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Liqun Zhang

Education

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"

M.S.,**B. S.,** Chemical Engineering
Zhejiang University Hangzhou, China

Research Experiences

Tennessee Technological University,Cookeville, TN Chemical Engineering
Assistant Professor 08/15-present

- Perform CHARMM and NAMD molecular dynamics simulations to investigate the structure, dynamics and functional properties of Human Beta Defensin type 3 interaction with EphA2 & EphrinA1 complex.
- Perform Monte Carlo and LAMMPS molecular dynamics simulations to understand the Processing-Structural-Performance Relationship in Asphalt Mix Technology .

Case Western Reserve University, Cleveland, OH School of Medicine
Postdoc Research Associate 07/09-02/15

- Perform CHARMM and NAMD molecular dynamics simulations to investigate the structure, dynamics and functional properties of human beta defensin type 3 interaction with C C chemokine receptors: CXCR4, CCR2b.
- Investigate 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.
- Work 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.
- Perform 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**
Postdoc 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.

Awards and Fellowships

- **Poster presentation 2nd place**, 2014 Annual Retreat Poster Award, Department of Physiology and Biophysics, 2014.
- **Ruth Kirschstein NRSA Postdoc Fellowship**, NIH, 2012-2014.
- **Travel awards to attend the Biophysics Society meeting,** sponsored by the Education, Minority Affairs, and Professional Opportunities for Women Committees. February, 15-19, San Francisco, California, 2014**.**
- **Travel awards to attend the Expanding Cross-Disciplinary Dialogue workshop,** sponsored by NSF, April, Arlington, VA, 2012.
- **Travel awards to attend the Engaging Difference: Diverse Women in STEM Building Careers, Creating Alliances workshop,** University of Virginia in Charlottesville, VA, 2011.
- **Travel awards to present seminar at Computational Biophysics to Systems Biology (CBSB10) Workshop**, Traverse City, MI, 2010.
- **Postdoc Travel awards for National Summit on Gender and Postdoctorate**, sponsored by NAP and NSF, March, Philadelphia, PA, 2010.
- **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.

Grants

- **New faculty startup package, Tennessee Technological University, 08/2015-07/2018**
- **K25, National Cancer Institute (NCI) Mentored Quantitative Research Career Development Awards, 2015.**

  Role: PI

  Project Title: "Investigation on hBD-3 Structure, Dynamics and Interactions with Chemokine and EPH Receptors"

  Status: Pending

Presentations

- 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. Baltimore, MD, 2015.

- 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.
- Liqun Zhang**,** Matthias Buck, "Structure and Dynamics of the Plexin-B1 Transmembrane Receptor bound to GTPases" Biophysical Society. San Francisco, CA, 2014.
- Liqun Zhang, Matthias Buck, "Investigation of the Structure and Dynamics of Heterodimeric Sam-Sam complexes using Microsecond Molecular Dynamics Simulations". Biophysical Society, Philadelphia, PA, 2013.
- Liqun Zhang, Alexander Sodt, Rick Venable, Richard W. Pastor, Matthias Buck, "Molecular dynamics prediction and refinement of transmembrane helix dimers", Biophysical Society, San Diego, CA, 2012.
- 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", Amer. Chem. Soc., Boston, MA, 2010.
- Liqun Zhang, Matthias Buck, "Differential dynamics coupling of plexin GTPase complexes in MD Simulations", ACS, Boston, MA, 2010.
- 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.
- 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.
- Liqun Zhang, Daniel J. Lacks, James Van Orman, "First principles simulations of noble gases dissolved in liquid silica", AIChE, 2008, Philadelphia, PA.
- Liqun Zhang, "Structure and Freezing of MgSiO3 Liquid in Earth's Lower Mantle", Science and Nature club, 2008, Case Western Reserve University, Cleveland, OH.
- Liqun Zhang, Michael L. Greenfield, "Viscosity calculation in model asphalt system", AIChE, 2006, San Francisco, CA.
- Liqun Zhang, Michael L. Greenfield. "Orientation calculation for model asphalt mixture using molecular simulation", AIChE, 2005, Cincinnati, OH.
- Liqun Zhang, Michael L. Greenfield, "Research on asphalt using molecular simulation", 2005, University of Rhode Island, Kingston
- Liqun Zhang, Michael L. Greenfield, "Developing model asphalt systems using molecular simulation", AIChE, 2004, Austin, TX.

Journal Publications

- Liqun Zhang, Susmita Borthakur, Matthias Buck "Molecular Simulations of a Dynamic Protein Complex: Role of Polar Interactions and Solvent in the Process of Protein Dissociation", submitted to ***Biophysical Journal***. 2015.
- 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**.
- 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**.
- 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**.

- 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**.
- 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**.
- Gaurav Goel, Liqun Zhang, Daniel J. Lacks, James A. Van Orman, "Isotope fractionation by diffusion in silicate melts: Insights from Molecular dynamics simulations", ***Geochim. Cosmochim. Acta***, 93, 205-213. **2012**.
- 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**.
- 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**.
- 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).
- 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**.
- Liqun Zhang, Michael L. Greenfield, "Rotational relaxation time of individual compounds from simulations of molecular asphalt models", ***Journal of Chemical Physics,*** 132,184502, **2010**.
- 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**.
- 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**.
- 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**.
- Liqun Zhang, Michael L. Greenfield, "Polymer modification effects to model asphalt systems", ***Energy & Fuels***, 22(5), 3363-3375. **2008.**
- 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**.
- Liqun Zhang**,** Michael L.Greenfield, "Analyzing properties of model asphalts using molecular simulation", ***Energy & Fuels***, 21, 1712-1716, **2007**.
- Liqun Zhang**,** Michael L.Greenfield, "Molecular orientation in model asphalts using molecular simulation", ***Energy & Fuels***, 21, 1102-1111, **2007**.
- 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

- 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.