring environmental contamination. We are developing new computational methods to relate physically motivated descriptors extracted from molecular dynamics simulations to experimental measurements through a reinforcement learning framework.

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

This award supports research activities centered on combining molecular simulations with machine learning techniques to guide the design of soft materials relevant to 3M interests. Two research directions include engineering interfacial hydrophobicity using active learning and screening solvent mixtures for polymer deconstruction using machine learning predictions of experimental outcomes.

Previous

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

The NSF-funded UW-Madison Materials Research Science and Engineering Center (MRSEC) supports annual seed projects designed to support a single student and nurture materials research on campus. This seed project funds a collaborative project with the Lynn and Blackwell group to uncover the physical principles behind the assembly and transport of amphiphilic quorum-sensing molecules to inform the design of soft materials that integrate and communicate with bacterial biofilms.

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

The NSF-funded UW-Madison Materials Research Science and Engineering Center (MRSEC) supports annual seed projects designed to support a single student and nurture materials research on campus. This seed project funds a collaborative project with the Lynn and Blackwell group to uncover the physical principles behind the assembly and transport of amphiphilic quorum-sensing molecules to inform the design of soft materials that integrate and communicate with bacterial biofilms.

Conference and Invited Presentations

1. *Molecular Foundry User Meeting (Invited)*, Lawrence Berkeley National Laboratory, Virtual, August 19, **2022**.
2. *Computational Chemistry and Materials Science Summer Institute Seminar Series*, Lawrence Livermore National Laboratory, Virtual, August 8-9, **2022**.

3. *Center for the Chemical Upcycling of Waste Plastics (CUWP) Annual Meeting (Invited)*, Madison, WI, June 7, **2022**.
4. *Department Seminar, Purdue Davidson School of Chemical Engineering*, West Lafayette, IN, March 24, **2022**.
5. *Biosciences Division Seminar, Oak Ridge National Laboratory*, Virtual, January 31, **2022**.
6. *PacifiChem, Experimental and Computational Analysis of the Nano-Bio Interface for Sustainable Nanotechnology (Invited)*, Virtual, December 21, **2021**.
7. *American Institute of Chemical Engineers Annual Meeting, Computational Molecular Science and Engineering Forum Plenary Session (Invited)*, Boston, MA, November 10, **2021**.
8. *3M Non-Tenured Faculty Award Forum (Invited)*, Virtual, November 4, **2021**.
9. *Department Seminar, Northwestern University Department of Chemical and Biological Engineering*, Evanston, IL, October 14, **2021**.
10. *Computing in Engineering Forum (Invited)*, Madison, WI, September 22, **2021**.
11. *Center for the Chemical Upcycling of Waste Plastics (CUWP) Annual Meeting*, Virtual, June 9, **2021**.
12. *Princeton Institute for the Science and Technology of Materials (PRISM)/Princeton Center for Complex Materials (PCCM) Seminar, Princeton University*, Virtual, April 28, **2021**.
13. *Department Seminar, University of Notre Dame, Department of Chemical and Biomolecular Engineering*, Virtual, April 13, **2021**.
14. *ACS Spring (Invited), Session on Surface Chemistry and Solvation Effects on Catalysis in Confined Environments*, Virtual, April 5, **2021**.
15. *Department Seminar, University of Illinois Urbana-Champaign Chemical and Biomolecular Engineering*, Virtual, March 30, **2021**.
16. *Department Seminar, University of Maine Department of Chemical and Biomedical Engineering*, Virtual, March 19, **2021**.
17. *3M Non-Tenured Faculty Award Forum (Invited)*, Virtual, February 5, **2021**.
18. *American Chemical Society Fall Meeting*, Virtual, August 17-21, **2020**.
19. *Bioenergy Research Centers Workshop on AI and Machine Learning (Invited)*, Washington DC, MD, February 27, **2020**.
20. *Department Seminar, Vanderbilt University Department of Chemical and Biomolecular Engineering*, Nashville, TN, February 24, **2020**.
21. *American Institute of Chemical Engineers Annual Meeting, Topical Plenary: Topical Conference in Molecular and Materials Data Science (Invited)*, Orlando, FL, November 11, **2019**.
22. *American Institute of Chemical Engineers Annual Meeting, Session on Spotlights in Thermodynamics and Computational Molecular Science (Invited)*, Orlando, FL, November 11, **2019**.
23. *Computing in Engineering Forum (Invited)*, Madison, WI, September 10-11, **2019**.
24. *Midwest Thermodynamics and Statistical Mechanics Meeting (Invited)*, Urbana, IL, June 2-4, **2019**.
25. *Materials Research Society Spring Meeting, Symposium on Nanomaterial Synthesis, Characterizations and Applications*, Phoenix, AZ, April 22-26, **2019**.
26. *American Chemical Society Spring Meeting, Symposium on Nanomaterials (Invited)*, Orlando, FL, March 31-April 4, **2019**.
27. *American Institute of Chemical Engineers Annual Meeting, Symposium on Modeling of Lipid Membranes and Membrane Proteins*, Pittsburgh, PA, October 28 - November 2, **2018**.
28. *Foundations of Molecular Modeling and Simulation*, Delavan, WI, July 15-19, **2018**.
29. *Midwest Thermodynamics & Statistical Mechanics Conference*, Pittsburgh, PA, June 10-12, **2018**.
30. *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**.
31. *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**.
32. *9th Sino-US Joint Conference of Chemical Engineering (Invited)*, Beijing, China, October 15-19, **2017**.
33. *Department Seminar, University of Wisconsin-Madison Department of Chemistry*, Madison, WI, September 26, **2017**.
34. *Department Seminar, University of Wisconsin-Madison Department of Materials Science and Engineering*, Madison, WI, September 7, **2017**.
35. *American Chemical Society Colloids & Surface Science Symposium*, New York, NY, July 9-12, **2017**.
36. *Midwest Thermodynamics and Statistical Mechanics Meeting*, Notre Dame, IN, June 4-6, **2017**.
37. *Materials Research Society Spring Meeting, Symposium on Computer-based Modeling and Experiment for the Design of Soft Materials*, Phoenix, AZ, April 20-21, **2017**.
38. *QBio Fall Seminar Series*, University of Wisconsin-Madison, Madison, WI, December 7, **2016**.
39. *Materials Research Society Fall Meeting, Symposium on Spatiotemporally and Morphologically-Controlled Biomaterials for Medical Applications*, Boston, MA, November 26-December 1, **2016**.
40. *American Institute of Chemical Engineers Annual Meeting, Symposium on Nanostructured, Biomimetic, and Biohybrid*

- Materials and Devices*, San Francisco, CA, November 14-18, **2016**.
41. *San Francisco Bay Area Nanotechnology Council Annual Fall Symposium*, Santa Clara, CA, November 15, **2016**.
 42. *Workshop on Biomaterials and their Interactions with Biological and Model Membranes*, Salou, Spain, September 30 – October 2, **2016**.
 43. *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**.
 44. *Materials Research Society Fall Meeting, Symposium on Modeling and Theory-Driven Design of Soft Materials*, Boston, MA, November 29-December 4, **2015**.
 45. *American Institute of Chemical Engineers Annual Meeting, Symposium on Protein Structure, Function, and Stability*, Salt Lake City, UT, November 8-13, **2015**.
 46. *American Institute of Chemical Engineers Annual Meeting, Symposium on Biomolecules at Biomaterial Interfaces*, Salt Lake City, UT, November 8-13, **2015**.
 47. *Materials Research Society Fall Meeting, Symposium on Medical Applications of Noble Metal Nanoparticles*, Boston, MA, November 29-December 4, **2014**.
 48. *Materials Research Society Spring Meeting, Symposium on Biomaterials for Biomolecule Delivery and Understanding Cell-Niche Interactions*, San Francisco, CA, April 21-25, **2014**.
 49. *American Physical Society March Meeting, DBIO Symposium on Assembly and Function of Biomimetic and Bioinspired Materials*, Denver, CO, March 3-7, **2014**.
 50. *Materials Research Society Fall Meeting, Symposium on Modeling and Theory-Driven Design of Soft Materials*, Boston, MA, December 1-6, **2013**.
 51. *American Physical Society March Meeting, DBIO Focus Session on Structure and Dynamics of Biomembranes*, Baltimore, MD, March 18-22, **2013**.
 52. *American Physical Society March Meeting, FIAP Symposium on Bionanotechnology*, Dallas, TX, March 21-25, **2011**.

Teaching

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

Mentorship

Current Graduate Student Researchers

Carlos Huang-Zhu, Chemical and Biological Engineering, UW-Madison	<i>Fall 2021 – Present</i>
Byunguk Park, Biophysics Training Program, UW-Madison	<i>Fall 2021 – Present</i>
Joshua Richardson, Chemical and Biological Engineering, UW-Madison	<i>Fall 2021 - Present</i>
Lisa Je, Chemical and Biological Engineering, UW-Madison <i>Co-advised with Prof. Victor Zavala</i>	<i>Summer 2021 – Present</i>
Panzheng Zhou, Chemical and Biological Engineering, UW-Madison	<i>Fall 2019 – Present</i>
Shiyi (Amy) Qin, Chemical and Biological Engineering, UW-Madison <i>Co-advised with Prof. Victor Zavala</i>	<i>Fall 2019 – Present</i>

Former Ph.D. Students

Dr. Benginur Demir, Chemical and Biological Engineering, UW-Madison <i>Co-advised with Prof. James Dumesic</i>	<i>Fall 2019 – Summer 2020</i>
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Dr. Alex Chew, Chemical and Biological Engineering, UW-Madison	<i>Fall 2016 – Summer 2021</i>
Dr. Bradley Dallin, Chemical and Biological Engineering, UW-Madison	<i>Fall 2016 – Summer 2021</i>
Dr. Samarhaben Patel, Chemical and Biological Engineering, UW-Madison	<i>Fall 2016 – Summer 2021</i>
Dr. Jonathan Sheavly, Chemical and Biological Engineering, UW-Madison	<i>Fall 2017 – Summer 2022</i>

Former M.S. Students

Atharva Kelkar, Chemical and Biological Engineering, UW-Madison	<i>Fall 2018 – Summer 2021</i>
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Current Postdoctoral Researchers

Dr. Juriti Rajbangshi, Chemical and Biological Engineering, UW-Madison	<i>Summer 2022 – Present</i>
Dr. Alvaro Posada-Borbón, Chemical and Biological Engineering, UW-Madison <i>Co-advised with Prof. Manos Mavrikakis and Prof. Victor Zavala</i>	<i>Fall 2021 – Present</i>
Dr. Jianping Li, Chemical and Biological Engineering, UW-Madison <i>Co-advised with Prof. Christos Maravelias</i>	<i>Summer 2020 – Present</i>

Former Postdoctoral Researchers

Dr. Zeynep Sümer, Chemical and Biological Engineering, UW-Madison	<i>Spring 2021 – Summer 2022</i>
Dr. Zhizhang Shen, Chemical and Biological Engineering, UW-Madison	<i>Fall 2018 – Fall 2020</i>

Undergraduate Researchers / Summer Interns

Nicole Babineau, REU student	<i>Summer 2022</i>
Natalia Ramos Acevedo, REU student	<i>Summer 2022</i>
Steven Yeo, UW-Madison undergraduate	<i>Fall 2021 - Present</i>
Dane Christiansen, Undergraduate Research Scholars student	<i>Fall 2021 - Present</i>
Elizabeth Griffin, REU student	<i>Summer 2021</i>
Mariela R. Rodriguez-Otero, REU student	<i>Summer 2021</i>
Luis Roberto Padilla, REU student	<i>Summer 2021</i>
Kourtney Reed, REU student	<i>Summer 2021</i>
Devesh Shah, UW-Madison Master's student (CS)	<i>Summer 2021</i>
Vedaant Tambi, UW-Madison undergraduate (CS)	<i>Spring 2020 – Spring 2021</i>
Wei He, UW-Madison undergraduate	<i>Spring 2020 – Fall 2020</i>
Isabella Wegner, UW-Madison undergraduate	<i>Summer 2019</i>
Herry Jin, UW-Madison undergraduate	<i>Spring 2019 – Summer 2020</i>
Ricardo Mathison, UW-Madison undergraduate	<i>Fall 2018 – Spring 2019</i>
Zhiwen Zhang, UW-Madison undergraduate	<i>Fall 2018 – Spring 2019</i>
Alexis Oswalt, REU student (Nanotechnology)	<i>Summer 2018</i>
Jack Euclide, UW-Madison undergraduate	<i>Spring 2018 – Summer 2018</i>
Geyao Gu, REU student (Theoretical Chemistry)	<i>Summer 2017</i>
Bret Wolter, UW-Madison undergraduate	<i>Summer 2017 – Fall 2018</i>
Seth Winger, UW-Madison undergraduate	<i>Summer 2017 – Fall 2018</i>
Sakura Kawano, UW-Madison undergraduate	<i>Fall 2016 – Spring 2018</i>
Collin Davda, Caltech undergraduate	<i>Summer 2015 – Spring 2016</i>
Sang Hyun Choi, MIT undergraduate	<i>Fall 2013 – Spring 2014</i>
Paul Jones, MIT-Imperial College exchange student	<i>Summer 2013</i>
Maxwell Plaut, MIT undergraduate	<i>Fall 2012</i>
Karthik Chellamuthu, Research Science Institute high school student	<i>Summer 2012</i>
Tiffany Tang, MIT undergraduate	<i>Fall 2011 – Spring 2012</i>
Alec Garza-Gallindo, MIT undergraduate	<i>Fall 2011 – Spring 2012</i>
Qian Lin, MIT undergraduate	<i>Fall 2010 – Spring 2011</i>
Eriko Iwatate, Center for Materials Science and Engineering REU Intern	<i>Summer 2010</i>

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), 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*, 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:

- Liaison Director for AIChE Computational Molecular Sciences and Engineering Forum *Fall 2021-Present*
- 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*

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*