VIVIANA MONJE

Assistant Professor
Chemical and Biological Engineering Department
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WORK ADDRESS
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EDUCATION

University of Maryland, College Park, MD

- PhD. in Chemical Engineering March, 2017

  Dissertation: "Computational Studies of Membrane Models and Their Interaction with a Peripheral Protein in Yeast, and Disruption of the Water-Oil Interface by a Hydrotrope"
  Advisor: Jeffery B. Klauda

- M.S. in Chemical Engineering November, 2014

  Thesis: "Computational Studies on Organelle-Specific Yeast Membrane Models"
  Advisor: Jeffery B. Klauda

- B.S. in Chemical Engineering May, 2012

  Minor in Project Management

EMPLOYMENT HISTORY

- **University at Buffalo, the State University of New York (SUNY).** Jan. 2021 – present

  Department of Chemical and Biological Engineering
  Assistant Professor

- **The University of Chicago.** Sept. 2017 – Jan. 2021

  Department of Chemistry
  Postdoctoral Scholar
  PI: Gregory A. Voth

- **University of Maryland - College Park, MD.** Sept. 2012 – Aug. 2017

  Chemical and Biomolecular Engineering
  Graduate Research Assistant
  Advisor: Jeffery B. Klauda

- **University of Alabama, Tuscaloosa, AL.** Summer 2011

  Chemical and Biological Engineering
  Undergraduate Research Assistant (REU participant. Mentor: Dr. Heath Turner)

- **University of Maryland - College Park, MD.** Summer 2010

  Center for Minorities in Science and Engineering
  Student Assistant (Supervisor: Lawanda Kamalidiin)

HONORS & AWARDS

- 2025 UB Exceptional Scholar: Young Investigator Award
- SoBLA Prize for Outstanding Service and Volunteering. Society of Biophysicists in Latin America. February, 2023 & 2024
- IDEAL Award from the American Institute of Chemical Engineering to the LatinXinChE leadership team. November, 2023
- SUNY PRODiG (Promoting Recruiting Opportunity, Diversity, Inclusion and Growth). 2020-2021 cohort

PEER-REVIEWED PUBLICATIONS

Full record: ORCiD | Google Scholar citations: 3551, h-index: 16, i20-index: 19 (by 06/30/2025)
[*] *indicates graduate student mentored by VM,*
[+] *indicates undergraduate student mentored by VM,*
[cl] *indicates VM as the computational lead in collaborative projects.*
[=] *denotes the corresponding author.*

Invited Book Chapters

Publications at UB

1. Campbell, O.[*], Allsopp, R.; Klauda, J.B., Monje, V. [=] "Atomistic simulations and analysis of peripheral membrane proteins with model lipid bilayers" in Methods in Molecular Biology Series, vol 2888. Intracellular Lipid Transport, 2nd Ed. Guillaume Drin, Ed. Springer, (2025) **Citations:** 1

Graduate work

2. Monje-Galvan, V. [=]; Warburton, L[+]; Klauda, J.B. "Setting-up all-atom molecular dynamics simulations to study the interactions of peripheral membrane proteins with model lipid bilayers" in Methods in Molecular Biology Series. Intracellular Lipid Transport. Guillaume Drin, Ed. Springer, (2019) **Citations:** 21
3. Khakbaz, P; Monje-Galvan, V.; Zhuang, X.; Klauda, J.B. [=] "Modeling Lipid Membranes" in Handbook of Hydrocarbon and Lipid Microbiology Series. Biogenesis of Fatty Acids, Lipids and Membranes. Otto Geiger, Ed. Springer, (2016) **Citations**: 7

Refereed Journal Articles

Publications at UB

1. Li. J. [*]; Thomson, S.[+]; Monje, V.[=] "Evaluating the influence of bilayer patch size on biophysical properties in multi-component lipid systems." (*Submitted*)
2. Campbell, O. [*]; Dahhan, D.[+]; Monje, V. [=] "Lipid-driven alignment and binding of p7 dimers in early oligomer assembly." (*Submitted, https://doi.org/10.1101/2025.06.13.659606*)

3. Ramirez, R.X. [*]; Bosch, A.M.; Perez, R.; Guzman, H.V.; Monje, V. [=] "2Danalysis: A toolbox for analysis of lipid membranes and biopolymers in two-dimensional space." Biophys J, (*In Press, https://doi.org/10.1016/j.bpj.2025.05.026*)
4. Jaramillo-Granada, A.M.; Li, J. [*]; Flores Villareal, A.; Lozano, O.; Ruiz-Suarez, J.C.; Monje-Galvan, V. [cl]; Sierra-Valdez, F.J.[=] "Modulation of phospholipase A_2 membrane activity by anti-inflammatory drugs." Langmuir, 40(13): 7038-7048 (2024)
5. Pradhan, A.J; Chitkara, S.; Ramirez, R.X. [*]; Monje-Galvan, V. [cl]; Sancak, Y.; Atilla-Gokcumen, G.E. [=] "Acylation of MLKL impacts its function in necroptosis." ACS Chem. Biol., 19(2): 407-418 (2024) **Citations:** 4
6. Campbell, O. [*]; Monje-Galvan, V. [=] "Lipid composition modulates interactions of p7 viroporin during membrane insertion." J. Struct. Biol. 215(3):108013 (2023) **Citations:** 3
7. Li. J. [*]; Monje-Galvan, V.[=] "In Vitro and In Silico Studies of Antimicrobial Saponins: A Review." Processes, 11(10): 2856 (2023). **Citations:** 11
8. Campbell, O. [*]; Le, V.[+]; Aguirre, A.[+]; Monje-Galvan, V. [=] "Realistic membrane modeling: using complex lipid mixtures in simulation studies." J. Vis. Exp., 199: e65712 (2023) **Citations:** 1
9. Li, J. [*]; Monje-Galvan, V. [=] "Effect of glycone diversity on the interaction of triterpenoid saponins and lipid bilayers." ACS Applied Bio. Mat, 7(2): 553-563 (2023) **Citations:** 9
10. Ramirez, R.X. [*]; Campbell, O. [*]; Pradhan, A.; Atilla-Gokcumen, G.E.; Monje-Galvan, V[=] "Modeling the molecular fingerprint of protein-lipid interactions of MLKL on complex bilayers." Frontier in Chem, 10: 1088058 (2023) **Citations:** 10
11. Campbell, O. [*]; Monje-Galvan, V. [=] "Protein-driven membrane remodeling: Molecular perspectives from Flaviviridae infections." Biophys. J, 122: 1-10 (2021) **Citations:** 6
12. Li, J. [*]; Kalyanram, P; Monje-Galvan, V. [cl]; Gupta, A. [=] "Interaction of Cyanine-D112 with binary lipid mixtures: molecular dynamics simulation and differential calorimetry study." ACS Omega, 7 (11): 9765-9774 (2022) **Citations:** 3
13. Pradhan, A.J; Lu, D.; Parisi, L.R.; Shen, S.; Berhane, I.A.; Galster, S.L.; Bynum, K.; Monje-Galvan, V.[cl]; Gokcumen, O.; Chemler, S.R.; Qu, J. ; Kay, J.G.; Atilla-Gokcumen, G.E. [=] "Protein acylation by saturated very long chain fatty acids and endocytosis are involved in necroptosis." Cell Chem. Biol., 28 (9): 1298-1309 (2021) **Citations:** 30

Postdoctoral work

14. Banerjee, P.; Monje-Galvan, V.; Voth, G.A. [=] "Cooperative membrane binding of HIV-1 matrix protein trimers." J. Phys. Chem. B., 128(11): 2595-2606 (2024) **Citations:** 4
15. Monje-Galvan, V; Voth, G.A. [=] "Molecular Interactions of the M and E integral membrane proteins of SARS-CoV-2." Faraday Disc., 232: 49-67 (2021) **Citations:** 26
16. Yu, A.; Pak, A.J.; He, P.; Monje-Galvan, V.; Casalino, L.; Gaieb, Z.; Dommer, A.C.; Amaro, R.E.; Voth, G.A. [=] "A multiscale coarse-grained model of the SARS-CoV-2 virion." Biophys. J., 120(6): 1097-1104 (2021) **Citations:** 1722
17. Monje-Galvan, V; Voth, G.A. [=] "Binding mechanism of the matrix domain of HIV-1 Gag on lipid membranes." eLife, 9:e58621 (2020) **Citations:** 38

Graduate work

18. Monje-Galvan, V.; Klauda, J.B. [=] "Interfacial properties of aqueous solutions of butanol isomers and cyclohexane." Fluid Phase Equilib., 513: 112551 (2020) **Citations**: 8
19. Leonard, A.N.; Wang, E.; Monje-Galvan, V.; Klauda, J.B[=]. "Developing and testing of lipid force fields with applications to modeling cellular membranes." Chem. Rev., 119(9): 6227-6269 (2019) **Citations:** 106
20. Wildermuth, K.; Monje-Galvan, V.; Klauda, J.B. [=] "Effect of membrane lipid packing on stable binding of the ALPS peptide." J. Chem. Theo. Comp., 15(2):1418-1429 (2019) **Citations:** 33
21. Monje-Galvan, V.; Klauda, J.B. [=] "Preferred binding mechanism of Osh4's amphipathic lipid-packing sensor motif, insights from molecular dynamics." J. Phys. Chem. B., 122(42): 9713-9723 (2018) **Citations:** 28
22. Novikov, A; Semenov, A.; Monje-Galvan, V; Kuryakov, V.; Klauda, J.B; Anisimov, M. [=] "Dual action of hydrotropes at the water/oil interface." J. Phys. Chem. C, 121(30): 16423-16431. (2017) **Citations:** 42
23. Boughter, C.T.; Monje-Galvan, V.; Im, W.; Klauda, J.B. [=] "Influence of Cholesterol on Phospholipid Bilayer Structure and Dynamics." J. Phys. Chem. B., 120(45): 11761-11772. (2016). **Citations:** 70
24. Monje-Galvan, V.; Klauda, J.B. [=] 2016. "Peripheral Membrane Proteins: Tying the Knot between Experiment and Computation." BBA: Biomembranes, 1858: 1584-1593 (2016). **Citations:** 69
25. Monje-Galvan, V.; Klauda, J.B. [=] 2015. "Modelling Yeast Organelle Membranes and How Lipid Diversity Influences Bilayer Properties." Biochemistry. 54(45), 6852-6861 (2015). **Citations:** 74
26. Wu, E.L.; Cheng, X.; Jo, S.; Rui, H.; Song, K.C.; Davila-Contreras, E.M.; Qi, Y.; Lee, J.; Monje-Galvan, V.; Venable, R.M.; Klauda, J.B.; Im, W. [=] "CHARMM_GUI Membrane Builder toward Realistic Biological Membrane Simulations." J. Comput. Chem. 35(27), 1997-2004 (2014). **Citations:** 2390
27. Jeong, J.C.; Jo, S.; Wu, E.L.; Qi, Y.; Monje-Galvan, V.; Yeom, M.S.; Gorenstein, L.; Chen, F.; Klauda, J.B.; Im, W. [=] "ST-Analyzer: A web-based user interface for simulation trajectory analysis." J. Comput. Chem. 35(12), 957-963 (2014). **Citations:** 15

<u>Conference Proceedings</u>

Publications at UB

1. Monje, V [=]; Li, J[*]; Ford Versypt, A.N.; Sanchez-Pena, M.L. "Work-in-progress: Evidence-based scope and selection of threshold concepts for the design of computational notebooks in undergraduate statistics courses for chemical engineering." *Proceedings of the ASEE Annual Conference*, Montreal, CA, 2025 (*Accepted*)

Graduate work

2. Monje-Galvan, V.; Klauda, J.B. [=] "Two sterols, two bilayers: Insights on Membrane Structure from Molecular Dynamics." *Molecular Simulation: Proceedings of the 4th*

International Conference on Molecular Simulation. 43(13-16): 1179-1188. (2017)
Citations: 11

TECHNICAL PRESENTATIONS (**since starting first independent position**)
*Presenter name is underlined, * indicates graduate student mentored by VM, + indicates undergraduate student mentored by VM*

Invited seminar speaker:

1. Monje, V. Center for Computational Biology Seminar. Simons Foundation Flatiron Institute, New York City, NY. April 16, 2025
2. Monje, V. Chemical and Biological Engineering Seminar Series. Iowa State University, Ames, IA. February 20, 2025.
3. Monje-Galvan, V. Chemical Engineering Department Seminar Series. Rochester Institute of Technology (RIT), Rochester, NY. April 18, 2024.
4. Monje-Galvan, V. Larry Mays Seminar Series in Bioinformatics. Department of Bioinformatics and Genomics (BIG), The University of North Carolina at Charlotte. virtual. October 6, 2023.
5. Monje-Galvan, V. Department of Biochemistry Seminar Series. Jacobs School of Medicine and Biomedical Sciences, University at Buffalo. August 29, 2023.
6. Monje-Galvan, V. "Fingerprinting protein-lipid interactions with molecular dynamics simulations." Buffalo Protein Science Group Seminar Series. Department of Structural Biology, University at Buffalo. April 19, 2023.

Invited talks:

1. Monje, V. "Molecular interactions at the cell membrane interface, predictions from simulations." Molecular Engineering of Soft Matter: Spanning Small Molecules to Macromolecules. Telluride Science & Innovation Center. Telluride, CO, May 27-31, 2025
2. Monje-Galvan, V. "Lipid sorting and the signature of protein-lipid interactions at the membrane interface." 34th International Conference in Science and Technology of Complex Fluids. San Luis Potosi, MX, June 29, 2023
3. Monje-Galvan, V. "Glycone diversity in small molecules and their interaction with lipid bilayers." Congreso de Bio-simulaciones del Cono Sur. Brazilian & Argentinian Biophysical Societies. Porto Alegre, Brasil, June 2, 2023
4. Monje-Galvan, V. "Diversidad lipídica en modelos de membranas celulares, estudios con dinámica molecular." VIII Encuentro Nacional de Químicos Teóricos y Computacionales & IV Escuela Colombiana de Teoría y Computación. Universidad Nacional de Colombia. virtual, May 2023
5. Monje-Galvan, V. "Molecular interactions at the cell membrane interface." II Simposio del Grupo de Investigación de Ciencias Básicas, Ibero Puebla & CIMAT-Monterrey, México. virtual, November 2022

6. Monje-Galvan, V. "Modelando la huella lipídica en enfermedades infecciosas." XX Curso Boliviano de Sistemas Complejos, Facultad de Física, Universidad Mayor de San Andrés, La Paz, Bolivia. virtual, September 2022
7. Monje-Galvan, V. "Modeling protein-lipid interactions in mechanisms of cell death." Biological Membranes and Membrane Proteins. Santa Fe, NM, June 2022
8. Monje-Galvan, V. "Modelaje de membranas lipídicas y su role n mecanismos de enfermedad." III International Congress in Biotechnology: Bolivia Innova, Universidad Católica Boliviana, Santa Cruz, Bolivia. virtual, June 2021

Conference Presentations
19 since starting first independent position (PI & mentees) | 7 as postdoctoral scholar | 10 as graduate research assistant

- American Institute of Chemical Engineers Annual meeting (2023, 2024)
- Biophysical Society Annual meeting (2022, 2023, 2024, 2025)
- NOBCChE Annual meeting (2022, 2023, 2024)
- American Society for Engineering Education (2025)
- UB Celebration of Academic Excellence (2024)
- UB Undergraduate Research Day (2022)
- Women in Bioinformatics & Data Science (3WBDS) LA Conference (virtual, 2022)
- Cell Bio 2021 of the American Society for Cell Biology (virtual, 2021)
- Gibbs Society of Biological Thermodynamics (virtual, 2021)

STUDENT MENTORING
Focus areas: computational biophysics; interfacial structure and thermodynamics; statistical thermodynamics; molecular modeling; lipid membrane modeling; high performance computing.
Group Website

Dissertations/Theses Progress

- Jinhui Li, PhD (Jan. 2021 – present), CBE. Expected graduation: December 2025.
- Ricardo X. Ramirez, PhD (Sept. 2021 – present), CBE. Expected graduation: May 2026
- Mahtab Firoozi, PhD (Sept. 2024 – present), CBE. Expected graduation: May 2029
- Mehmet Hozaat, MS. (May 2025 – present), CBE. Expected graduation: August 2025

Research Group Alumni (l*ast known position in italics*)

Graduate Students

- Oluwatoyin Campbell, PhD. 2025.
- Laura Sweezy, M.Eng. 2021. *Thermo Fisher Scientific, Grand Island, NY, USA*

Undergraduate Students

- Dina Dahhan (January 2024 – present), BMS University at Buffalo, sponsored by GWIS fellowship (*graduate mentor: Oluwatoyin Campbell*)

- Seth Thomson (January 2023 – December 2024), *Process Engineer @ Andritz, Glens Falls, NY*
- Trey Lewis (Summer 2024, CLIMB UP alumni), UB *Neuroscience undergraduate.*
- Angela Aguirre (June 2022 – May 2024), *Graduate Student at Purdue University*
- Shane Varner (June 2021 – December 2022, LSAMP alumni) *Process Engineer @ Linde, Tonawanda, NY*
- Van Le (November 2022 – June 2023), *CSE graduate 2023*
- Jocelyn Mendez (June 2022 – Aug. 2022 as LSAMP fellow) *CBE graduate 2023.*

Career Development Mentoring

- Juan D. Mendez. Remote research intern (June 2023 – present). *B.S. in Chemistry, Universidad Icesi, Cali, Colombia.*
- Ivan Felsztyna, PhD. Remote research intern (January 2023 – May 2024) *Instituto de Investigaciones Biologicas y Tecnologicas (IIByT), CONICET, Universidad Nacional de Cordoba (UNC), Cordoba, Argentina.*
- Dahlia Andres. Undergraduate Mentee (January 2021 – August 2021) *through the Center for Minorities in Science and Engineering at the University of Maryland-College Park*

PROFESSIONAL SERVICE

Offices / Boards

- Chair elect of the AIChE Affinity group LatinXinChE (January 2025 – December 2025, *elected position*)
- Treasurer of the Theory and Computation Subgroup of the Biophysical Society (2024-2026, *nominated*)
- Early Careers Committee Member for the Biophysical Society (appointment position from July 2023 – June 2026)
- Board member of the Advisory Board to the Center for Minorities in Science and Engineering at the University of Maryland (2023-2026)
- Secretary of the AIChE Affinity group LatinXinChE (June 2022 – December 2024)
- Liaison director for the Computational Molecular Science and Engineering Forum (CoMSEF) of the AIChE. (2022-2024, *elected position*)
- Review Editor for Bioengineering and Biotechnology - Biochemical Engineering (2022-2024).

Conference Session Chair/Co-chair

- Co-Chair for the "*Protein-Lipid Interactions*" session at the Biophysical Society annual meeting (Feb. 2022, San Francisco, CA)

- Co-Chair for the "*Physical, Chemical & Systems Cell Biology*" poster session in the ASCB Cell Bio 2021 conference with Dr. Fernanda Marconi Roversi. (Dec. 2021, virtual)

Sessions Organized

- BPS-sponsored mini-symposium with the Society for Latinoamerican Biophysicists (SoBLA) "*Building Bridges in Computational Biophysics*".
  Co-organizer with Dr. P. Soto, Creighton University, NE, USA; Dr. C. Bores Quijano, Union College, NY, USA; and Dr Priscila Gomes, Auburn University, AL, USA. (Held virtually on an annual basis on the second week of October since 2022)
- Biophysics Week 2023. "*Foro de Estudiantes en Biofisica.*" Co-organizer with Dr. A. D. Reyes-Figueroa, CIMAT-Monterrey, MX. (March 20, 2023 - virtual)

Reviewer for scientific journals (since 2020)

ACS Omega | Biophys. J. | Nat. Comm. | MDPI Membranes | MDPI Pharmaceutics | ACS JPCB | ACS JPC Letters | Molec. Sim. | J. Struc. Biol. | Springer Nat. Comm. Biol. | Structure | J. Molec. Graph. Model. | Nat. Comp. Sci.

Proposal Review Panels

- NIH: *mail reviewer* for RM1 (10/2024); *ad hoc reviewer* for Biochemistry and Biophysics of Membranes (BBM) (06/2024); *Early Career Reviewer* for BBM (10/2022)
- NSF: GRFP (2022, 2023, 2025); CTMC Bio (01/2022)
- ACS Petroleum Research Fund (Aug. 2021)
- Referee for the National Academy of Engineering initiatives *EngineerGirl Writing Contest* & *Ambassadors Program* (2014 – present on an annual basis)

Service at the University at Buffalo (UB)

- JEDI for Faculty Mentoring SubCommittee Member. SubCommittee lead: Dr. Negar Elhami-Khorasani. Lead: Dr. Kristen R. Moore (2023 – present)
- Faculty Senate IT Committee Member. Lead: Dr. Jessica Kruger. (2022 – present)
- Undergraduate mentor for incoming SEAS first-year students, EAS 202 (2021 – present)
- CLIMB UP undergraduate research mentor (2024, 2025).
- WiSE Open Lab outreach, undergraduate students visit to the Monje Group, Q&A session on research and graduate school. (2022, 2024, 2025)
- Committee member of the *Teaching Faculty Search for the Institute for Artificial Intelligence and Data Science*. (multiple positions to fill). Committee chair: Dr. Johannes Hachmann. (Dec. 2022 – Spring 2024)
- Committee member of the *Tenure-track Faculty Search in Computational Chemistry Related to Health*. Committee chair: Dr. John Richard, Dept. of Chemistry. (Oct. 2022 – March 2023)
- Louise Stokes Alliance for Minority Participation (LSAMP) mentor (2021 – 2023)

Service in the Department of Chemical and Biological Engineering (CBE) @ UB

- CBE Graduate Committee member (Jan. 2022 – present)
- Co-organizer for the annual CBE Graduate Research Symposium (Nov. 2021 - present)
- CBE Seminar Series Coordinator (Spring 2022 – Fall 2025)
- Member of PhD Dissertation Committees (9) & Master Thesis Committees (2)
- Undergraduate faculty advising (8)

Professional memberships

American Institute of Chemical Engineers (AIChE) | Biophysical Society (BPS) | American Chemical Society (ACS) | Society of Latin-American Biophysicist (SoBLA)

TEACHING ACTIVITIES

Formal courses at UB

CE 305: Probability, Statistics, and Data Analysis (undergraduate course, 3 credit hrs.)

Fall 2021, 2022, 2023, 2024, 2025. Enrollment: 44-54 students

CE 410 / CE 530: Molecular Modeling (cross-listed graduate & undergraduate, 3 credit hrs.)

Spring 2022, 2023, 2024, 2025. Enrollment: 10-21 students

Other courses taught at UB

CE498 Undergraduate Research

CE501, CE502, CE 503, CE 504 (MS level research credits)

CE601, CE602, CE 659, CE 660 (PhD level research credits)

These courses constitute several additional credit hours per semester and are offered on a rolling basis to satisfy CBE elective credits for undergraduates, or research credits for graduate students to satisfy their degree requirements. The following students have registered for these credits under my supervision: 4 PhD; 1 MEng; 5 Undergraduates.

Other courses taught

Universidad Nacional de Quilmes, Argentina (joint instructor, virtual 9-week course with Dr. Juliana Palma): "Alcances y limitaciones de las simulaciones de dinámica molecular." Lectures available online. Fall 2021. Enrollment: 33

Universidad Mayor de San Andres, La Paz-Bolivia. (Keynote lecturer): "Modern Topics in Biophysics." XVIII Curso Boliviano de Sistemas Complejos. Lectures & workshops available online. Dec. 2-4, 2020). Enrollment: 55

Formal courses at the University of Chicago

Biophysical Research Immersion (modular course offered to 1st year graduate students)

- Module 1: Hands-on workshop on molecular dynamics simulations (Sept. 2018)
- Module 2: Journal club & Communications in Biophysics (Autumn Quarter 2018)

RESEARCH GRANTS

- Human Frontier Science Program (HFSP) Research Grant
  Award: RGEC28/2025
  Role: co-PI (*computational lead*)
  Total Amount: $1,200,000; Monje share: $400,000
  Period: 09/2025-08/2028
  "*MetaCrystal: Metabolic principles of intracellular crystallization"*

- National Science Foundation RIEF
  Award: EEC-2407487
  Role: PI
  Total Amount: $199,810; Monje share: $116,906
  Period: 09/2024-08/2026
  "*Research Initiation: Computational notebooks as scaffolds to consolidate threshold concepts in an undergraduate introductory statistics course in chemical engineering*"

COMPUTATIONAL AWARDS

- *BIO240088*. 750,000 ACCESS Credits. **ACCESS Allocations** computing and data resource program supported by NSF. (March 2024 – March 2025).

- *MCB200093P*. 345,000 MD simulation units (6 computer days). **Anton2** at Pittsburgh Supercomputing Center (PSC), dedicated supercomputer for the simulation of biological systems. (2023-2024)

- *MCB200093P*. 230,000 MD simulation units (4 computer days). **Anton2** at Pittsburgh Supercomputing Center (PSC), dedicated supercomputer for the simulation of biological systems. (2022-2023)

- *BIO220003*. 50,000 GPU hours on ***Bridges-2*** computer at PSC & 2,500 core-hours ***Bridges-RM*** at PSC. XSEDE Educational allocation (2022-2023). Allocation used during the Spring 2022 semester, CE 410/530 course (enrollment: 10). Corresponding awarded value: $17,886

- *MCB200093P*. 230,000 MD simulation units (4 computer days). **Anton2** at Pittsburgh Supercomputing Center, dedicated supercomputer for the simulation of biological systems. (2020-2021)

Prior to UB

- *MCB180125.* 2,500 GPU hours on ***Bridges*** computer at PSC & 50,000 CPU node-hours on ***Comet*** at PSC. XSEDE Educational allocation (2018-2019). Allocation used during a two-week introductory workshop on molecular dynamics (enrollment: 9). Corresponding awarded value: $1,578.