VIVIANA MONJE

Assistant Professor
Chemical and Biological Engineering Department

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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

- 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

Prior to UB

- Ann G. Wylie Dissertation Fellowship (Univ. of MD). Fall 2016
- LSAMP Bridge to the Doctorate Fellow (NSF). 2012 – 2014
- LSAMP Undergraduate Program Fellow (NSF). 2010 – 2012
- ACCESS Engineering Scholar (NSF). 2009 – 2012

PEER-REVIEWED PUBLICATIONS

Google Scholar citations: 3401, h-index: 15, i10-index: 19 (as of 04/15/2025)
Google Scholar | ORCiD

[*] *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. 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, (*accepted*) **IF: 3.2. Q1 Biophysics**
2. 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) **IF: 3.9. Q1 Condensed Matter Physics. Surfaces & interfaces.**
3. 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) **IF: 4.0. Q1 Biochemistry. Citations: 4**
4. Campbell, O. [*]; Monje-Galvan, V. [=] "Lipid composition modulates interactions of p7 viroporin during membrane insertion." J. Struct. Biol. 215(3): 108013 (2023) **IF: 3.0 Q1 Struct. Biol. Citations: 3**
5. Li. J. [*]; Monje-Galvan, V.[=] "In Vitro and In Silico Studies of Antimicrobial Saponins: A Review." Processes, 11(10): 2856 (2023). **IF: 3.5. Q2 Chem. Eng. Citations: 11**
6. 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) **IF: 1.2. Q2 Chem. Eng. Citations: 1**
7. 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) **IF: 4.7. Q1 Chem. Q2 Biomaterials. Citations: 9**
8. 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) **IF: 5.5. Q1 Chemistry. Citations: 10**
9. Campbell, O. [*]; Monje-Galvan, V. [=] "Protein-driven membrane remodeling: Molecular perspectives from Flaviviridae infections." Biophys. J, 122: 1-10 (2021) **IF: 4.0. Q1 Biophysics. Citations: 6**
10. 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) **IF: 4.1. Q1 Chem. Eng. Citations: 3**
11. 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) **IF: 9.0. Q1 Biochem. Q1 Molec. Biol. Citations: 30**

Postdoctoral work

12. 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) **IF: 3.3. Q1 Phys. Theo. Chem. & Surfaces, Coatings, and films. Citations: 4**

13. 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) **IF: 4.0. Q1 Phys. & Theo. Chem. Citations: 26**

14. 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) **IF: 4.0. Q1 Biophysics. Citations: 1722**

15. Monje-Galvan, V; Voth, G.A. [=] "Binding mechanism of the matrix domain of HIV-1 Gag on lipid membranes." eLife, 9:e58621 (2020) **IF: 8.7. Q1 Biochem. Genetics & Molec. Biol. Citations: 38**

Graduate work

16. Monje-Galvan, V.; Klauda, J.B. [=] "Interfacial properties of aqueous solutions of butanol isomers and cyclohexane." Fluid Phase Equilib., 513: 112551 (2020) **IF: 2. 8. Q1 Chem. Eng. Citations: 8**

17. 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) **IF: 60.6. Q1 Chemistry. Citations: 106**

18. 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) **IF: 6.0. Q1 Phys & Theo. Chem. Citations: 33**

19. 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) **IF: 3.5. Q1 Phys & Theo. Chem. Citations: 28**

20. 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) **IF: 4.2. Q1 Phys & Theo. Chem. Citations: 42**

21. 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). **IF: 3.5. Q1 Phys & Theo. Chem. Citations: 70**

22. Monje-Galvan, V.; Klauda, J.B. [=] 2016. "Peripheral Membrane Proteins: Tying the Knot between Experiment and Computation." BBA: Biomembranes, 1858: 1584-1593 (2016). **IF: 3.7. Q1 Biophysics. Citations: 69**

23. Monje-Galvan, V.; Klauda, J.B. [=] 2015. "Modelling Yeast Organelle Membranes and How Lipid Diversity Influences Bilayer Properties." Biochemistry. 54(45), 6852-6861 (2015). **IF: 3.2. Q1 Biochem. Citations: 74**

24. 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). **IF: 3.7. Q1 Chem. Q2 Comp. Mathematics. Citations: 2390**

25. 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). **IF: 3.7. Q1 Chem. Q2 Comp. Mathematics. Citations: 15**

Undergraduate work

26. Spencer, J.D.; Moton, J.M.; Gibbons, W.T.; Gluesenkamp, K.; Ahmed, I.I.; Taverner, A.M.; McGahagan, D.; Tesfaye, M.; Gupta, C.; Bourne, T.P; Monje, V.; Jackson, G.S. [=] "Design of a combined heat, hydrogen, and power plant for university campus waste streams." Int. J. of Hydrogen Energy. 38(12), 4889-4900. (1st place in the 2012 Hydrogen Student Design Contest) **IF: 6.7**. **Q1. Condensed Matter Phys. Q1 Fuel Tech. Citations**: **17**

27. Klauda, J.B.; Monje, V.; Kim, T.; Im, W. [=] "Improving the CHARM Force Field for Polyunsaturated Fatty Acid Chains." J. Phys. Chem. B. 116(31), 9424-9431 (2012). **IF: 3.5. Q1 Phys & Theo. Chem. Citations: 185**

Conference Proceedings

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) **IF: 2.05. Q2 Chem. Eng. Citations: 11**

TECHNICAL PRESENTATIONS

*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 Engineering of Soft Matter: Spannign Small Molecules to Macromolecules. Telluride Science & Innovation Center. Telluride, CO, May 27-31, 2025 (scheduled)
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

Prior to UB

8. "Computers and Cells – Biophysics of Lipid Membranes at the Atomic Scale." 2020 Seminar Series Grupo de Investigadores Latitud Cero. virtual, July 2020
9. "Molecular interactions in cellular processes, a perspective from simulations." XVI LAWNP. La Paz, Bolivia, October 2019

10. "Modelos simétricos y asimétricos para membranas de la levadura, nociones sobre la interacción de lípidos." Universidad Mayor de San Andrés - Instituto de Investigaciones Físicas. La Paz, Bolivia, May 2017
11. "Comportamiento de hidrotropos en la interfaz de soluciones aquosas." Universidad Mayor de San Andrés – Facultad de Ingeniería – Ingeniería Química. La Paz, Bolivia, May 2017
12. "Mejorando el campo de fuerza para simulaciones moleculares de ácidos grasos poliinsaturados en membranas celulares." Universidad Mayor de San Andrés - Instituto de Investigaciones Físicas. La Paz, Bolivia, 2013

Conference Presentations

1. Ramirez, R.X.[*]; Monje, V. "BPS2025 – Molecular dynamics simulations of conformational changes in MLKL induced by phosphorylation." Biophysical Society, San Diego, CA, February 2025
2. Li, J.[*]; Monje, V. "BPS2025 – Permeation of triterpenoid glycosides through lipid bilayers" Biophysical Society, San Diego, CA, February 2025
3. Li, J.[*]; Thomson, S.[+]; Monje, V. "BPS2025 – Effect of membrane patch size on the simulation of complex lipid bilyaers." Biophysical Society, San Diego, CA, February 2025
4. Campbell, O[*]; Monje-Galvan, V. "Modeling the effect of Surface tension on neutral lipid mixtures on the Surface of lipid monolayer interfaces." AIChE, San Deigo, CA. October 2024
5. Campbell, O[*]; Monje-Galvan, V. "Mechanisms of protein and lipid interplay during molecular pathogenesis of Hepatitis C and Liver cancer." NOBCChE, Orlando, FL, September 2024
6. Thomson, S.[+]; Monje-Galvan, V. "Realistic lipid membrane modeling using all-atom molecular dynamics simulation." UB Celebration of Academic Excellence, Buffalo, NY, May 2, 2024
7. Li, J.[*]; Monje-Galvan, V. "Effects of anti-inflammatory drugs on lipid bilayers." UB Celebration of Academic Excellence, Buffalo, NY, May 2, 2024
8. Monje-Galvan, V.; Ramirez, R.X.[*], Felsztyna, I.; Kanduc, M.; Guzman, H.V. "RNA adsorption dynamics onto membrane models for lipid nanoparticles." Biophysical Society, Philadelphia, PA, February 2024
9. Campbell, O[*]; Monje-Galvan, V. "Protein-mediated remodeling of membranas by the Hepatitis C viroporin." NOBCChE, New Orleans, LO, September 2023
10. Campbell, O.[*]; Monje-Galvan, V. "Molecular dynamics simulations of Hepatitis C viroporin and lipid membranes." Biophysical Society, San Diego, CA, February 2023
11. Li, J.[*]; Monje-Galvan, V. "Clustering and binding of oleanolic acid saponins with bacterial membranes." Biophysical Society, San Diego, CA, February 2023

12. Ramirez, R.X.[*]; Monje-Galvan, V. "Modeling the molecular fingerprint of protein-lipid interactions of MLKL on complex bilayers." Biophysical Society, San Diego, CA, February 2023
13. Campbell, O.[*]; Monje-Galvan, V. "Lipid fingerprint in chronic viral infections: learning from simulations of the viroporin protein of Hepatitis C virus." 3rd Women in Bioinformatics & Data Science (3WBDS) LA Conference. virtual, September 2022
14. Campbell, O.[*]; Monje-Galvan, V. "Modeling protein-lipid interactions in Hepatitis C viral infection." NOBCChE, Orlando, FL, September 2022
15. Varner, S.[+]; Monje-Galvan, V. "Molecular dynamics simulations of GM3 in the plasma membrane." UB Undergraduate Research Day, Buffalo, NY, August 2022
16. Mendez, J.[+]; Monje-Galvan, V. "Structural properties of viral protein H in bacteriophage φX174." UB Undergraduate Research Day, Buffalo, NY, August 2022
17. Li, J.[*]; Monje-Galvan, V. "Interactions of antibiotic organic molecules with lipid bilayers." Biophysical Society, San Francisco, CA, February 2022
18. Li, J. [*]; Monje-Galvan, V. "Interactions of antibacterial compounds and lipid membranes." Cell Bio 2021 of the American Society for Cell Biology. virtual, December 2021
19. Monje-Galvan, V. "Membrane permeabilization during necroptosis: Insights from molecular dynamics studies." Gibbs Society of Biological Thermodynamics, 35th conference. virtual, September 2021

Postdoctoral work

20. Monje-Galvan, V.; Pak, A.J.; Voth, G.A. "Modeling protein-lipid interactions during viral assembly of SARS-CoV-2." Biophysical Society, virtual, February 2021
21. Monje-Galvan, V.; Voth, G.A. "The role of lipids on transmembrane protein interactions in viral infections." AIChE National Meeting, virtual, November 2020
22. Monje-Galvan, V.; Swanson, J.; Lippincott-Schwartz, J.; Sengupta, P.; Voth, G.A. "Modeling protein-lipid sorting at the HIV-1 viral assembly site." AIChE National Meeting, Orlando, FL, November 2019
23. Monje-Galvan, V.; Voth, G.A. "Lipid-lipid and lipid-protein interactions of the matric domain of HIV-1 Gag at the viral assembly site." Biophysical Society, Baltimore, MD, 2019
24. Monje-Galvan, V.; Pak, A.; Voth, G.A. "Computational modeling of protein interactions of the matrix domain of HIV-1 Gag." AIChE National Meeting, Pittsburgh, PA, 2018
25. Monje-Galvan, V. & Voth, G.A. "Protein aggregation and protein-membrane interactions of the matrix domain of HIV1- Gag." EuriSciCon, Structural Biology Conference, Barcelona, Spain, 2018
26. Monje-Galvan, V. & Voth, G.A. "Molecular interactions of the Matrix domain of HIV-1 Gag protein at the membrane interface." Biophysical Society, San Francisco, CA, 2018

Graduate work

27. Monje-Galvan, V. & Klauda, J.B. "Asymmetric models for the trans-Golgi Network and plasma membranes of S. cerevisiae, insights from molecular dynamics." American Chemical Society, Washington, DC, 2017
28. Novikov, A; Semenov, A.; Monje-Galvan, V.; Kuryakov, V.; Klauda, J.B.; Anisimov, M. "Interfacial behavior of hydrotropes in aqueous solutions." American Chemical Society, Washington, DC, 2017
29. Monje-Galvan, V. & Klauda, J.B. "Asymmetric membrane models for the PM and TGN of yeast, an all-atom molecular dynamics study." Biophysical Society, New Orleans, LA, 2017
30. Monje-Galvan, V. & Klauda, J.B. "Lo/Ld Phase Coexistence and Interaction in Model Membranes with IPC Lipids." Biophysical Society, Los Angeles, CA, 2016
31. Monje-Galvan, V. & Klauda, J.B. "Membrane binding of the Osh4 curvature-sensing peptide." Biophysical Society, Baltimore, MD, 2015
32. Monje-Galvan, V. & Klauda, J.B. "Binding studies of a Saccharomyces Cerevisiae peripheral protein Osh4" American Chemical Society, Denver, CO, 2015
33. Monje-Galvan, V. & Klauda, J.B. "Membrane binding of a curvature-sensing peptide of a lipid transport protein in yeast." XL Congress of Theoretical Chemists of the Latin Expression QUITEL, Galapagos, Ecuador, 2014
34. Monje-Galvan, V. & Klauda, J.B. "Molecular dynamic studies on organelle-specific yeast membrane models and amphipathic lipid packing sensor motif binding mechanism." Biophysical Society, San Francisco, CA, 2014
35. Monje-Galvan, V. & Klauda, J.B. "Simulation studies on organelle-specific yeast membrane models and amphipathic lipid packing sensor motif binding mechanism." AIChE National Meeting, San Francisco, CA, 2013
36. Monje-Galvan, V. & Klauda, J.B. "Improved CHARMM Force Field for Polyunsaturated Fatty Acid Chains, a Study on DAPC Membranes." Biophysical Society, Philadelphia, PA, 2013

GRADUATE STUDENTS

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

Group Website

Dissertations/Theses Progress

- Oluwatoyin Campbell, PhD (Jan. 2021 – present), CBE University at Buffalo. Expected graduation: May 2025.
- Jinhui Li, PhD (Jan. 2021 – present), CBE University at Buffalo. Expected graduation: December 2025.

- Ricardo X. Ramirez, PhD (Sept. 2021 – present), CBE University at Buffalo. Expected graduation: May 2026
- Mahtab Firoozi, PhD (Sept. 2024 – present), CBE University at Buffalo. Expected graduation: May 2029

Undergraduate Students

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

Special Achievement of Graduate Students

- Oluwatoyin Campbell. *PhD Candidate at CBE at University at Buffalo*. **Graduate Women in Science** (Sept. 2023 – May 2024). Graduate fellowship given to outstanding graduates students to promote participation and professional development in the sciences.
- Oluwatoyin Campbell. *PhD Candidate at CBE at University at Buffalo*. **Presidential Fellow** (Sept. 2020 – present). UB scholarship given to outstanding incoming graduates students to the PhD program for their high academic achievement.
- Oluwatoyin Campbell. *PhD Candidate at CBE at University at Buffalo*. **CLIMB HI Impact Scholar** (Sept. 2020 – June 2022). Professional Development Program for the initial two years of graduate schools.

Research Group Alumni
Last known position in italics

Graduate Students

- Laura Sweezy, M.Eng. (Jan. 2021 – Dec. 2021). *Thermo Fisher Scientific, Grand Island, NY, USA*

Undergraduate Students

- Seth Thomson (January 2023 – December 2024), *CBE University at Buffalo*
- 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) *Linde, Tonawanda, NY, USA*
- Van Le (Nov. 2022 – June 2023), *CSE graduate 2023*
- Jocelyn Mendez (June 2022 – Aug. 2022 as LSAMP fellow) *CBE graduate 2023.*

Career Development Mentoring

- Juan D. Mendez (since Summer 2023 as a remote research intern – work in progress with experimental collaborators). *B.S. in Chemistry, Universidad Icesi, Cali, Colombia.*
- Ivan Felsztyna (January 2023 – May 2024) as a remote research intern – manuscript under preparation). *Doctoral candidate at the Instituto de Investigaciones Biologicas y*

Tecnologicas (IIByT), Consejo nacional de investigaciones cientificas y tecnicas (CONICET), Universidad Nacional de Cordoba (UNC), Cordoba, Argentina.

- Dahlia Andres (Jan. 2021 – Aug. 2021 as mentee through the Center for Minorities in Science and Engineering, CMSE, at the University of Maryland-College Park) *Undergraduate in Mechanical Engineering at UMD, Vehicle Engineering Intern at Northrop Grumman*

Undergraduate Students – prior to UB

- Ms. Lidiya Gavrilenko (June 2016 – Aug. 2017 at the University of Maryland-College Park, mentee) *Engineer at Federal Aviation Administration*
- Ms. Linnea Warburton (Jan 2017 – Aug. 2018 at University of Maryland-College Park, mentee & co-author) *PhD student in Mechanical Eng. At UC Berkley*
- Mr. Edgar I. Sanchez Medina (June 2016 – Aug. 2016 as summer intern at the University of Maryland-College Park, mentee) *PhD student at Max Planck Institute for Dynamics of Complex Technical Systems*
- Christopher Boughter, Ph.D. (June 2015 – Nov. 2016 at the University of Maryland-College Park, mentee & co-author) *NIH IRTA Postdoctoral Fellow at NIAID (NIH)*
- Mr. Kyle Wildermuth (June 2015 – Sept. 2017 at the University of Maryland-College Park, mentee & co-author) *Partner & Developer at Lifelike Labs, Chicago, IL, USA.*

PROFESSIONAL DEVELOPMENT

- UB SEAS Faculty Launch & Mentoring Program (FLMP) Fellow (2024 cohort)
- 2024 NSF Engineering CAREER Proposal Workshop (virtual, May 15-17, 2024)
- Community of Practice in Action (CoPA): Addressing Social Responsibility in the Curriculum. (2022-2023 cohort)
- ASEE / AIChE *Faculty Summer School*. Colorado School of Mines. (July 25-29, 2022)
- "*Write Winning NIH Grant Proposals Workshop*" by Grant Writer's Seminars & Workshops (GWSW) (Jan 13-14, 2022)

PROFESSIONAL MEMBERSHIPS

- American Institute of Chemical Engineers (AIChE), since 2012.
- Biophysical Society (BPS), since 2013.
- American Chemical Society (ACS), since 2012.
- Society of Latin-American Biophysicist (SOBLA), since 2013.
- Consultant with the *Complex Systems Group* at the Physics Research Institute of UMSA (La Paz, Bolivia), since 2019.

UNIVERSITY SERVICE

- JEDI for Faculty Mentoring SubCommittee Member. SubCommittee lead: Dr. Negar Elhami-Khorasani. JEDI Committee lead: Dr. Kristen R. Moore (2023 – present)
- Faculty Senate IT Committee Member. Committee lead: Dr. Jessica Kruger. (2022 – present)
- Reviewer with Women in Science and Engineering (WiSE) for the Gresky Award & Arnold Family Scholarship (2022 – 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. (April 2022, April 2024, April 2025 scheduled)
- 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)
- UB SEAS graduate poster competition. (2022, 2023)
- WiSE early move-in events (Fall 2021, Fall 2022)
- WiSE STEM Outreach Program, faculty visitor & panelist with high school students; Amazon sponsored project. (Fall 2022)
- WiSE & Shine panelist (March 2022)
- Undergraduate mentor for incoming SEAS first-year students (Spring 2021)
- Poster judge for the CSTEP 15th Annual Research Poster Symposium (July 2021)

DEPARTMENTAL SERVICE

- CBE Graduate Committee member (Jan. 2022 – present)
- Co-organizer for the annual CBE Graduate Research Symposium (Nov. 2021 - present)
- Judge for graduate poster presentations at CBE Graduate Symposium (Nov. 2020 - present)
- CBE Seminar Coordinator (Spring 2022 – Fall 2025)
- CBE Graduate Recruitment virtual open house (Nov. 8, 2022 – international students; Nov. 30, 2022 – domestic students)
- CBE Graduate Student Recruitment Fair, AIChE Annual meeting (virtual, Nov. 2020; Phoenix, AZ, Nov. 2022)
- Member of PhD Dissertation committees of:

Student	*Degree*	*Department*	*Principal Advisor*
Carley Cook	PhD granted	CBE	A. Ford-Versypt
Mahasweta Bhattacharya	PhD granted	CBE	R. Gunawan
Peter Zhang	PhD candidate	Chemistry	H. Nguyen
Oluwatoyin Campbell	PhD candidate	CBE	V. Monje
Jinhui Li	PhD candidate	CBE	V. Monje
Ricardo X. Ramirez	PhD candidate	CBE	V. Monje
Eduardo A. Chacin Ruiz	PhD candidate	CBE	A. Ford-Versypt
Mahtab Firoozi	PhD student	CBE	V. Monje
Daniel Guiggey	PhD student	CBE	N. Parashurama

- Member of Master Thesis committees of:

Student	*Degree*	*Department*	*Principal Advisor*
Ritik R. Konduskar	M.S.	CBE	J. Hachmann
Samia Noor	M.S.	Chemistry	H. Nguyen

- Faculty advisor for undergraduates:

Year	*Spring*	*Fall*
2021	-	4
2022	4	4
2023	4	4
2024	2	6
2025	4	

OTHER SERVICE

Professional 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 Biofísica.*" Co-organizer with Dr. A. D. Reyes-Figueroa, CIMAT-Monterrey, MX. (March 20, 2023 - virtual)

Reviewer for scientific journals (since 2020)

ACS Omega | Biophysical Journal | Nature Communications | MDPI Membranes | MDPI Pharmaceutics | ACS Journal of Physical Chemistry B | ACS Journal of Physical Chemistry Letters | Molecular Simulation | Journal of Structural Biology | Springer Nature Communications Biology | Structure | Journal of Molecular Graphics and Modelling | Nature Computational Science

Proposal Reviewer

- NIH mail reviewer for the NIGMS Collaborative Program for Multidisciplinary Teams (RM1). (September 2024)
- NIH *ad hoc* reviewer for the Biochemistry and Biophysics of Membranes (BBM) study section. (June 2024)
- NIH Early Career Reviewer (ECR) for the Biochemistry and Biophysics of Membranes (BBM) study section. (Oct. 2022)
- NSF Graduate Research Fellowships Program (GRFP) (2022, 2023, 2025)
- NSF Chemical Theory, Models, and Computational Methods (CTMC Bio) (Jan. 2022)
- ACS Petroleum Research Fund (Aug. 2021)
- Referee for the National Academy of Engineering *EngineerGirl Writing Contest* & *Ambassadors Program* from the (2014 – present, annual basis)

Poster Judge

- Student Research Achievement Award (SRAA) competition judge at the Biophysical Society meeting (2022, 2023)
- Undergraduate student poster judge at the AIChE national meeting (2019)

Panelist

- Panelist for LatinXinChE Resume building Workshop, virtual (Feb 2025)
- Panelist for LatinXinChE Graduate School Applications, virtual (Oct 2023)
- Panelist for LSAMP & bridge to the Doctorate Program with the Center for Minorities in Science and Engineering (CMSE), and Women in Engineering (WIE) at the University at Maryland-College Park (2009 – 2021)
- Panelist for ACCESS scholarship at Montgomery College (2009 – 2017)

TEACHING ACTIVITIES

Formal courses at UB

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

Fall 2024; enrollment: 47 students
Fall 2023; enrollment: 54 students
Fall 2022; enrollment: 53 students
Fall 2021 (as CE 327); enrollment: 44 students

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

Spring 2025; enrollment: 14 students
Spring 2024; enrollment: 21 students
Spring 2023; enrollment: 2 students
Spring 2022; enrollment: 10 students

Other courses taught at UB

CE498 & BMS498, Undergraduate Research

CE501 & CE502, Individual Problems (MS level)

CE503 & CE504, Engineering Projects (MEng level)

CE601 & CE602, Individual Problems (PhD level)

CE659 & CE660, Dissertation (PhD level)

These courses constitute several additional credit hours per semester and are offered on a rolling basis to satisfy CBE elective credits for undergraduates (CE498), or research credits for graduate students to satisfy their degree requirements. The following students have registered for these credits under my supervision: 3 PhD; 1 MEng; 4 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 Biophysical Research (Autumn Quarter 2018)

Prior to UB

Teaching assistant at the University of Maryland-College Park

- CHBE 440 (Process Engineering Economics & Design II: Spring 2016)
- CHBE 468/648 (Molecular Dynamics Simulations: Spring 2015)
- CHBE 410 (Statistics and Experimental Design: Fall 2011, Fall 2014)
- ENCH 400 (Chemical and Biomolecular Engineering Thermodynamics II: Spring 2012)

ESTEEM Student Mentor with the Center for Minorities in Science and Engineering, High School student outreach (Summer 2010)

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.

TRAVEL GRANT AWARDS

- Biophysical Society 2022 early career scientists travel award (2022)

Prior to UB

- Kharasch Postdoctoral Travel Award, issued by the University of Chicago (2018)
- Chemical Society of Washington Travel Award, issued by the American Chemical Society CSW chapter (2015)