

LIU, JINCHAN**EDUCATION BACKGROUND**

01.2023 – present	Ph.D. Candidate in Molecular Biophysics & Biochemistry PI: Dr. Victor S. Batista	Yale University
08.2020 – 01.2023	M.S. in Molecular Biophysics & Biochemistry Overall GPA: 4.0/4.0	Yale University
08.2016 – 06.2020	B.S. in Chemistry Overall GPA: 3.8/4.0	Jilin University

PROJECTS ONGOING

12.2021 – present Interrogating the water oxidation mechanism in the photosystem II computationally.

Nature oxidizes water to dioxygen with the oxygen evolving complex (OEC) during photosynthesis in the photosystem II (PSII), which serves as the blueprints for future clean energy technologies. To learn the strategy of oxidizing water from nature, (1) I use Quantum Mechanics/Molecular Mechanics (QM/MM) calculations to study the catalytic mechanism of the OEC, especially how the substrate water is delivered to the OEC. (2) I use Molecular Dynamics (MD) to study the water dynamics in the water channel of PSII. (3) I am currently developing a novel force field for Mn ions in the OEC to reproduce a precise potential of binding of ligand to the Mn ions, enabling the computational study on water exchange and ligand binding with DFT precision.

PUBLICATIONS

Online Academic Profiles: [Google Scholar](#), [ResearchGate](#)

Journal Articles

15. S. Liu, **J. Liu**, A. Foote, H. Ogasawara, **V. S. Batista**, and K. Salaita. A tunable genetically encoded tension sensor based on engineered coiled-coil motifs. *In Prep.*
14. **J. Liu**, K. R. Yang, Z. Long, W. H. Armstrong, G. W. Brudvig, **V. S. Batista**. Substrate water delivery to the oxygen-evolving complex of photosystem II. *In Prep.*
13. D. A. Flesher, **J. Liu**, J. Wang, C. J. Gisriel, K. R. Yang, **V. S. Batista**, R. J. Debus, and G. W. Brudvig. Structure of a mutated photosystem II complex reveals perturbation of the oxygen-evolving complex. *Submitted.*
12. E. D. Huseman, A. Lo, O. Fedorova, J. L. Elia, S. E. Gueble, K. Lin, R. Sundaram, D. M. Burgenske, J. Oh, **J. Liu**, F. Menges, M. G. Rees, M. M. Ronan, J. A. Roth, **V. S. Batista**, J. M. Crawford, J. N. Sarkaria, A. M. Pyle, R. S. Bindra, and Seth B. Herzon. Mechanism of Action of KL-50, a Novel Imidazotetrazine for the Treatment of Drug-Resistant Brain Cancers. *Submitted.*
11. C. J. Gisriel, D. A. Flesher, Z. Long, **J. Liu**, J. Wang, D. A. Bryant, **V. S. Batista**, G. W. Brudvig. (2023) A quantitative assessment of (bacterio)chlorophyll assignments in the cryo-EM structure of the *Chloracidobacterium thermophilum* reaction center. *Photosynth. Res.*
10. K. M. Kuo, **J. Liu**, A. Pavlova, **J. C. Gumbart**. (2023) Drug binding to BamA targets its lateral gate. *J. Phys. Chem. B.*
9. Y. Li*, A. Acharya*, L. Yang, **J. Liu**, E. Tajkhorshid, H. Zgurskaya, M. Jackson, **J. C. Gumbart**. (2023) Insights into substrate transport and water permeation in the mycobacterial transporter MmpL3. *Biophys. J.*
8. A. M. Fredericks, K. W. East, Y. Shi, **J. Liu**, F. Maschietto, A. Ayala, W. G. Cioffi, M. Cohen, W. G. Fairbrother, C. T. Lefort, G. J. Nau, M. M. Levy, J. Wang, **V. S. Batista**, G. P. Lisi, and S. F. Monaghan. (2022)

- Identification and mechanistic basis of non-ACE2 blocking neutralizing antibodies from COVID-19 patients with deep RNA sequencing and molecular dynamics simulations. *Front. Mol. Biosci.*
7. R. J. Wei, U. Khaniya, J. Mao, **J. Liu**, **V. S. Batista**, M. R. Gunner. (2022) Tools for analyzing protonation states and for tracing proton transfer pathways with examples from the *Rb. sphaeroides* photosynthetic reaction centers. *Photosynth. Res.*
 6. J. Wang, **J. Liu**, C. J. Gisriel, S. Wu, F. Maschietto, D. A. Flesher, E. Lolis, G. P. Lisi, G. W. Brudvig, Y. Xiong, **V. S. Batista**. (2022) How to correct relative voxel scale factors for calculations of vector-difference Fourier maps in cryo-EM. *J. Struct. Biol.*
 5. C. Stevens, S. Babii, A. N. Pandya, W. Li, Y. Li, J. Mehla, R. Scott, P. Hegde, P. K. Prathipati, A. Acharya, **J. Liu**, **J. C. Gumbart**, J. North, M. Jackson, H. I. Zgurskaya. (2022) Proton transfer activity of the reconstituted Mycobacterium tuberculosis MmpL3 is modulated by substrate mimics and inhibitors. *Proc. Natl. Acad. Sci. U.S.A.*
 4. D. A. Flesher*, **J. Liu***, J. M. Wiwczar*, K. M. Reiss, K. R. Yang, J. Wang, M. Askerka, C. J. Gisriel, **V. S. Batista** and G. W. Brudvig. (2022) Glycerol binding at the narrow channel of photosystem II stabilizes the low-spin S₂ state of the oxygen-evolving complex. *Photosynth. Res.*
 3. C. J. Gisriel, J. Wang, **J. Liu**, D. A. Flesher, K. M. Reiss, H. Huang, K. R. Yang, W. H. Armstrong, M. R. Gunner, **V. S. Batista**, R. J. Debus, and G. W. Brudvig. (2022) High-resolution cryo-electron microscopy structure of photosystem II from the mesophilic cyanobacterium, *Synechocystis* sp. PCC 6803." *Proc. Natl. Acad. Sci.*
 2. **J. Liu**, and **J. C. Gumbart**. (2020) Membrane thinning and lateral gating are consistent features of BamA across multiple species. *PLoS Comput. Biol.*
 1. J. Cao, M. Ma, **J. Liu**, Y. Yang, H. Liu, X. Xu, J. Huang, H. Yue, **G. Tian**, and S. Feng. (2019) Highly effective transformation of carbohydrates to 5-Hydroxymethylfurfural with Al-montmorillonite as catalyst. *Appl. Catal. A-Gen.*

Posters and Presentations at Conferences

6. "The PSII Express: the Atomistic Mechanism of Water Delivery to the OEC of PSII." **J. Liu**, K. R. Yang, Z. Long, G. W. Brudvig, V. S. Batista. **Poster & Presentation** at *Photosynthesis Gordon Research Conference*. July 23rd-28th, 2023. Newry, ME.
5. "The PSII Express: the Atomistic Mechanism of Water Delivery to the OEC of PSII." **J. Liu**, K. R. Yang, Z. Long, G. W. Brudvig, V. S. Batista. **Poster & Presentation** at *Photosynthesis Gordon Research Seminar*. July 22nd-23rd, 2023. Newry, ME.
4. "Redox Leveling of the Kok Cycle of Photosystem II Established by Water Ligand Binding to the Oxygen Evolving Complex." **J. Liu**, K. R. Yang, G. W. Brudvig, V. S. Batista. **Poster** at *Biophysics Society Meeting*. Feb. 20th, 2023. San Diego, CA.
3. "Glycerol binding at the narrow channel of PSII stabilizes the low-spin S₂ state of the OEC." **J. Liu**, D. A. Flesher, K. R. Yang, J. Wang, C. J. Gisriel, G. W. Brudvig, V. S. Batista. **Presentation** at *Eastern Regional Photosynthesis Conference*. April 23rd, 2022. Woods Hole, MA.
2. "Revealing the allosteric pathways of the protein-tyrosine phosphatase 1B: a combined mutagenesis-computational study." **J. Liu**, E. Wang, J. P. Loria, and V. S. Batista. **Platform** at *Biophysics Society Meeting*. Feb. 21st, 2022. San Francisco, CA.
1. "Dynamic lateral gate of BamA and TamA regulated by POTRA domains." **J. Liu**, and J. C. Gumbart. **Poster** at *Biophysics Society Meeting*. Feb. 18th, 2020. San Diego, CA.

Book Chapter

1. Y. Li, **J. Liu**, **J. C. Gumbart**. (2021) Preparing membrane proteins for simulation using CHARMMGUI. *Structure and Function of Membrane Proteins*. Humana, New York, NY.

Online Tutorial

1. Y. Li, J. Liu, J. C. Gumbart. (2020) [Membrane Proteins Tutorial \(Introductory\)](#). [UIUC Theoretical and Computational Biophysics Group Tutorials](#).

TEACHING EXPERIENCE

Fall 2023 MB&B 435 Teaching Assistant for Quantitative Approaches in Biophysics and Biochemistry
Spring 2023 BIOL 101 Teaching Assistant for Biochemistry and Biophysics
Fall 2022 MB&B 435 Teaching Assistant for Quantitative Approaches in Biophysics and Biochemistry
Spring 2022 BIOL 101 Teaching Assistant for Biochemistry and Biophysics

HONORS AND AWARDS

07.2023 Best Poster Award, Photosynthesis Gordon Research Conference 2023. (4/123)
06.2023 Graduate Student Assembly Conference Travel Fellowship, Yale Univ. (\$800)
06.2020 Top 10 students of 2019, Jilin Univ. (7/1000)
06.2019 Second Prize, *Tang Aoqing Honors Program of Research & Practice*, Jilin Univ. (5000 RMB)
07.2018 Outstanding Student Award of the Chemistry Division, *10th Anniversary Meeting of the National Training Plan for Talent in Basic Science*, USTC (1/20)
06.2018 Second Prize, *Tang Aoqing Honors Program of Research & Practice*, Jilin Univ. (5000 RMB)
09.2017 Second Class Scholarship, Jilin Univ. (2000 RMB)
09.2017 Jingying Scholarship, Jilin Univ. (2000 RMB)

RESEARCH SKILLS

Coding and Scripting: tcl/tk, bash, python, matlab

Computational Software: VMD, GView; NAMD, AMBER, openMM, Gaussian; ChemDraw, CHARMMGUI

Writing and Plotting: Microsoft, EndNote, LaTeX, Adobe Illustrator, xmgrace, python