VIVIANA MONJE

Assistant Professor Chemical and Biological Engineering Department

WORK ADDRESS

506 Furnas Hall,
The State University of New York at Buffalo
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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
- 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: 2850, h-index: 15, i10-index: 17 (as of 06/14/2024)

Google Scholar | ORCiD

Invited Book Chapters

Publications at UB

1. Campbell, O.*, Allsopp, R.; Klauda, J.B., Monje-Galvan, V. = "Best practices for all-atom molecular dynamics of protein-lipid interaction studies" in Methods in Molecular Biology Series. Intracellular Lipid Transport, 2nd Ed. Guillaume Drin, Ed. Springer, (*Submitted*)

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:** 10
- 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:** 4

^{*} indicates graduate student mentored by VM, + indicates undergraduate student mentored by VM, = denotes the corresponding author.

Refereed Journal Articles

Publications at UB

- 1. Jaramillo-Granada, A.M.; Li, J.*; Flores Villareal, A.; Lozano, O.; Ruiz-Suarez, J.C.; Monje-Galvan, V.=; Sierra-Valdez, F.J. "Modulation of phospholipase A₂ membrane activity by anti-inflammatory drugs." Langmuir, 40(13): 7038-7048 (2024) **IF: 3.9. Q1 Condensed Matter Physics. Surfaces & interfaces.**
- 2. Pradhan, A.J; Chitkara, S.; Ramirez, R.X.*; Monje-Galvan, V.=; 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.**
- 3. 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.**
- 4. 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.**
- 5. 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. O2 Chem. Eng.**
- 6. 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.**
- 7. Ramirez, R.X.*; Campbell, O.*; Pradhan, A.; Atilla-Gokcumen, G.E.; Monje-Galvan, V. = "Modeling the molecular fingerpring of protein-lipid interactions of MLKL on complex bilayers." Frontier in Chem, 10: 1088058 (2023) **IF: 5.545. Q1 Chemistry. Citations: 1**
- 8. Campbell, O. *; Monje-Galvan, V. = "Protein-driven membrane remodeling: Molecular perspectives from Flaviviridae infections." Biophys. J, 122: 1-10 (2021) **IF: 4.033. Q1 Biophysics. Citations: 2**
- 9. Li, J.*; Kalyanram, P; Monje-Galvan, V; 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: 4.132. Q1 Chem. Eng. Citations: 1**
- 10. Pradhan, A.J; Lu, D.; Parisi, L.R.; Shen, S.; Berhane, I.A.; Galster, S.L.; Bynum, K.; Monje-Galvan, V.; 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: 9.039. Q1 Biochem. Q1 Molec. Biol. Citations: 15**

Postdoctoral work

11. 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**

- 12. 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: 4.008. Q1 Phys. & Theo. Chem. Citations: 19**
- 13. 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: 4.033. Q1 Biophysics. Citations: 122**
- 14. Monje-Galvan, V; Voth, G.A. = "Binding mechanism of the matrix domain of HIV-1 Gag on lipid membranes." eLife, 9:e58621 (2020) **IF: 8.713. Q1 Biochem. Genetics & Molec. Biol. Citations: 14**

Graduate work

- 15. Monje-Galvan, V.; Klauda, J.B. = "Interfacial properties of aqueous solutions of butanol isomers and cyclohexane." Fluid Phase Equilib., 513: 112551 (2020) **IF: 2.778. Q1 Chem. Eng. Citations: 6**
- 16. 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: 60.620. Q1 Chemistry. Citations: 76**
- 17. 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: 6.006. Q1 Phys & Theo. Chem. Citations: 22**
- 18. 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: 3.466. Q1 Phys & Theo. Chem. Citations: 14**
- 19. 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: 4.177. Q1 Phys & Theo. Chem. Citations: 28**
- 20. 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: 3.466. Q1 Phys & Theo. Chem. Citations: 56**
- 21. Monje-Galvan, V.; Klauda, J.B. = 2016. "Peripheral Membrane Proteins: Tying the Knot between Experiment and Computation." BBA: Biomembranes, 1858: 1584-1593 (2016). **IF: 3.720. Q1 Biophysics. Citations: 50**
- 22. 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: 3.162. Q1 Biochem. Citations: 59**
- 23. 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: 3.672. Q1 Chem. Q2 Comp. Mathematics. Citations: 1612**
- 24. 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: 3.672. Q1 Chem. Q2 Comp. Mathematics. Citations: 15

Undergraduate work

- 25. 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: 6.730**. **Q1. Condensed Matter Phys. Q1 Fuel Tech. Citations: 16**
- 26. 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:** 3.466. Q1 Phys & Theo. Chem. Citations: 154

Conference Proceedings

Graduate work

1. 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: 10**

TECHNICAL PRESENTATIONS

Presenter name is underlined, * indicates graduate student mentored by VM, + indicates undergraduate student mentored by VM

<u>Invited seminar speaker</u>:

- 1. <u>Monje-Galvan, V.</u> Chemical and Biological Engineering Seminar Series. Iowa State University, Ames, IA (*Spring 2025, scheduled*)
- 2. <u>Monje-Galvan, V.</u> Physics Colloquium. Union College, Schenectady, NY (*Fall 2024, scheduled*)
- 3. Monje-Galvan, V. Chemical Engineering Department Seminar Series. Rochester Institute of Technology (RIT), Rochester, NY. April 18, 2024
- 4. <u>Monje-Galvan, V.</u> Department of Biochemistry Seminar Series. Jacobs School of Medicine and Biomedical Sciences, University at Buffalo. August 29, 2023
- 5. <u>Monje-Galvan, V.</u> "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. <u>Monje-Galvan, V.</u> "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

- 2. <u>Monje-Galvan, V.</u> "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
- 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
- 4. <u>Monje-Galvan, V.</u> "Molecular interactions at the cell membrane interface." II Simposio del Grupo de Investigación de Ciencias Básicas, Ibero Puebla & CIMAT-Monterrey, México. virtual, November 2022
- 5. <u>Monje-Galvan, V</u>. "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
- 6. <u>Monje-Galvan, V.</u> "Modeling protein-lipid interactions in mechanisms of cell death." Biological Membranes and Membrane Proteins. Santa Fe, NM, June 2022
- 7. <u>Monje-Galvan, V.</u> "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. <u>Thomson, S.</u>⁺; Monje-Galvan, V. "Realistic lipid membrane modeling using all-atom molecular dynamics simulation." UB Celebration of Academic Excellence, Buffalo, NY, May 2, 2024
- 2. <u>Li, J.*</u>; Monje-Galvan, V. "Effects of anti-inflammatory drugs on lipid bilayers." UB Celebration of Academic Excellence, Buffalo, NY, May 2, 2024
- 3. <u>Campbell, O.*</u>; Monje-Galvan, V. "Molecular dynamics simulations of Hepatitis C viroporin and lipid membranes." Biophysical Society, San Diego, CA, February 2023

- 4. <u>Li, J.</u>*; Monje-Galvan, V. "Clustering and binding of oleanolic acid saponins with bacterial membranes." Biophysical Society, San Diego, CA, February 2023
- 5. <u>Ramirez, R.X.</u>*; Monje-Galvan, V. "Modeling the molecular fingerprint of protein-lipid interactions of MLKL on complex bilayers." Biophysical Society, San Diego, CA, February 2023
- 6. 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
- 7. <u>Campbell, O.*</u>; Monje-Galvan, V. "Modeling protein-lipid interactions in Hepatitis C viral infection." NOBCChE, Orlando, FL, September 2022
- 8. <u>Varner, S.</u>⁺; Monje-Galvan, V. "Molecular dynamics simulations of GM3 in the plasma membrane." UB Undergraduate Research Day, Buffalo, NY, August 2022
- 9. Mendez, J.⁺; Monje-Galvan, V. "Structural properties of viral protein H in bacteriophage φ X174." UB Undergraduate Research Day, Buffalo, NY, August 2022
- 10. <u>Li, J.</u>*; Monje-Galvan, V. "Interactions of antibiotic organic molecules with lipid bilayers." Biophysical Society, San Francisco, CA, February 2022
- 11. 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
- 12. <u>Monje-Galvan, V</u>. "Membrane permeabilization during necroptosis: Insights from molecular dynamics studies." Gibbs Society of Biological Thermodynamics, 35th conference. virtual, September 2021

Postdoctoral work

- 13. 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
- 14. Monje-Galvan, V.: Voth, G.A. "The role of lipids on transmembrane protein interactions in viral infections." AIChE National Meeting, virtual, November 2020
- 15. 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
- 16. 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
- 17. 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
- 18. <u>Monje-Galvan, V.</u> & Voth, G.A. "Protein aggregation and protein-membrane interactions of the matrix domain of HIV1- Gag." EuriSciCon, Structural Biology Conference, Barcelona, Spain, 2018

19. 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

- 20. <u>Monje-Galvan, V.</u> & 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
- 21. Novikov, A; Semenov, A.; <u>Monje-Galvan, V.</u>; Kuryakov, V.; Klauda, J.B.; Anisimov, M. "Interfacial behavior of hydrotropes in aqueous solutions." American Chemical Society, Washington, DC, 2017
- 22. 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
- 23. Monje-Galvan, V. & Klauda, J.B. "Lo/Ld Phase Coexistence and Interaction in Model Membranes with IPC Lipids." Biophysical Society, Los Angeles, CA, 2016
- 24. Monje-Galvan, V. & Klauda, J.B. "Membrane binding of the Osh4 curvature-sensing peptide." Biophysical Society, Baltimore, MD, 2015
- 25. Monje-Galvan, V. & Klauda, J.B. "Binding studies of a Saccharomyces Cerevisiae peripheral protein Osh4" American Chemical Society, Denver, CO, 2015
- 26. <u>Monje-Galvan, V.</u> & 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
- 27. 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
- 28. 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
- 29. 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

<u>Undergraduate Students</u>

- Seth Thomson (January 2023 December 2024), CBE University at Buffalo
- Dina Dahhan (Spring 2024 present), BMS University at Buffalo, sponsored by GWIS fellowship (*graduate mentor: Oluwatoyin Campbell*)
- Trey Lewis (Summer 2024), Neuroscience University at Buffalo, sponsored by CLIMB-UP summer program at the University at Buffalo.

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

- 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) CBE graduate 2024
- 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 colaborators). *B.S. in Chemistry, Universidad Icesi, Cali, Colombia.*
- Ivan Felsztyna (since Spring 2023 as a remote research intern manuscript under preparation). Doctoral candidate at the Instituto de Investigaciones Biologicas y Tecnologicas (IIByT), Consejo nacional de investigaciones científicas y tecnicas (CONICET), Universidad Nacional de Cordoba (UNC), Cordoba, Argentina.
- Dahlia Andres (Jan. 2021 Aug. 2021 as <u>mentee</u> 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

- 2024 NSF Engineering CAREER Proposal Workshop (virtual, May 15-17, 2024)
- UB SEAS Faculty Launch & Mentoring Program (FLMP) Fellow (2024 cohort)
- 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)
- 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 Open Lab outreach, undergraduate students visit to the Monje Group, Q&A session on research and graduate school. (April 2022, April 2024)
- 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)
- CBE Seminar Coordinator (Spring 2022 present)
- Co-organizer for the annual CBE Graduate Research Symposium (Nov. 2021 present)
- Judge for graduate poster presentations at 23rd CBE Graduate Symposium (2020 present)
- 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

• Faculty advisor for undergraduates:

Year	Spring	Fall
2021	-	4
2022	4	4
2023	4	4
2024	2	5

OTHER SERVICE

Professional Offices / Boards

- Treasurer of the <u>Theory and Computation Subgroup</u> of the Biophysical Society (2024-2026, *nominated*)
- <u>Early Careers Committee Member</u> for the Biophysical Society (appointment position from July 2023 June 2026)
- Board member of the Advisory Board to the <u>Center for Minorities in Science and</u> Engineering at the University of Maryland (2023-2026)
- Secretary of the <u>AIChE Affinity group LatinXinChE</u> (June 2022 December 2024)
- Liaison director for the Computational Molecular Science and Engineering Forum (CoMSEF) of the AIChE. (2022-2024 term, *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; and Dr. C. Bores Quijano, Union College, NY, USA. (Held virtually the second week of October 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

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 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 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

• 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). <u>Corresponding</u> 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)