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Liqun (Laura) Zhang

Education

Postdoc, Physiology and Biophysics 02/2015
Case Western Reserve University Cleveland, OH, USA
Advisor: Matthias Buck

Postdoc, Chemical Engineering 07/2009
Case Western Reserve University Cleveland, OH, USA
Advisor: Daniel J. Lack

Ph.D., Chemical Engineering 12/2007
University of Rhode Island Kingston, Rhode Island, USA
Advisor: Michael L. Greenfield
Thesis title: "Physical and Mechanical Properties of Model Asphalt Systems Calculated Using Molecular Simulation"

B.S,M.S.,Chemical Engineering 04/2003
Zhejiang University Hangzhou, China

Research Experiences

University of Rhode Island, Kingston, RI Chemical Engineering
Assistant Professor Research 06/2023-current

- Investigated the structure, dynamics and functional properties of SARS-CoV-2 and accessory proteins binding with ACE2 receptor and natural antimicrobial peptides Human Beta Defensins in collaboration with experimentalists and bioinformatics in Univeristy of Tennesee Chattanooga and Case Western Reserve University

1910 Genetics Inc., Boston, MA Computational Chemistry
Computational Chemist 05/2022-Current

- Apply molecular dynamics simulations and different drug design programs to design drugs to combat cancer and Alzheimer diseases using structure-based and ligand-based drug design methods in collaboration with AI and biology teams in the company

Tennessee Technological University,Cookeville, TN Chemical Engineering
Assistant Professor 08/2015-05/2022

- Investigated the structure, dynamics and functional properties of Human Beta Defensin type 3 interaction with lipid membrane, and chemokine receptor CXCR4 receptor in collaboration with experimentalists in Louisiana State University and Case Western Reserve University
- Studied the structure, dynamics, and interaction of human defensin and covid-19 viruses in collaboration with experimentalists in the Medical School and Dental School in Case Western Reserve University
- Performed LAMMPS and CHARMM molecular dynamics simulations to study the chemical composition, microstructure and physical and mechanical properties of biomass modified asphalt at different temperatures; collaborated with a lithium ion battery startup company working on microstructure design of anodes

Case Western Reserve University, Cleveland, OH School of Medicine
Postdoctoral Research Associate 07/09-07/15

- Investigated the structure and dynamics of the complexes between transmembrane protein plexin and Rho family GTPases using both CHARMM and NAMD molecular dynamics simulations, and docking programs: HADDOCK, Rosettadock, XPLOR-NIH
- Worked on plexin transmembrane monomer/dimmer/trimer in lipid bilayers by performing CHARMM, NAMD, and Anton molecular dynamics simulations to understand the relationships among plexin dynamics, structure, and functional mechanism
- Performed microsecond-long molecular dynamics simulations on EphA2-SHIP2 SAM:SAM heterodimer to investigate its dynamics and structure properties, and the diverse functional mechanism

Case Western Reserve University, Cleveland, OH Chemical Engineering and Geological Science
Postdoctoral Research Scholar 01/08- 06/09

- Performed Ab Initio VASP simulation on silicate melts and minerals with/without a noble gas；analyzed sitting and dynamic properties of noble gas in silicate melts and minerals at different temperature and pressure conditions
- Calculated thermodynamic properties of binary silica joins using both first principles and empirical molecular dynamics simulations; Analyzed factors influencing neutral species and charged small particles transport behavior inside silica melts; investigated isotopes transport behavior in silicate

University of Rhode Island, Kingston, RI Chemical Engineering
Graduate Assistant 09/03-12/07

- Worked on Linux system and multiple CPU platforms; implemented molecular simulation source code using Fortran; extended atom-based OPLS-aa force field in Monte Carlo simulation (Towhee)
- Created model asphalt mixtures for molecular simulation input; performed molecular simulation on original and polymer modified asphalt system using parallel molecular dynamics (Lammps) and Monte Carlo (Towhee) methods
- Calculated transport properties by relaxation autocorrelation function analysis; calculated density, heat capacity, isothermal compressibility and expansion coefficient of pure compounds and mixtures; analyzed molecular orientation, radial distribution function and solubility parameters of molecules in the system

Teaching Experience

- **Developed** and taught graduate and undergraduate level class CHE6810 (Protein Biophysics & Simulations) in Fall of 2015, 2017, 2018, 2019, Spring of 2022
- Taught undergraduate level class CHE3010 (Thermodynamics of Chemical Process) in Fall of 2016, 2020
- Taught undergraduate level class CHE3021 (Separation and Solution Thermodynamics) in Spring of 2016, 2017, 2018, 2019, and 2020
- Team taught undergraduate level class CHE4420: Process Design II in the Spring of 2016, 2017, 2018, 2019 and 2020
- Taught graduate level class CHE6010 (Advanced Chemical Engineering Thermodynamics) in Fall of 2019, 2021
- Taught undergraduate level class CHE3730/3735 (Chemical Engineering Operations) in Spring of 2021

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Awards and Fellowships

- **Ruth Kirschstein NRSA Postdoc Fellowship**, NIH, 2012-2014
- **Poster presentation 2nd place**, 2014 Annual Retreat Poster Award, Department of Physiology and Biophysics, Case Western Reserve University, 2014
- **Excellence in Doctoral Research in the Area of Science, Technology, Engineering and Mathematics**, University of Rhode Island, 2008
- **New England Institute of Chemists Graduate Student Award**, American Institute of Chemists, 2006-2007
- **Excellent student scholarship**, Zhejiang University, 2000-2001

Professional Activities

Editorial Board

- Reviewer board member of Membrane (ISSN 2077-0375) (2020-current)
- Guest Editor of the "Computational Data-Driven Design and Modeling of Biomolecules and Biomimetics" in the honor of Professor Ruth Nussinov special issue (2020-current)

Conference Chair

- Session co-chair of Computational Molecular Science and Engineering Forum program, Annual Meeting of the American Institute of Chemical Engineering. Event title:" "Molecular Simulation of Protein Adsorption and Molecular Recognition Processes" (2017)
- Session chair/co-chair of Engineering Sciences and Fundamentals program, Annual Meeting of the American Institute of Chemical Engineers. Event title: "Effects of Confinement on Molecular Properties" (2018- present)

Membership

- Society of Woman Engineers (SWE) (2016-current)
- American Institute of Chemical Engineers (2003-current)
- American Chemical Society (2005-current)
- Biophysical Society (2009-current)
- Affiliated Member of American Association of Cancer Research (AACR) (2016-current)

Funding Endeavors

External Funding (including Resource Funding) Awarded

- NSF Predictive Intelligence for Pandemic Prevention (PIPP) Phase I (2022-2024)
- NSF SBIR Phase I (2020-2022)
- CWRU COVID-19 Patients grant (2020- 2021)
- DOD Department of Army STTR Phase I (2019 –2020)
- Burroughs Wellcome Fund, Collaborative Research Travel Grant (2018-2019)
- Extreme Science and Engineering Discovery Environment (XSEDE), Supercomputer time award (2015-2022)
- Pittsburgh Supercomputing Center - Anton Supercomputer Time (2018-2022)

Internal Funding Awarded

- Faculty Research Award, TTU (2017-2018, 2019-2020, 2021-2022)

Supervised students/visiting scholar

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Alumni

- Rabeta Yeasmin (2016-2020)
- Kolawole Sonibare (2017-2019)
- Yilun Lee (2017-2019)
- Chuanxing Zhan (2017-2019)
- Jackson Penfield (2019-2021)
- George Rucker (2020-2022)
- In total 13 undergraduate researchers each was trained in Dr. Zhang lab for more than 1 year, including Joshua Berry (2015-2017), Lela Fine (2019-2021), Ann Brewer (2020-2022)

Visiting scholar

- Prof. Chuansheng Wu, Chongqing Jiaotong University, Chongqing, China, 400074 (12/2016-05/2017)

Invention Disclosure

- Liqun Zhang, Aaron Weinberg, Matthias Buck, Parameswaran Ramkrishnan, Santosh K. Ghosh, Arnold Caplan, Tracey Bonfield, "Antimicrobial peptides and their derivatives as novel therapeutics to treat viral related illness", filed in Case Western Reserve University, 03/24/2020.

Publications

Journal

1. Liqun Zhang, Santosh K. Ghosh, Shrikanth C. Basavarajappa, Jeannine Muller-Greven, Jackson Penfield, Ann Brewer, Parameswaran Ramakrishnan, Matthias Buck, and Aaron Weinberg, "HBD-2 binds SARS-CoV-2 RBD and blocks viral entry: Strategy to combat COVID-19", ***iScience***, **2022**, Volume 25, Issue 3, 103856.
2. Liqun Zhang," Interaction of Human β Defensin Type 3 (hBD-3) with Different PIP2-containing Membranes, a Molecular Dynamics Simulation Study", ***Journal of Chemical Information and Modeling***, **2021,** 61, 9, 4670–4686. doi:10.1021/acs.jcim.1c00805.
3. Liyanage D Fernando, Malitha C Dickwella Widanage, Jackson Penfield, Andrew S Lipton, Nancy Washton, Jean-Paul Latgé, Ping Wang, Liqun Zhang, Tuo Wang," Structural Polymorphism of Chitin and Chitosan in Fungal Cell Walls from Solid-State NMR and Principal Component Analysis", ***Frontiers in Molecular Biosciences***, **2021**. Volume 8, 727053. https://doi.org/10.3389/fmolb.2021.727053.
4. Ann Brewer, Liqun Zhang, "Binding Free Energy Calculation of Human Beta Defensin 3 with Negatively Charged Lipid Bilayer Using Free Energy Perturbation Method", ***Biophysical Chemistry***, 277, 106662, **2021**.
5. Rabeta Yeasmin, Ann Brewer, Lela Fine, Liqun Zhang, "Molecular Dynamics Simulations on Human Beta Defensin Type 3 Crossing Different Lipid Bilayers", ***ACS Omega***, 6, 21, 13926–13939, **2021**.
6. Kolawole Sonibare, George Rucker, Liqun Zhang, "Molecular Dynamics Simulation on Vegetable Oil Modified Model Asphalt", ***Construction and Building Materials***, 270, 121687, **2021**.
7. Jianying Hu, Liqun Zhang, Xijin Zhang, Yuan Guo, Xiong Yu,"Comparative evaluation of moisture susceptibility of modified asphalt and foamed asphalt using surface free energy approach", ***Construction and Building Materials***, 256, 119429, **2020**.
8. Liqun Zhang,"Disulfide Bonds Affect the Binding Sites of Human beta Defensin Type 3 On Negatively Charged Lipid Membranes", ***Journal of Chemical Physics B***. 124, 11, 2088–2100. **2020**. https://doi.org/10.1021/acs.jpcb.9b10529.

9. George Rucker, Yu Xiong, Liqun Zhang, "Molecular Dynamics Investigation on n-Alkane-Air/Water Interfaces", ***Fuel***, 267, 117252, **2020**. https://doi.org/10.1016/j.fuel.2020.117252.
10. Kolawole Sonibare, Lasantha Rathnayaka, Liqun Zhang, "Comparison of CHARMM and OPLS-aa forcefield predictions for components in one model asphalt mixture", ***Construction and Building Materials***, 236,117577, **2020**. https://doi.org/10.1016/j.conbuildmat.2019.117577.
11. Xue Kang, Christopher Elson, Jackson Penfield, Alex Kirui, Adrian Chen, Liqun Zhang+, Tuo Wang+, "Integrated solid-state NMR and molecular dynamics modeling determines membrane insertion of human β-defensin analog". ***Commun Biol***, 2, 402, **2019**.(+ shared corresponding authorship)
12. Rabeta Yeasmin, Matthias Buck, Aaron Weinberg, and Liqun Zhang, "Translocation of Human β Defensin Type 3 through a Neutrally Charged Lipid Membrane: A Free Energy Study", ***J. Phys. Chem. B***, 122 (50), 11883–11894. **2018**.
13. Liqun Zhang, "Investigation on two human defensin dimers: structure prediction and refinement using a combined simulation strategy", ***Molecular Simulation***, 44, 757-768, **2018**.
14. ChaoWang, BimingMo, Zhenfeng He,XiaofengXie, Cindy XinxinZhao, LiqunZhang, QianShao, XingkuiGuo, Evan K.Wujcik, ZhanhuGuo," Hydroxide ions transportation in polynorbornene anion exchange membrane", ***Polymer***,138,363-368, **2018**.
15. Jinbo Zhao, Lili Wu, Chuanxing Zhan, Qian Shao, Zhanhu Guo, Liqun Zhang,"Overview of polymer nanocomposites: Computer simulation understanding of physical properties", **Polymer**, 133, 272-287, **2017**. (Journal cover page)
16. Liqun Zhang, "Different Dynamics and Pathway of Disulfide Bonds Reduction of Two Human Defensins, a Molecular Dynamics Simulation Study". ***Proteins***. 85(4):665-681. doi: 10.1002/prot.25247. **2017**.
17. Liqun Zhang, Matthias Buck, "Molecular Dynamics Simulations Reveal Isoform Specific Contact Dynamics Between the Plexin Rho GTPase Binding Domain (RBD) and Small Rho GTPases Rac1 and Rnd1". ***J. Phys. Chem. B.***DOI: 10.1021/acs.jpcb.6b11022. **2017**.
18. Liqun Zhang, Susmita Borthakur, Matthias Buck, "Dissociation of a Dynamic Protein Complex Studied by All-Atom Molecular Simulations", ***Biophysical Journal***. 110, 877–886. **2016**.
19. Liqun Zhang, Anton Polyanski and Matthias Buck, "Modeling Transmembrane Domain Dimers/Trimers of Plexin Receptors: Implications for Mechanisms of Signal Transmission across the Membrane", ***PLOS ONE***., 10(4):e0121513. **2015**.
20. Liqun Zhang, Thomas Centa, Matthias Buck "Structure and Dynamics Analysis on Plexin-B1 Rho-GTPase Binding Domain Monomer and Dimer", ***J. Phys. Chem. B.*** 118(26):7302-11, **2014**.
21. Liqun Zhang, Matthias Buck "Molecular Simulations of a Dynamic Protein Complex: Role of Salt-Bridges and Polar Interactions in Configurational Transitions". ***Journal of Biophysics***. 105(10), 2421-2417, **2013**.
22. Mirco Zerbetto, Ross Anderson, Sabine Bouguet-Bonnet, Mariano Rech, Liqun Zhang, Eva Meirovitch, Antonino Polimeno, Matthias Buck,"Analysis of 15N-1H NMR relaxation in proteins by a combined experimental and molecular dynamics simulation approach: Picosecond-nanosecond dynamics of the Rho GTPase binding domain of plexin-B1 in the dimeric state", ***J. Chem. Phys. B***, 117(1), 174-184, **2013**.
23. Liqun Zhang, Alexander Sodt, Rick M.Venable, Richard W. Pastor, Matthias Buck, "Prediction and Refinement of ErbB1/B2 and EphA1 Transmembrane Dimers from Microsecond MD Simulations", ***Proteins***. 81(3), 365-76. **2013**.

24. Gaurav Goel, Liqun Zhang, Daniel J. Lacks, James Van Orman, "Isotope fractionation by diffusion in silicate melts: Insights from molecular dynamics simulations", ***Geochimica et Cosmochimica Acta***, 93(15), 205-213, **2012**.
25. HyeongJu Lee, Prasanta K. Hota, Preeti Chugha, Hui Miao, Liqun Zhang, SoonJeung Kim, Rebecca S. Alviani, Lukas Stetzig, Bing-Cheng Wang, B, Matthias Buck "Refined NMR structure of a heterodimeric SAM:SAM complex. Characterization and manipulation of the EphA2 interface leads to new cellular functions of SHIP2." ***Structure***, 20, 41-55, **2012**.
26. Mehdi Bagheri Hamaneh+, Liqun Zhang+, Matthias Buck, "A direct coupling between global and internal motions in a single domain protein? A molecular dynamics investigation of extreme case scenarios", ***Biophysical Journal***, 101, 196-204, **2011** (+ shared first authorship).
27. Liqun Zhang, "Thermodynamic properties calculation for MgO-SiO2 liquids using both empirical and first-principle molecular simulations", ***Physical Chemistry Chemical Physics***, 13, 21009-21015, **2011**.
28. Liqun Zhang, James Van Orman, Daniel J. Lacks, "Molecular dynamics investigation of liquid MgO-CaO-SiO2 as a function of composition and pressure", ***Chemical Geology***, 275, 50-57, **2010**.
29. Liqun Zhang, Michael L. Greenfield, "Rotational relaxation time of individual compounds from simulations of molecular asphalt models", ***Journal of Chemical Physics,*** 132,184502, **2010**.
30. Liqun Zhang, James Van Orman, Daniel J. Lacks, "The influence of atomic size and charge of dissolved species on the diffusivity and viscosity of silicate melts", ***American Mineralogist Letter***, 94, 1735-1738, **2009**.
31. Liqun Zhang, Daniel J. Lacks, James Van Orman, "Diffusivity calculation on noble gas silica systems using first principles molecular simulations", ***Molecular Simulation***, 35, 942-952, **2009**.
32. Liqun Zhang, Daniel J. Lacks, James Van Orman, "Effective radii of noble gas atoms in silicates from first principles molecular simulation", ***American Mineralogist***, 94, 600-608, **2009**.
33. Liqun Zhang, Michael L. Greenfield, "Polymer modification effects to model asphalt systems", ***Energy & Fuels***, 22(5), 3363-3375. **2008.**
34. Liqun Zhang, Michael L. Greenfield, "Relaxation time, diffusion, and viscosity analysis of model asphalt systems using molecular simulation", ***Journal of Chemical Physics***, 127, 194502, **2007**.
35. Liqun Zhang**,** Michael L.Greenfield, "Analyzing properties of model asphalts using molecular simulation", ***Energy & Fuels***, 21, 1712-1716, **2007**.
36. Liqun Zhang**,** Michael L.Greenfield, "Molecular orientation in model asphalts using molecular simulation", ***Energy & Fuels***, 21, 1102-1111, **2007**.
37. Liqun Zhang, Bo Lu, Zhirong Cheng, "Study on mechanism and kinetics of oxidizing reaction of pinane to hydroperoxide", ***Chemical Reaction Engineering and Technology***, 18, 225-230, **2002**.

Book Chapter

38. Liqun Zhang, Sabine Bouguet-Bonnet, Matthias Buck, "Combining NMR and Molecular Dynamics Studies for Insights into the Allostery of Small GTPase–Protein Interactions", Allostery Methods in Molecular Biology, 2012, Volume 796, Part 3, 235- 259, DOI: 10.1007/978-1-61779-334-9_13.

Manuscripts In Review

39. Jackson Penfield, Liqun Zhang, "Comparative Study on the Structure and Dynamics of Chemokine Receptor CXCR4 with CXCL12 and hBD-3", submitted to ***ACS Pharmacology & Translational Science***, 2023.
40. George R Rucker, Jackson Penfield, Mouhmad Elayyan, and Liqun Zhang, "Structure and Dynamics of Human Beta Defensin Type 3 in Different Negatively Charged Lipid Membranes", Submitted to ***Protein***, 2023.
41. George Rucker, Liqun Zhang, "Comparison of the Interaction and Structure of Lignin in Pure System and in Asphalt Media by Molecular Dynamics Simulations", Submitted to ***ACS Sustainable Chem. Eng.***, 2023.
42. George Rucker, Liqun Zhang, "Molecular Dynamics Simulation on Polymer Modified Model Asphalt", Submitted to ***Environmental Science and Pollution Research***, 2023.
43. George Rucker, Hong Qin, Liqun Zhang, "Structure, Dynamics and Free Energy Studies on the Effect of Spot Mutations on SARS-CoV-2 Spike Protein Binding with ACE2 Receptor", submitted to ***Plos One***, 2023.

Conferences

1. George Rucker, John Choy, Letu Qingge, Ziwei Ma, Qin Hong, Liqun Zhang, "Molecular Dynamics Simulation on Spike Protein Mutants Binding with ACE2 Receptor and Human β Defensin Type 2", ACS Northeast Regional Meeting (NERM), Boston, MA, 2023.
2. Praveen Pilyanam , Liqun Zhang, "Molecular Dynamics Investigation on Branched Alkane-Air/Water Interfaces", AIChE meeting, Phoenix, AZ, 2022.
3. Jackson Penfield, Liqun Zhang, "Molecular Dynamics Simulation on Human β Defensin Type 3 Binding with the CXCR4 Receptor", AIChE meeting, Boston, MA, 2021.
4. George Rucker, Liqun Zhang, "Molecular Dynamics Study of Asphalt-Water/Air Interface Systems", AIChE meeting, Boston, MA, 2021.
5. Ann Brewer, Liqun Zhang," Free Energy Calculation on Human Beta Defensin Translocation through Bacterial Lipid Membranes", AIChE meeting, Boston, MA, 2021.
6. Wentao Li, Yue Zhou, Liqun Zhang, Brett Lucht, Xiao-Guang Sun, et al, "Solving Lithium Dendrite Problems through Structure Design of Advanced Metal Anodes for Lithium Metal Batteries", The Electrochemical Society (ECS) virtual meeting, 2021.
7. Jackson Penfield, Matthias Buck, Parameswaran Ramakrishnan, Santosh Ghosh, Aaron Weinberg, Liqun Zhang, "Interaction and Binding of Human Beta Defensin Type 2 with SARS-CoV-2 RBD", ACS virtual meeting, 2021.
8. Jackson Penfield, Mouhmad Elayya, George Rucker, Liqun Zhang,"Binding of Human β defensin with Different Lipid Membranes During Translocation", Finding Your Inner Modeler Virtual Conference, 2021.
9. Jackson Penfield and Liqun Zhang, "Molecular dynamics simulation on human beta-defensin type 3 binding with CXCR4 receptor", AIChE virtual meeting, 2020.
10. George Rucker and Liqun Zhang, "Molecular Dynamics Simulation on Original and Polymer Modified Asphalt Mixtures", AIChE virtual meeting, 2020.
11. Rabeta Yeasmin and Liqun Zhang, "Binding Free Energy Calculation on Human Beta Defensin Type 3 on Bacterial Membrane", AIChE virtual meeting, 2020.
12. Nutchanok Keerakiatwong and Liqun Zhang, "Structure and Dynamics of Human Beta Defensin Interacting with Bacterial Lipid Membranes", AIChE virtual meeting, 2020.
13. Liqun Zhang, "Binding and Interaction of Human Beta Defensin Type with Mixed PIP2 Lipid Membranes", Biophysical Society meeting, San Diego, CA, 2020.

14. Mouhmad Elayyan, George Rucker, Yilun Lee, Rabeta Yeasmin, Liqun Zhang," Molecular Dynamics Simulation on Interaction of Human Beta Defensin Type 3 with Different Lipid Bilayers", AIChE meeting, Orlando, FL, 2019.
15. Jackson S. Penfield, Liqun Zhang," Molecular Dynamics Simulation on Human Beta-Defensin Type 3 Binding with CXCR4 Receptor", AIChE meeting, Orlando, FL, 2019.
16. Rabeta Yeasmin and Liqun Zhang," Free Energy Calculation on Human β Defensin Type 1 in Different Redox Conditions", AIChE meeting, Orlando, FL, 2019.
17. Kolawole Sonibare, Loukas Petridis, and Liqun Zhang, "Molecular Dynamics Simulations of Biomass-Modified Model Asphalt", AIChE meeting, Orlando, FL, 2019.
18. Yilun Lee, Liqun Zhang, "Molecular Dynamic Simulation Study on the Air/Water-Alkanes Interface Systems", AIChE meeting, Orlando, FL, 2019.
19. Rabeta Yeasmin, Mouhmad Elayya, George Rucker, Yilun Lee, Liqun Zhang, "Molecular Dynamic Simulations on Human β Defensin Type 3 Embedded in Different Lipid Bilayers", Finding Your Inner Modeler III workshop, University of Alabama at Birmingham, Birmingham, AL, 2019.
20. Christopher Elson, Liqun Zhang, "Molecular Simulation on Human Beta Defensin Type 3 Interaction with Lipid Membranes", AIChE meeting, Pittsburg, PA, 2018.
21. Rabeta Yeasmin, Liqun Zhang, "Translocation Energy Calculation on Human β Defensin Type 3 through Bacterial Lipid Membranes", AIChE meeting, Pittsburg, PA, 2018.
22. Liqun Zhang, "Free Energy Study on hBD-3 Translocation on Lipid Membrane", Biophysical Society Meeting, San Francisco, CA, 2018.
23. Rabeta Yeasmin, Liqun Zhang, "Study of Interaction and Transpassing of Human Beta Defensin-3 with Popg and Pops Membrane", AIChE meeting, Minneapolis, 2017.
24. Liqun Zhang, "Predicting the Dimer Structure of Defensins Using a Combined Simulation Strategy", AIChE meeting, Minneapolis, 2017.
25. Liqun Zhang, Zhiming Feng, Aaron Weinberg, "Human Beta Defensin Type 3 Interaction with Chemokine Receptor CXCR4", Biophysical Society meeting, New Orleans, LA, 2017.
26. Liqun Zhang, "Investigation on the Pathway of Disulfide Bonds Reduction on Human Defensins Using Molecular Dynamics Simulations", AIChE, San Francisco, CA, 2016.
27. Liqun Zhang, Esmaeel Azadian, "Investigation on the Interaction between Human Beta Defensin Type 3 (hBD-3) and Ectodomain of EphA2 Receptor using Molecular Dynamics Simulation Method", American Association of Cancer Research, New Orlands, LA, 2016.
28. Liqun Zhang, Thomas Centra, Matthias Buck, "Investigation on Plexin Rho GTPase Binding Domain Binding with Small Rho GTPases using Molecular Dynamics Simulations", Biophysical Society meeting, Los Angeles, CA. 2016.
29. Liqun Zhang, Matthias Buck, "Investigation on the Interaction between Plexin Intracellular Plus Transmembrane Domains with GTPases and with the Lipid Bilayer Using All-atom Molecular Dynamics Simulations", Biophysical Society meeting, Baltimore, MD. 2015.
30. Liqun Zhang, Matthias Buck, "Structure and dynamic properties analysis of plexin-B1 Rho-GTPase binding domain as a monomer and dimer", ACS. Dallas,TX. 2014.
31. Liqun Zhang**,** Matthias Buck, "Structure and Dynamics of the Plexin-B1 Transmembrane Receptor bound to GTPases" Biophysical Society meeting, San Francisco, CA. 2014.
32. Liqun Zhang, Matthias Buck, "Investigation of the Structure and Dynamics of Heterodimeric Sam-Sam complexes using Microsecond Molecular Dynamics Simulations". Biophysical Society meeting, Philadelphia, PA. 2013.

33. Liqun Zhang, Alexander Sodt, Rick Venable, Richard W. Pastor, Matthias Buck, "Molecular dynamics prediction and refinement of transmembrane helix dimers", Biophysical Society meeting, San Diego, CA. 2012.
34. Liqun Zhang, James Van Orman, Daniel Lacks, "Molecular dynamics investigation of MgO-CaO-SiO2 melts: influence of pressure and composition on density and transport properties", ACS. Boston, MA. 2010.
35. Liqun Zhang, Matthias Buck, "Differential dynamics coupling of plexin GTPase complexes in MD Simulations", ACS. Boston, MA. 2010.
36. Liqun Zhang, Matthias Buck, "Molecular dynamics simulations of the plexin Trans- and Juxta-membrane region in a DPPC lipid bilayer: application of the primary hydration shell model", Computational Biophysics to Systems Biology Workshop. Traverse city, MI. 2010.
37. Liqun Zhang, Daniel J. Lacks, James Van Orman, "Investigation on transport properties of generic species in silicate melts using molecular simulations". Midwest Thermodynamics and Statistical Mechanics Conference. Detroit, MI. 2009.
38. Liqun Zhang, Daniel J. Lacks, James Van Orman, "First principles simulations of noble gases dissolved in liquid silica", AIChE. Philadelphia, PA. 2008.
39. Liqun Zhang, Michael L. Greenfield, "Viscosity calculation in model asphalt system", AIChE. San Francisco, CA. 2006.
40. Liqun Zhang, Michael L. Greenfield. "Orientation calculation for model asphalt mixture using molecular simulation", AIChE, Cincinnati, OH. 2005.
41. Liqun Zhang, Michael L. Greenfield, "Developing model asphalt systems using molecular simulation", AIChE. Austin, TX. 2004.

Invited Presentations

1. Jackson Penfield, Liqun Zhang, "SARS-Covid-19 virus RBD domain binding and interaction with human beta defensin type 2", invited by "Pandemic Advance Capabilities and Engineering" session of AIChE virtual meeting, Nov. 18th, 2021.
2. Liqun Zhang, "Free-energy studies on human β defensin type 3 through a neutrally charged lipid membrane", ACS Spring 2019 National Meeting & Exposition, April 4th, 2019, invited by the "Simulation of protein-membrane interfaces" symposium chair and co-chair Prof. Matthias buck and Prof. Alemayehu Gorfe.
3. Liqun Zhang, "Binding and Interaction of Human Beta Defensin Type 3 with Lipid Membranes". University of Tennessee, Graduate School of Medicine, Oct. 16th, 2018.
4. Liqun Zhang, "Investigation on Model Asphalt and Human β Defensin Type 3 Using Molecular Dynamics Simulations", invited by Prof. Wenyin Li, Taiyuan University of Technology, Taiyuan, China, May, 30th, 2018.
5. Liqun Zhang, "Molecular Dynamic Simulations on Human β Defensin Type 3", invited by Prof. Yi He, Zhejiang University, Hangzhou, China, May, 18th, 2018.
6. Liqun Zhang, "Molecular Dynamic Simulations on Human β Defensin Type 3", invited by Prof. Dapeng Cao, Beijing University of Technology, Beijing, China, May, 24th, 2018.
7. Liqun Zhang, "Molecular Dynamic Simulations on Human β Defensin Type 3", invited by Prof. Zhending Su, Hubei University of Technology, Wuhan, China, May, 28th, 2018.
8. Liqun Zhang, "Molecular Dynamics Simulation on Model Asphalt and Silica Melts", Case Western Reserve University, Cleveland. OH. 2017(Invited by Dr. Yu Xiong).
9. Liqun Zhang, "Investigation on Human Beta Defensin Type 3 Using Computer Simulation Methods". University of Tennessee, Graduate School of Medicine, Nov. 21st, 2017.

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10. Liqun Zhang, "Molecular Dynamics Simulation on Human Beta Defensin Type 3", Oak Ridge National Lab, Dec. 11th, 2017 (Invited by Dr. Jeremy Smith).
11. Liqun Zhang, "Investigation on Model Asphalts and Silica Melts Using Molecular Dynamics Simulations". University of Tennessee, Knoxville, TN. 2015 (Invited by Dr. Baoshan Huang).