Ruibin Liang

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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

Adjunct Assistant Professor 2021-present
Department of Cell Physiology and Molecular Biophysics
Texas Tech University Health Sciences Center, 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

College of Arts and Sciences Research Award, Texas Tech University 2026
Chancellor's Distinguished Research Award, Texas Tech University **2025**
Poster award in Laboratory Head category, The Welch Conference 2024
Maximizing Investigators' Research Award, NIGMS, NIH 2023
Apple Polishing Award, Texas Tech University 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

Research Experience

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

- As an independent researcher at Texas Tech University, I have successfully published **19** peer-reviewed research articles, **18** of which I served as the corresponding author, in highly reputable journals in the fields of theoretical and computational chemistry and biophysics. These include high-quality publications in journals such as *ACS Cent. Sci., J. Chem. Theory Comput.*, *J. Phys. Chem*, *J. Chem. Phys.*, *Phys. Chem. Chem. Phys.*, *eLife*, *J. Mol. Biol.*, *J. Biol. Chem.*, and *Research*. The rigorous peer review processes and long-standing reputations of these journals ensure the high quality and groundbreaking nature of the research published in them.
- My research group has been awarded two prestigious grants: the highly competitive Welch research grant and the NIH Maximizing Investigators' Research Award (MIRA, i.e., the R35 award). As the sole PI on both awards, I have secured over $2 million in funding for my research group. *Notably, the Welch research grants currently have a low funding rate of less than 10% after competition among leading academic research institutions across Texas. In 2022, I was the only PI at Texas Tech University to receive this grant, and I am one of the only two PIs in our department with an active standard Welch research grant.*
- My group focuses on developing and applying multiscale simulation methods to explore photochemical processes in photoactive biomolecules. This research is crucial for understanding fundamental biological processes, such as vision and photosynthesis, and for advancing biomedical applications, such as the design of drugs with low side effects and sensitive probes for bioimaging. Our work has deepened the understanding of the photochemistry of molecular photoswitches—used in light-regulated drugs and bioimaging agents—as well as the photoinduced electron transfer in cryptochromes, a key protein for circadian rhythms and biological magnetic sensing. (**10 publications as corresponding author**).

- My group has designed a multiscale simulation framework to investigate the catalytic mechanism of unspecific peroxygenases through multiscale simulations. My study offers new insights into the enzyme's catalytic mechanism at atomic-level details, aiding the design of new biocatalysts for sustainable chemical transformations of feedstocks. My study also contributed to a in-depth understanding of the limitations of currently widely used computational protocols for studying enzyme catalysis. (**2 publications as corresponding author**)
- My group has systematically characterized the functional cycle of melibiose permease (MelB), a key model of cation-coupled symporter in the Major Facilitator Superfamily (MFS) that is crucial for various physiological and pathological processes. The research project unravels the molecular origin of cation-coupled transport mechanisms in MFS symporters. (**4 publications, 3 as corresponding author**)
- My group conducted quantum mechanics simulations to explore a novel type of chirality, termed "turbo chirality", in organic chemistry, leading to a fundamental transformation of the current textbook understanding of chirality in organic compounds. (**3 publications as corresponding author**)

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" to undergraduate students at TTU.
- Taught the course CHEM5340 "Computational Chemistry and Biomolecular Modeling" to graduate students at TTU.
- Taught the course GMBP 5321 "Biochemistry and Biophysics of Membranes" to graduate students at TTU Health Sciences Center.
- Mentored multiple research projects of 7 graduate students, 7 postdoctoral scholars, 2 undergraduate students, and 1 high-school student.
- Served as a thesis committee member for 7 graduate students.
- Recipient of the "Apple Polishing Award" from Texas Tech University, a prestigious award for teaching and mentoring undergraduate 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.

Services

Departmental Service

Graduate Affairs Committee (2021-2022) in the Department of Chemistry and Biochemistry

Space and Infrastructure Committee (2022-now) in the Department of Chemistry and Biochemistry

College and University Service

Served as a panelist in a workshop on dissertation writing hosted by the Graduate Writing Center at TTU (2021)

Reviewer service

Reviewer of 37 research articles in reputable journals in theoretical and computational chemistry since joining Texas Tech University (Nature Chemistry, Nature Communication, ACS Central Science, PNAS, Journal of Chemical Theory and Computation, Journal of Physical Chemistry, Journal of Chemical Physics, Physical Chemistry and Chemical Physics, Biophysical Journal, PLOS computational biology, Nanoscale, RSC advances, Langmuir, ChemPhotoChem, ChemBioChem, Advanced Materials, New Journal of Chemistry, Cells).

Member of review panel of NSF in CHE division in 2021

Member of review panel of NIH NIGMS in 2025

Ad hoc reviewer of NSF proposal in CHE division in 2024

Poster session reviewer in American Chemical Society Southwest Regional Meeting, Oklahoma City, OK, 2023

Conference and workshops
Session chair in Biophysical Society Conference on Proton Reactions, 2025
Session chair in Virtual Conference on Theoretical Chemistry, 2020

Presentations

Gordon Research Conference, Photosensory Receptors and Signal Transduction, Ventura, CA 2026
Decrypting the Nonadiabatic Photoinduced Electron Transfer Mechanism in Light-Sensing Cryptochrome
(Invited talk)

Stony Brook University, Department of Chemistry, Stony Brook, NY 2025
Unraveling the functional mechanisms and design principles of photoactive biomolecular systems through multiscale simulations
(Invited talk)

The University of Utah, Department of Chemistry, Salt Lake City, UT 2025
Unraveling the functional mechanisms and design principles of photoactive biomolecular systems through multiscale simulations
(**Invited talk)**

Bowling Green State University, Department of Chemistry, Bowling Green, OH 2025
Unraveling the functional mechanisms and design principles of photoactive biomolecular systems through multiscale simulations
(**Invited talk)**

Georgia State University, Department of Chemistry, Atlanta, GA 2025
Unraveling the functional mechanisms and design principles of photoactive biomolecular systems through multiscale simulations
(**Invited talk)**

Lehigh University, Department of Chemistry, Bethlehem, PA 2025
Unraveling the functional mechanisms and design principles of photoactive biomolecular systems through multiscale simulations
(**Invited talk)**

Wayne State University, Department of Chemistry, Detroit, MI 2025
Unraveling the functional mechanisms and design principles of photoactive biomolecular systems through multiscale simulations
(**Invited talk)**

The Biophysical Society (BPS) Conference -- Proton Reactions: From Basic Science to Biomedical Applications, Estes Park, CO 2025

Decrypting the Non-Adiabatic Photoinduced Electron Transfer Mechanism in Light-Sensing Cryptochrome
(Invited talk)

Virginia Commonwealth University, Department of Chemistry, Richmond, VA 2025
Unraveling the functional mechanisms and design principles of photoactive biomolecular systems through multiscale simulations
(**Invited talk)**

University of Nevada, Department of Chemistry, Reno, NV 2025
Unraveling the functional mechanisms and design principles of photoactive biomolecular systems through multiscale simulations
(**Invited talk)**

CMPR XVI Annual Symposium,
Texas Tech University Health Sciences Center, Lubbock, TX 2025
Atomic-Level Free Energy Landscape Reveals Cooperative Symport Mechanism of Melibiose Transporter
(**Invited talk)**

Oklahoma State University, Department of Chemistry, Stillwater, OK 2025
Unraveling the functional mechanisms and design principles of photoactive biomolecular systems through multiscale simulations
(**Invited talk)**

American Chemical Society Southwest Regional Meeting, Waco, TX 2024
Development of Multiscale Simulation Approaches for the Characterization of Photochemical Reactivities in Biomolecules
(**Invited talk)**

The Welch Conference, Houston, TX 2024
Development of Multiscale Simulation Approaches for the Characterization of Photochemical Reactivities in Biomolecules
(**Poster award in laboratory-head group**)

The University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK 2024
Development of Multiscale Simulation Approaches for the Characterization of Photochemical Reactivities in Biomolecules
(**Invited talk)**

The University of New Mexico, Department of Chemistry and Chemical Biology, Albuquerque, NM 2024
Development of Multiscale Simulation Approaches for the Characterization of Photochemical Reactivities in Biomolecules
(**Invited talk)**

Telluride Conference on Proton Transfer in Biology, Telluride, CO 2024
Understanding the Multifaceted Mechanism of Compound I Formation and Reactivity in Unspecific Peroxygenases through Multiscale Simulations
(**Invited talk)**

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**)

Publications

#co-first author *corresponding author

Independent Research at Texas Tech University (Under review)

1. Rashidniyaghi, E.; Khavani, M.; Coerver, C.; **Liang, R.***; Ravanfar, R*. Mechanistic Understanding of Protein–MOF Integration through Surfactant-Driven Interfacial Design. *bioRxiv* **2025**, 2025.2011.2011.687871. DOI: 10.1101/2025.11.11.687871. (Submitted)
2. Yuan, Q.; Pandey, A.; Liu, H.; Bouley, B.; Li, Z.; Zhu, H.; **Liang, R.*;** Li, G.* A New Chirality Phenomenon in Amino Acid and Peptide Derivatives. *ChemRxiv* **2026** (0109). DOI: 10.26434/chemrxiv-2026-kncjf.

Independent Research at Texas Tech University (Peer-reviewed and Published)

3. Khavani, M.; Bakhtiiari, A.; Khalvati, L; Leurs, R; **Liang, R.*** A Systematic Benchmark Study of Free Energy Methods for Quantifying Light-Responsive Binding Affinities of Photoswitchable Antagonists of Beta-Adrenergic Receptors. *J. Med. Chem*. **2026** (Accepted).
4. Hariharan, P.; Shi, Y.; Bakhtiiari, A.; **Liang, R.**; Viner, R.; Guan, L*. Allosteric effects of the coupling cation in melibiose transporter MelB. *eLife* **2026**, *14*, RP108335. DOI: 10.7554/eLife.108335.
5. Bakhtiiari, A.; Khavani, M.; Costa, G. J.; **Liang, R.*** A Multiscale Simulation Framework for Elucidating Photochemical Structure–Activity Relationships of Photoswitchable Ligands in Complex Biomolecular Environments. *J. Chem. Inf. Model*. **2025**, *65* (23), 12861–12878. DOI: 10.1021/acs.jcim.5c01831.
6. Costa, G. J.; **Liang, R***. Decrypting the Nonadiabatic Photoinduced Electron Transfer Mechanism in Light-Sensing Cryptochrome. *ACS Cent. Sci.* **2025**, *11* (7), 1071-1082. DOI: 10.1021/acscentsci.5c00376.
7. Pandey, A.; Costa, G. J.; Alam, M.; Poirier, B.*; **Liang, R.*** Development of Parallel On-the-Fly Crystal Algorithm for Reaction Discovery in Large and Complex Molecular Systems. *J. Chem. Theory Comput.* **2025**, *21* (9), 4704-4717. DOI: 10.1021/acs.jctc.5c00324.
8. Bakhtiiari, A.; **Liang, R.*** Unraveling Solvent and Substituent Effects in the Photodynamics of Light-Dependent Microtubule Inhibitors for Cancer Phototherapy. *J. Comput. Chem*. **2025**, *46* (7), e70076. DOI: https://doi.org/10.1002/jcc.70076
9. Wang, Y.; Xu, T.; Pandey, A.; Jin, S.; Yan, J. X.; Yuan, Q.; Zhang, S.; Wang, J.-Y.; **Liang, R.***; Li, G.* Enantiopure Turbo Chirality Targets in Tri-Propeller Blades: Design, Asymmetric Synthesis, and Computational Analysis. *Molecules* **2025**, *30* (3). DOI: 10.3390/molecules30030603.
10. Rahman, A. U.; Wang, Y.; Xu, T.; Reddy, K. D.; Jin, S.; Yan, J. X.; Yuan, Q.; Unruh, D.; **Liang, R.***; Li, G.* Discovery of Staircase Chirality through the Design of Unnatural Amino Acid Derivatives. *Research* **2024**, *7*, 0550. DOI: 10.34133/research.0550.
11. **Liang, R**.*; Guan, L.* Atomic-Level Free Energy Landscape Reveals Cooperative Symport Mechanism of Melibiose Transporter. *eLife* **2024**, 13:RP103421. DOI: https://doi.org/10.7554/eLife.103421.1. (Peer-reviewed preprint)
12. Xu, T.; Wang, Y.; Jin, S.; Rahman, A. U.; Yan, X.; Yuan, Q.; Liu, H.; Wang, J.-Y.; Yan, W.; Jiao, Y.; **Liang, R.***; Li, G.* Amino Turbo Chirality and Its Asymmetric Control. *Research* **2024**, *7*, 0474. DOI: 10.34133/research.0474.
13. Hariharan, P.; Bakhtiiari, A.; **Liang, R.***; Guan, L.* Distinct roles of the major binding residues in the cation-binding pocket of the melibiose transporter MelB. *J. Biol. Chem*. **2024**, *300* (7), 107427. DOI: 10.1016/j.jbc.2024.107427.
14. 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**, *20* (11), 4778-4789. DOI: 10.1021/acs.jctc.4c00292.
15. 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
16. 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

17. 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.
18. 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.
19. **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.
20. 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.
21. **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.
22. **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.
23. **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 joining Texas Tech University

24. **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.
25. 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.
26. 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.
27. 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.
28. 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.
29. **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.
30. **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)**
31. 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.

32. 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)**
33. **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.
34. 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.
35. **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.
36. **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.
37. **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.
38. **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.
39. 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.