

**VIVIANA MONJE-GALVAN**  
Assistant Professor  
Chemical and Biological Engineering Department

**WORK ADDRESS**

506 Furnas Hall,  
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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
- 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: 2307, h-index: 14, i10-index: 17 (as of 7/1/2023)

[Google Scholar](#) | [ORCID](#)

\* indicates graduate student mentored by VMG, + indicates undergraduate student mentored by VMG, = denotes the corresponding author.

### Invited Book Chapters

#### *Graduate work*

1. Monje-Galvan, V. <sup>=</sup>; Warburton, L<sup>+</sup>; 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
2. 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

### Refereed Journal Articles

#### *Publications at UB*

1. Campbell, O. <sup>\*</sup>; Monje-Galvan, V. = “Lipid composition modulates interactions of p7 viroporin during membrane insertion.” J. Struct. Biol. (*Under Review*)

2. Campbell, O. \*; Le, V.+; Aguirre, A.+; Monje-Galvan, V. = “Realistic membrane modeling: using complex lipid mixtures in simulation studies.” *JoVE (Under Review)*
3. Li, J. \*; Monje-Galvan, V. = “Effect of glycone diversity on the interaction of triterpenoid saponins and lipid bilayers.” *ACS Applied Bio. Mat*, [2c00928](#) (2023) **IF: 3.250. Q1 Chem. Q2 Biomaterials.**
4. 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: 5.545. Q1 Chemistry. Citations: 1**
5. 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**
6. 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**
7. 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*

8. Banerjee, P.; Monje-Galvan, V.; Voth, G.A. = “Cooperative membrane binding of HIV-1 matrix protein trimers.” (*in preparation*)
9. 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**
10. 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**
11. 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*

12. 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**
13. 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**

14. 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**
15. 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**
16. 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**
17. 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**
18. 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**
19. 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**
20. 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**
21. 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*

22. 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. (1<sup>st</sup> place in the 2012 Hydrogen Student Design Contest) **IF: 6.730. Q1. Condensed Matter Phys. Q1 Fuel Tech. Citations: 16**
23. 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 4<sup>th</sup> 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 VMG, + indicates undergraduate student mentored by VMG*

Invited seminar speaker:

1. Monje-Galvan, V. Chemical and Biological Engineering Seminar Series. Iowa State University, Ames, IA (*Spring 2024, scheduled*)
2. Monje-Galvan, V. Physics Colloquium. Union College, Schenectady, NY (*Fall 2023, scheduled*)
3. Monje-Galvan, V. “Fingerprinting protein-lipid interactions with molecular dynamics simulations.” Buffalo Protein Science Group seminar series. Dept. of Structural Biology, UB. April 19, 2023

Invited talks:

1. Monje-Galvan, V. “Lipid sorting and the signatura of protein-lipid interactions at the membrane interface.” 34<sup>th</sup> International Conference in Science and Technology of Complex Fluids. San Luis Potosi, MX, June 29, 2023
2. 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
3. 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. 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
5. 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
6. 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*

4. “Computers and Cells – Biophysics of Lipid Membranes at the Atomic Scale.” 2020 Seminar Series Grupo de Investigadores Latitud Cero. virtual, July 2020
5. “Molecular interactions in cellular processes, a perspective from simulations.” XVI LAWNP. La Paz, Bolivia, October 2019
6. “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
7. “Comportamiento de hidrotropos en la interfaz de soluciones acuosas.” Universidad Mayor de San Andrés – Facultad de Ingeniería – Ingeniería Química. La Paz, Bolivia, May 2017
8. “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. Campbell, O.\*; Monje-Galvan, V. “Molecular dynamics simulations of Hepatitis C viroporin and lipid membranes.” Biophysical Society, San Diego, CA, February 2023
2. Li, J.\*; Monje-Galvan, V. “Clustering and binding of oleanolic acid saponins with bacterial membranes.” Biophysical Society, San Diego, CA, February 2023
3. 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
4. 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
5. Campbell, O.\*; Monje-Galvan, V. “Modeling protein-lipid interactions in Hepatitis C viral infection.” NOBCCHE, Orlando, FL, September 2022
6. Varner, S.+; Monje-Galvan, V. “Molecular dynamics simulations of GM3 in the plasma membrane.” UB Undergraduate Research Day, Buffalo, NY, August 2022
7. Mendez, J.+; Monje-Galvan, V. “Structural properties of viral protein H in bacteriophage  $\phi$ X174.” UB Undergraduate Research Day, Buffalo, NY, August 2022
8. Monje-Galvan, V. “Modeling protein-lipid interactions in mechanisms of cell death.” Biological Membranes and Membrane Proteins. Santa Fe, NM, June 2022
9. Li, J.\*; Monje-Galvan, V. “Interactions of antibiotic organic molecules with lipid bilayers.” Biophysical Society, San Francisco, CA, February 2022
10. 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

11. Monje-Galvan, V. “Membrane permeabilization during necroptosis: Insights from molecular dynamics studies.” Gibbs Society of Biological Thermodynamics, 35th conference. virtual, September 2021

*Postdoctoral work*

12. 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
13. Monje-Galvan, V.; Voth, G.A. “The role of lipids on transmembrane protein interactions in viral infections.” AIChE National Meeting, virtual, November 2020
14. 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
15. Monje-Galvan, V.; Voth, G.A. “Lipid-lipid and lipid-protein interactions of the matrix domain of HIV-1 Gag at the viral assembly site.” Biophysical Society, Baltimore, MD, 2019
16. 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
17. 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
18. 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*

19. 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
20. 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
21. 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
22. Monje-Galvan, V. & Klauda, J.B. “Lo/Ld Phase Coexistence and Interaction in Model Membranes with IPC Lipids.” Biophysical Society, Los Angeles, CA, 2016
23. Monje-Galvan, V. & Klauda, J.B. “Membrane binding of the Osh4 curvature-sensing peptide.” Biophysical Society, Baltimore, MD, 2015
24. Monje-Galvan, V. & Klauda, J.B. “Binding studies of a *Saccharomyces Cerevisiae* peripheral protein Osh4” American Chemical Society, Denver, CO, 2015
25. 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

26. 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
27. 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
28. 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

### Undergraduate Students

- Shane Varner (June 2021 – December 2022, LSAMP alumni), CBE University at Buffalo
- Angela Aguirre (June 2022 – June 2023), CBE University at Buffalo
- Van Le (Nov. 2022 – present), CSE University at Buffalo
- Seth Thomson (January 2023 – present), CBE University at Buffalo

### Special Achievement of Graduate Students

- Oluwatoyin Campbell. *PhD Candidate at CBE at University at Buffalo*. **Presidential Fellow** (Sept. 2020 – present). UB scholarship given to outstanding incoming graduate 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). *R&D Associate, Regeneron, Tarrytown, NY, USA*

### *Undergraduate Students*

- Jocelyn Mendez (June 2022 – Aug. 2022 as LSAMP fellow) *CBE Undergraduate at University at Buffalo.*

### *Career Development Mentoring*

- Ivan Felsztyna (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 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**

- 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 (2023-2024 academic year)
- Louise Stokes Alliance for Minority Participation (LSAMP) mentor (2021 – present)
- Faculty Senate IT Committee Member. Committee lead: Dr. Jessica Kruger. (2022-2023 academic year)
- Committee member of the *Teaching Faculty Search for the Institute for Artificial Intelligence and Data Science*. Committee chair: Dr. Johannes Hachmann. (Dec. 2022 – June 2023)
- 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)
- UB SEAS graduate poster competition. (2022, 2023)
- Reviewer with Women in Science and Engineering (WiSE) for the Gresky Award (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 Open Lab outreach, undergraduate students visit to the Monje Group, Q&A session on research and graduate school. (April 2022)
- WiSE & Shine panelist (March 2022)
- Undergraduate mentor for incoming SEAS first-year students (Spring 2021)
- Poster judge for the CSTEP 15<sup>th</sup> 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)

- 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)
- Judge for graduate poster presentations at 23<sup>rd</sup> CBE Graduate Symposium (Nov. 2020 - virtual)
- Member of PhD Dissertation committees of:

<i>Student</i>	<i>Degree</i>	<i>Department</i>	<i>Principal Advisor</i>
Carley Cook	PhD candidate	CBE	A. Ford-Versypt
Mahasweta Bhattacharya	PhD candidate	CBE	R. Gunawan
Oluwatoyin Campbell	PhD candidate	CBE	V. Monje-Galvan
Jinhui Li	PhD candidate	CBE	V. Monje-Galvan
Ricardo X. Ramirez	PhD candidate	CBE	V. Monje-Galvan

- Faculty advisor for undergraduates:

<i>Year</i>	<i>Spring</i>	<i>Fall</i>
2021	-	4
2022	4	4
2023	4	4

## OTHER SERVICE

### Professional Offices / Boards

- Early Careers Committee Member for the Biophysical Society (appointment position from July 2023 – June 2026)
- Review Editor for Bioengineering and Biotechnology - Biochemical Engineering (2022-2024).
- Liaison director for the Computational Molecular Science and Engineering Forum ([CoMSEF](#)) of the AIChE. (2022-2024 term, elected position)
- Board member of the [AIChE Affinity group LatinXinChE](#) (June 2022 – Dec. 2023)

### 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

- Biophysics Week 2023. “*Foro de Estudiantes en Biofísica*.” Co-organizer with Dr. A. D. Reyes-Figueroa, CIMAT-Monterrey, MX. (March 20, 2023 - virtual)

- 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. (Oct. 12, 2022 - 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

#### Proposal Reviewer

- 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)
- 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 on an 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 – present)
- 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 2023; enrollment: 51 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 2023; enrollment: 2 students

Spring 2022; enrollment: 10 students

Other courses taught at UB

*CE498*, 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 1<sup>st</sup> 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)

**COMPUTATIONAL AWARDS**

- *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)