

# Ruibin Liang

Department of Chemistry and Biochemistry  
CHEM 232A  
Texas Tech University  
1204 Boston Ave, Lubbock, TX 79409

Email: [rliang@ttu.edu](mailto:rliang@ttu.edu)  
[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. Martinez**

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

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

A total of 14 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

- As an independent researcher at Texas Tech University, I have successfully published 12 peer-reviewed research articles, 11 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 *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. **(6 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. (**1 publication 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**

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

- Taught the course CHEM3310 “Introduction to Biochemistry” to undergraduate students.
- Taught the course CHEM5340 “Computational Chemistry and Biomolecular Modeling” to graduate students.
- Mentored multiple research projects of 4 graduate students, 5 postdoctoral scholars and 2 undergraduate students.
- 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**

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### **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 36 academic articles since joining Texas Tech University in 2020:

- Nature Chemistry: 1 time
- Nature Communication: 2 times
- ACS Central Science: 1 time
- PNAS: 1 time.
- Journal of Chemical Theory and Computation: 4 times
- Journal of Physical Chemistry: 4 times
- Journal of Chemical Physics: 6 times
- Physical Chemistry and Chemical Physics: 5 times
- Biophysical Journal: 1 time
- PLOS computational biology: 1 time
- Nanoscale: 1 time

- RSC advances: 1 time
- Langmuir: 1 time
- ChemPhotoChem: 1 time
- ChemBioChem: 1 time
- Advanced Materials: 1 time
- New Journal Chemistry: 2 times
- Cells: 1 time

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 Virtual Conference on Theoretical Chemistry, 2020

### **Presentations**

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Oklahoma State University, Department of Chemistry, Stillwater, OK <i>Unraveling the functional mechanisms and design principles of photoactive biomolecular systems through multiscale simulations</i> <b>(Invited talk)</b>	2025
American Chemical Society Southwest Regional Meeting, Waco, TX <i>Development of Multiscale Simulation Approaches for the Characterization of Photochemical Reactivities in Biomolecules</i> <b>(Invited talk)</b>	2024
The Welch Conference, Houston, TX Development of Multiscale Simulation Approaches for the Characterization of Photochemical Reactivities in Biomolecules <b>(Poster)</b>	2024
The University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK <i>Development of Multiscale Simulation Approaches for the Characterization of Photochemical Reactivities in Biomolecules</i> <b>(Invited talk)</b>	2024
The University of New Mexico, Department of Chemistry and Chemical Biology Albuquerque, NM <i>Development of Multiscale Simulation Approaches for the Characterization of Photochemical Reactivities in Biomolecules</i> <b>(Invited talk)</b>	2024
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)**

8<sup>th</sup> 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)**

4<sup>th</sup> 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 Marcos, TX  
*The coupling between photochemistry and protein-ligand interactions in photopharmacology*  
**(Invited talk)**

4<sup>th</sup> 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. 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. *ChemRxiv* **2025**. DOI: 10.26434/chemrxiv-2025-9hcdq.



- Costa, G. J.; **Liang, R.\*** Decrypting the Non-Adiabatic Photoinduced Electron Transfer Mechanism in Light-Sensing Cryptochrome. *ChemRxiv* **2025**. DOI: 10.26434/chemrxiv-2025-golg7

### Independent Research at Texas Tech University (Peer-reviewed)

- 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>
- 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.
- 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.
- 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)
- 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.
- 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.
- 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.
- 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<sup>+</sup>-coupled symport in an MFS sugar transporter. *eLife* **2024**, *12*:RP92462. DOI: <https://doi.org/10.7554/eLife.92462.3>
- 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.jpcc.3c06311>
- 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.jpcc.3c04589.
- 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.
- 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.
- 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>.
- 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.jpcc.1c10819.

17. **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.
18. **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

19. **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.
20. 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.
21. 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  $n\pi^*$  and  $\pi\pi^*$  Excited States. *J. Am. Chem. Soc.* **2020**, *142* (49), 20680-20690. DOI: 10.1021/jacs.0c09056.
22. 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.
23. 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.
24. **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.jpcclett.9b00701.
25. **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)**
26. 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.
27. 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)**
28. **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.
29. 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.

30. **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.
31. **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.
32. **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.
33. **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.
34. 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.