Ruibin Liang

Department of Chemistry and Biochemistry
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Google Scholar webpage
Personal Webpage

Professional Experience

Assistant Professor 2020-present
Department of Chemistry and Biochemistry
Texas Tech University, Lubbock, TX

Postdoctoral Scholar 2017-2020
Department of Chemistry, **Stanford University,** Stanford, CA
Research advisor: **Professor Todd J. Martínez**

Postdoctoral Scholar 2016-2017
Department of Chemistry**, University of California, Berkeley,** Berkeley, CA
Research advisor: **Professor William H. Miller**

Education

Ph.D. in Theoretical and Computational Chemistry 2016
The University of Chicago, Chicago, IL
Research advisor: **Professor Gregory A. Voth**

M.S. in Theoretical and Computational Chemistry 2012
The University of Chicago, Chicago, IL

B.S. in Chemical Biology 2011
Tsinghua University, Beijing, China

Honors and Awards

Maximizing Investigators' Research Award, National Institutes of Health 2023
Research Grant from the Welch Foundation 2022
Chemical Computing Group Excellence Award 2015
American Chemical Society National Meeting

The Windt Memorial Fund Graduate Fellowship 2015
The University of Chicago

Outstanding Young Researcher Award 2015
From Computational Biophysics to Systems Biology" (CBSB) conference

Zongcheng Zheng Academic Excellent Scholarship 2010

Tsinghua University

Wang Yong Academic Excellent Scholarship 2009

Tsinghua University

Zengjue Sun Academic Excellent Scholarship 2008

Tsinghua University

Funding

National Institutes of Health (Grant No. 1R35GM150780), $1,788,834 2023-2028

The Welch foundation (Grant No. D-210-20220331), $300,000 2022-2025

Total of 12 grant applications as PI and Co-PI since Sept 2020

Research Experience

Assistant Professor 2020-present

Department of Chemistry and Biochemistry, **Texas Tech University,** Lubbock, TX

- Developed and applied multiscale simulation methods to study the biochemical processes involved in photoactive biological systems. Research projects include molecular photoswitches as therapeutics in photopharmacology, organic molecules with aggregation-induced-emission characteristics as bioimaging probes for disease diagnosis, and catalytic mechanisms of unspecific peroxygenases for sustainable chemical transformations of feedstocks.
- Applied *ab initio* simulation to study the enzymatic mechanism of DNAase, in collaboration with Prof. Roger B. Sutton at TTUHSC.
- Applied molecular dynamics and free energy simulation to study the functional mechanism of melibiose transporter, in collaboration with Prof. Lan Guan at TTUHSC.

Postdoctoral Scholar with **Professor Todd J. Martínez** 2017-2020

Department of Chemistry**, Stanford University**, Stanford CA

- Applied restricted-spin ensemble Kohn-Sham (REKS) method in combination with *ab initio* multiple spawning (AIMS) method to simulate the photodynamics of channelrhodopsin 2 and bacteriorhodopsin.
- Applied quantum mechanics/molecular mechanics (QM/MM) simulation to study hydrogen bond structures in ketosteroid isomerase, resulting in a successful collaboration with the experimentalist Prof. Daniel Herschlag.

Postdoctoral Scholar with **Professor William H. Miller** 2016-2017

Department of Chemistry, **University of California, Berkeley**, Berkeley, CA

- Developed the symmetrical quasi-classical windowing model applied to the Meyer-Miller Hamiltonian (the SQC/MM simulation method) to investigate the photochemical processes in complex conjugated systems, such as ultrafast exciton transfer in organic semiconductors.

Graduate student with **Professor Gregory A. Voth** 2012-2016

Department of Chemistry, **The University of Chicago**, Chicago, IL

- Developed new multiscale reactive molecular dynamics methods to study proton transport mechanism in influenza A virus M2 channel and cytochrome c oxidase, resulting in many successful collaborations with several experimentalists, such as Prof. William F. DeGrado, Prof. Mei Hong and Prof. Mårten Wikström.
- Identified the inaccuracy of the self-consistent charge density functional tight binding method (SCC-DFTB) for simulating hydroxide and proton transport in aqueous and biological systems, which led to improvements of the method.

Teaching and Mentoring Experience

Assistant Professor 2020-present

Department of Chemistry and Biochemistry, **Texas Tech University,** Lubbock, TX

- Taught the course CHEM3310 "Introduction to Biochemistry" for undergraduate students.
- Mentored graduate students and postdoctoral scholars' projects.
- Served as thesis committee member for six graduate students.

Teaching Assistant for General Chemistry 2011-12

Department of Chemistry, **The University of Chicago**, Chicago, IL

- Prepared and led discussion and laboratory sessions for 30 undergraduate students, graded homework assignments and exams.
- Mentored one Ph.D. student's research, resulting in one publication on JACS.

Postdoctoral Scholar with **Professor Todd J. Martínez** 2017-2020

Department of Chemistry, **Stanford University**, Stanford CA

- Mentored two Ph.D. students' research, resulting in three publications on JACS.

Presentations

American Chemical Society National Meeting, New Orleans, LA 2024
Understanding the photochemical reactions in biomolecules through multiscale simulations
(**Invited talk)**

8th International Conference on Catalysis and Chemical Engineering 2024
Boston, MA
Understanding the Multifaceted Mechanism of Compound I Formation in Unspecific Peroxygenases through Multiscale Simulations
(**Invited talk)**

Texas Tech University, Department of Physics and Astronomy, Lubbock, TX 2024
Understanding the photochemical reactions in biomolecules through multiscale simulations
(**Invited talk)**

4th International Conference on Photopharmacology, Hong Kong 2023

Multiscale simulations reveal the coupling between photochemistry and protein-ligand interactions in photopharmacology
(**Invited talk)**

American Chemical Society Southwest Regional Meeting, Oklahoma City, OK 2023
Multiscale simulations reveal the coupling between photochemistry and protein-ligand interactions in photopharmacology
(**Invited talk)**

Texas Tech University Health Science Center, Department of Cell Physiology and Molecular Biophysics, Lubbock, TX 2023
Multiscale simulations reveal the coupling between photochemistry and protein-ligand interactions in photopharmacology
(**Invited talk)**

New York University Shanghai, Department of Chemistry, Shanghai, China 2023
The coupling between photochemistry and protein-ligand interactions in photopharmacology
(**Invited talk)**

Texas State University, Department of Chemistry and Biochemistry 2022
San Macros, TX
The coupling between photochemistry and protein-ligand interactions in photopharmacology
(**Invited talk)**

4th International Conference on Catalysis and Chemical Engineering 2022
San Francisco, CA
Effects of enzyme-ligand interactions on the photoisomerization of a light-regulated chemotherapeutic drug
(**Invited talk)**

Center for Membrane Protein Research 13th Annual Virtual Symposium 2021
Texas Tech University Health Science Center, Lubbock, TX
Towards understanding photoactive biomolecular systems through multiscale simulation
(**Invited talk)**

Purdue University, Department of Chemistry, West Lafayette, IN 2021
Towards understanding photoactive biomolecular systems through multiscale simulation
(**Invited talk)**

American Chemical Society National Meeting, Atlanta, GA 2021
First-principles non-adiabatic dynamics simulation of azobenzene photodynamics in solutions
(**Contributed talk**)

American Chemical Society National Meeting, Atlanta, GA 2021
Light activation mechanism of channelrhodopsin 2
(**Contributed talk**)

Workshop "Principles of Light-Induced Charge Transfer for Optogenetics" 2021

Light activation mechanism of channelrhodopsin 2
(**Contributed talk**)

Virtual Conference on Theoretical Chemistry 2020
Light activation mechanism of channelrhodopsin 2
(**Contributed talk**)

Texas Tech University, Lubbock, TX 2020
Understanding the quantum mechanical effects in biochemical reactions with multiscale simulation
(**Invited talk**)

Vanderbilt University, Nashville, TN 2020
Understanding the quantum mechanical effects in biochemical reactions with multiscale simulation
(**Invited talk**)

Syracuse University, Syracuse, NY 2020
Understanding the quantum mechanical effects in biochemical reactions with multiscale simulation
(**Invited talk**)

Northeastern University, Boston, MA 2020
Understanding the quantum mechanical effects in biochemical reactions with multiscale simulation
(**Invited talk**)

University of Alabama, Tuscaloosa, AL 2020
Understanding the quantum mechanical effects in biochemical reactions with multiscale simulation
(**Invited talk**)

34th William S. Johnson Symposium, Stanford, CA 2019
Nonadiabatic photodynamics of retinal protonated Schiff base in channelrhodopsin 2
(**poster**)

Gordon Research Conferences on Proteins, Holderness, NH 2019
Nonadiabatic photodynamics of retinal protonated Schiff base in channelrhodopsin 2
(**Invited talk**)

The 29th International Conference on Photochemistry, Boulder, CO 2019
Nonadiabatic photodynamics of retinal protonated Schiff base in channelrhodopsin 2
(**contributed talk**)

Northern California Theoretical Chemistry, Berkeley, CA 2019
Nonadiabatic photodynamics of retinal protonated Schiff base in channelrhodopsin 2
(**poster**)

Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing, China 2019
Molecular dynamics simulation of chemical reactions in proteins
(**Invited talk**)

University of Waterloo, Waterloo, ON, Canada 2018
Molecular dynamics simulation of chemical reactions in proteins
(**Invited talk**)

Tsinghua University, Beijing, China 2018
Molecular dynamics simulation of chemical reactions in biomolecules

(**Invited talk**)

West Coast Theoretical Chemistry Symposium, Stanford, CA 2018
Nonadiabatic photodynamics of retinal protonated Schiff base in channelrhodopsin 2
(**poster**)

American Chemical Society National Meeting, Boston, MA 2015
Mechanism of Proton Permeation through Influenza A M2 Channel
(**poster**)

Midwest Theoretical Chemistry Conference, Ann Arbor, MI 2015
Multiscale simulations reveal the proton pumping mechanism in cytochrome c oxidase
(**poster**)

From Computational Biophysics to Systems Biology (CBSB), Oklahoma City, OK 2015
Mechanism of Proton Permeation through Influenza A M2 Channel
(**Invited talk**)

Gordon Research Conferences on Protons & Membrane Reactions, Ventura, CA 2014
Mechanism of Proton Permeation through Influenza A M2 Channel
(**poster**)

Midwest Theoretical Chemistry Conference, Evanston, IL 2014
Mechanism of Proton Permeation through Influenza A M2 Channel
(**poster**)

Technical Skills

Programming: Python, C/C++, Fortran, Mathematica, Matlab, Perl, Bash, GPU computing, Tensorflow

Software packages: Schrödinger, CP2K, TeraChem, CHARMM, AMBER, NAMD, LAMMPS, VMD, etc.

Computational chemistry methods: structure-based ligand design, homology modeling, docking simulation, molecular dynamics, free energy calculation, reactive force-field development, quantum chemistry calculation, quantum dynamics, non-adiabatic dynamics simulation, etc.

Publications

#co-first author *corresponding author

Research at TTU

1. **Liang, R.***; Guan, L.* Atomic-level free energy landscape unravels the cooperative carbohydrate-cation transport coupled with conformational transition in melibiose permease. (*In preparation*)
2. Hariharan, P.; Bakhtiiari, A.; **Liang, R.***; Guan, L.* Distinct roles of the major binding residues in the cation-binding pocket of MelB. *J. Biol. Chem.* **2024**. DOI: https://doi.org/10.1101/2024.02.27.582382 *(Accepted)*
3. Pandey, A.; Poirier, B.*; **Liang, R.*** Development of Parallel On-the-Fly Crystal Algorithm for Global Exploration of Conical Intersection Seam Space. *J. Chem. Theory Comput.* **2024.** DOI: 10.1021/acs.jctc.3c00451.

4. Hariharan, P.; Shi, Y.; Katsube, S.; Willibal, K.; Burrows, N. D.; Mitchell, P.; Bakhtiiari, A.; Stanfield, S.; Pardon, E.; Kaback, H. R.; **Liang, R.**; Steyaert, J.; Viner, R.; Guan, L.* Mobile barrier mechanisms for Na+-coupled symport in an MFS sugar transporter. *eLife* **2024,** 12:RP92462. DOI: https://doi.org/10.7554/eLife.92462.3
5. Costa, G. J.; Egbemhenghe, A.; **Liang, R.*** Computational Characterization of the Reactivity of Compound I in Unspecific Peroxygenases. *J. Phys. Chem. B* **2023,** *127* (51), 10987–10999. DOI: https://doi.org/10.1021/acs.jpcb.3c06311
6. Costa, G. J.; **Liang, R.*** Understanding the Multifaceted Mechanism of Compound I Formation in Unspecific Peroxygenases through Multiscale Simulations. *J. Phys. Chem. B* **2023**, *127* (41), 8809-8824. DOI: 10.1021/acs.jpcb.3c04589.
7. Bakhtiiari, A.; Costa, G. J.; **Liang, R.*** On the Simulation of Thermal Isomerization of Molecular Photoswitches in Biological Systems. *J. Chem. Theory Comput.* **2023**, *19* (18), 6484-6499. DOI: 10.1021/acs.jctc.3c00451.
8. **Liang, R.***; Bakhtiiari, A. Multiscale simulation unravels the light-regulated reversible inhibition of dihydrofolate reductase by phototrexate. *J. Chem. Phys.* **2022**, *156* (24), 245102. DOI: 10.1063/5.0096349.
9. Katsube, S.; **Liang, R.***; Amin, A.; Hariharan, P.; Guan, L.* Molecular Basis for the Cation Selectivity of Salmonella typhimurium Melibiose Permease. *J. Mol. Biol.* **2022**, *434* (12), 167598. DOI: https://doi.org/10.1016/j.jmb.2022.167598.
10. **Liang, R.***; Bakhtiiari, A. Effects of Enzyme–Ligand Interactions on the Photoisomerization of a Light-Regulated Chemotherapeutic Drug. *J. Phys. Chem. B* **2022**, *126* (12), 2382-2393. DOI: 10.1021/acs.jpcb.1c10819.
11. **Liang, R.***; Das, D.; Bakhtiiari, A. Protein confinement fine-tunes aggregation-induced emission in human serum albumin. *Phys. Chem. Chem. Phys.* **2021**, *23* (46), 26263-26272, 10.1039/D1CP04577F. DOI: 10.1039/D1CP04577F.
12. **Liang, R.*** First-Principles Nonadiabatic Dynamics Simulation of Azobenzene Photodynamics in Solutions. *J. Chem. Theory Comput.* **2021**, *17* (5), 3019-3030. DOI: 10.1021/acs.jctc.1c00105.

Research before TTU

13. **Liang, R.**; Yu, J. K.; Meisner, J.; Liu, F.; Martinez, T. J.* Electrostatic Control of Photoisomerization in Channelrhodopsin 2. *J. Am. Chem. Soc.* **2021**, *143* (14), 5425-5437. DOI: 10.1021/jacs.1c00058.
14. Pinney Margaux, M.; Mokhtari Daniel, A.; Akiva, E.; Yabukarski, F.; Sanchez David, M.; **Liang, R.**; Doukov, T.; Martinez, T. J.; Babbitt Patricia, C.; Herschlag, D*. Parallel molecular mechanisms for enzyme temperature adaptation. *Science* **2021**, *371* (6533), eaay2784. DOI: 10.1126/science.aay2784.
15. Yu, J. K.; Bannwarth, C.; **Liang, R.**; Hohenstein, E. G.; Martínez, T. J.* Nonadiabatic Dynamics Simulation of the Wavelength-Dependent Photochemistry of Azobenzene Excited to the nπ* and ππ* Excited States. *J. Am. Chem. Soc.* **2020**, *142* (49), 20680-20690. DOI: 10.1021/jacs.0c09056.
16. Yu, J. K.; **Liang, R.**; Liu, F.; Martínez, T. J.* First-Principles Characterization of the Elusive I Fluorescent State and the Structural Evolution of Retinal Protonated Schiff Base in Bacteriorhodopsin. *J. Am. Chem. Soc.* **2019**, *141* (45), 18193-18203. DOI: 10.1021/jacs.9b08941.
17. Watkins, L. C.; **Liang, R.**; Swanson, J. M. J.; DeGrado, W. F.; Voth, G. A.* Proton-Induced Conformational and Hydration Dynamics in the Influenza A M2 Channel. *J. Am. Chem. Soc.* **2019**, *141* (29), 11667-11676. DOI: 10.1021/jacs.9b05136.
18. **Liang, R.**; Liu, F.; Martínez, T. J.* Nonadiabatic Photodynamics of Retinal Protonated Schiff Base in Channelrhodopsin 2. *J. Phys. Chem. Lett.* **2019**, *10* (11), 2862-2868. DOI: 10.1021/acs.jpclett.9b00701.

19. **Liang, R.**[#]; Cotton, S. J.[#]; Binder, R.[#]; Hegger, R.; Burghardt, I.*; Miller, W. H.* The symmetrical quasi-classical approach to electronically nonadiabatic dynamics applied to ultrafast exciton migration processes in semiconducting polymers. *J. Chem. Phys.* **2018**, *149* (4), 044101. DOI: 10.1063/1.5037815. **(Editor's Pick, Cover Article)**
20. Pinney, M. M.; Natarajan, A.; Yabukarski, F.; Sanchez, D. M.; Liu, F.; **Liang, R.**; Doukov, T.; Schwans, J. P.; Martinez, T. J.; Herschlag, D.* Structural Coupling Throughout the Active Site Hydrogen Bond Networks of Ketosteroid Isomerase and Photoactive Yellow Protein. *J. Am. Chem. Soc.* **2018**, *140* (31), 9827-9843. DOI: 10.1021/jacs.8b01596.
21. Cotton, S. J.; **Liang, R.**; Miller, W. H.* On the adiabatic representation of Meyer-Miller electronic-nuclear dynamics. *J. Chem. Phys.* **2017**, *147* (6), 064112. DOI: 10.1063/1.4995301.**(Editor's Choice)**
22. **Liang, R.**; Swanson, J. M. J.*; Wikström, M.; Voth, G. A.* Understanding the essential proton-pumping kinetic gates and decoupling mutations in cytochrome c oxidase. *Proc. Natl. Acad. Sci. U. S. A.* **2017**, *114* (23), 5924-5929. DOI: 10.1073/pnas.1703654114.
23. Lee, S.[#]; **Liang, R.** [#]; Voth, G. A.; Swanson, J. M. J.* Computationally Efficient Multiscale Reactive Molecular Dynamics to Describe Amino Acid Deprotonation in Proteins. *J. Chem. Theory Comput.* **2016**, *12* (2), 879-891. DOI: 10.1021/acs.jctc.5b01109.
24. **Liang, R.**; Swanson, J. M. J.; Madsen, J. J.; Hong, M.; DeGrado, W. F.*; Voth, G. A.* Acid activation mechanism of the influenza A M2 proton channel. *Proc. Natl. Acad. Sci. U. S. A.* **2016**, *113* (45), E6955-E6964. DOI: 10.1073/pnas.1615471113.
25. **Liang, R.**; Swanson, J. M. J.; Peng, Y.; Wikström, M.; Voth, G. A.* Multiscale simulations reveal key features of the proton-pumping mechanism in cytochrome c oxidase. *Proc. Natl. Acad. Sci. U. S. A.* **2016**, *113* (27), 7420-7425. DOI: 10.1073/pnas.1601982113.
26. **Liang, R.**; Li, H.; Swanson, J. M. J.; Voth, G. A.* Multiscale simulation reveals a multifaceted mechanism of proton permeation through the influenza A M2 proton channel. *Proc. Natl. Acad. Sci. U. S. A.* **2014**, *111* (26), 9396-9401. DOI: 10.1073/pnas.1401997111.
27. **Liang, R.**; Swanson, J. M. J.; Voth, G. A.* Benchmark Study of the SCC-DFTB Approach for a Biomolecular Proton Channel. *J. Chem. Theory Comput.* **2014**, *10* (1), 451-462. DOI: 10.1021/ct400832r.
28. Choi, T. H.[#]; **Liang, R.**[#]; Maupin, C. M.; Voth, G. A.* Application of the SCC-DFTB Method to Hydroxide Water Clusters and Aqueous Hydroxide Solutions. *J. Phys. Chem. B* **2013**, *117* (17), 5165-5179. DOI: 10.1021/jp400953a.