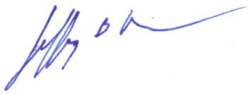
CURRICULUM VITAE
Jeffery B. Klauda

Notarization. I have read the following and certify that this curriculum vitae is a current and accurate statement of my professional record.

Signature:  Date: 6/4/2024

I. Personal Information

Jeffery B. Klauda
Department of Chemical and Biomolecular Engineering
Associate Chair and Graduate Director in ChBE (July 2015-current)
Co-Director of the Biophysics Program (IPST) (August 2020-current)
Professor (July 2021-current)
Associate Professor (July 2014-June 2021)
Assistant Professor (August 2007-June 2014)
Biophysics Program (July 2014-current)
Institute for Physical Science & Technology (January 2022 – current)

Education/Employment

University or Institute	Location	Dates	Degree/Appointment	Research Advisor
Rensselaer Polytechnic Institute	Troy, NY	1994-1998	B.S. Chemical Eng.	Prof. Michael Abbott
Rensselaer Polytechnic Institute	Troy, NY	1994-1998	B.S. Applied Mathematics	
University of Delaware	Newark, DE	1998-2003	Ph.D. Chemical Eng.	Prof. Stanley Sandler (NAE)
National Institutes of Health	Bethesda, MD	2003-2007	Post-doctoral Fellow	Dr. Bernard Brooks

II. Research, Scholarly, Creative, and/or Professional Activities

II.B. Chapters

II.B.1 Invited and Refereed Chapters in Books.

1. **Klauda, J.B.,** R.M. Venable, A.D. MacKerell, & R.W. Pastor. Consideration for Lipid Force Field Development. *Curr. Top. In Memb.*: *Computational Modeling of Membrane Bilayers.* **60**, 1-48 (2008). **(Cit.=67)**
2. Jo, S., E. L. Wu, D. Stuhlsatz, **J. B. Klauda**, A. D. MacKerell, G. Widmalm, and W. Im. Lipopolysaccharide Membrane Building and Simulation. In *Glycoinformatics: Methods in Molecular Biology*. J. M. Walker, editor. Springer Science, New York. **1273**: 391-406 (2015).

3. Khakbaz, P.[‡], V. Monje-Galvan[‡], X. Zhuang[‡] and **J.B. Klauda**[*]. Modeling Lipid Membranes. In *Biogenesis of Fatty Acids, Lipids and Membranes, Handbook of Hydrocarbon and Lipid Microbiology*. O. Geiger, editor. Springer International Publishing, **p. 1-19** (2017).
4. Jarboe, L.R., **J.B. Klauda**, Y. Chen, K.M. Davis, and M.C. Santoscoy. Engineering the Microbial Cell Membrane to Improve Bioproduction. In *Green Polymer Chemistry: New Products, Processes, and Application ACS Symposium Series*. H.N. Cheng, R.A. Gross and P.B. Smith, editors. American Chemical Society, **p 25-39** (2018).
5. Monje-Galvan, V.,[‡] L.M. Warburton,[†] and **J.B. Klauda**. Setting Up All-Atom Molecular Dynamics Simulations to Study the Interactions of Peripheral Membrane Proteins with Model Lipid Bilayers. In *Intracellular Lipid Transport. Methods in Molecular Biology.* G. Drin, editor, Humana Press: New York, NY. Vol 1949 **p 325-339** (2019).

II.C. Refereed Journals

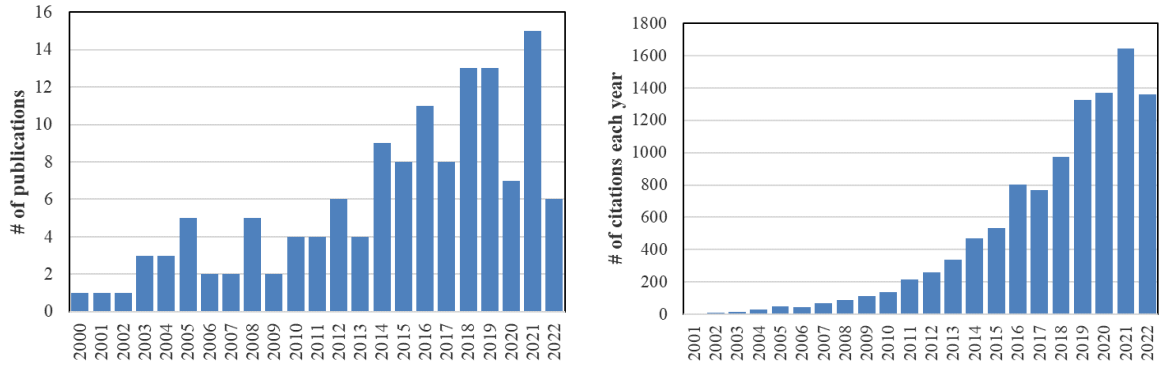
II.C.1 Referred Journal Articles

Listed chronologically below are articles which I am an author. My name is bolded for clarity and followed by an [*] when I am the corresponding author. Research based on work at the University of Maryland is delineated by a section title. Researchers in my lab are denoted as follows: [o]high school, [†]undergraduate, [‡]graduate, and [I]postdoctoral. All contain citations per article shown in **red** as of June 27, 2023 based on the Web of Science database (except overall citations were updated June 27, 2023). Also shown in the table below is a list of journals that I have published, their InCites Impact factor for 2018, and quartile list with grouping when appropriate (based on field that I publish in).

Journal	Impact Factor	Quartile	# of pubs	# invited
Chemical Reviews	54.3	Q1	1	1
Journal of the American Chemical Society	14.7	Q1	1	0
Proceedings of the National Academy of Sciences (USA)	9.58	Q1	1	0
ACS Applied Materials & Interfaces	8.456	Q1	1	0
Metabolic Engineering	7.808	Q1	1	0
Nanoscale	6.97	Q1	1	0
Journal of Chemical Theory and Computation	5.313	Q1	7	0
Journal of Molecular Biology	5.067	Q1	4	0
Analyst	4.019	Q1	1	0
Journal of Chemical Information and Modeling	3.966	Q1-Chem. Medicinal	2	0
Biochimica et Biophysica Acta-Biomembranes	3.79	Q1-Biophys	8	2
Marine and Petroleum Geology	3.538	Q1	1	0
Industrial & Engineering Chemistry Research	3.375	Q1	3	0
Chemical Engineering Science	3.372	Q1	1	0
Journal of Physical Chemistry C	4.309	Q2	2	0
Faraday Discussions	3.861	Q2	1	0
Journal of Structural Biology	3.754	Q2	1	0

Langmuir	3.683	Q2	2	0
Biophysical Journal	3.665	Q2	15	0
Journal of Computational Chemistry	3.224	Q2	3	0
Energy & Fuels	3.021	Q2-Chem. Eng.	1	0
Journal of Chemical Physics	2.997	Q2	5	1
Biochemistry	2.952	Q2	2	0
Journal of Physical Chemistry B	2.923	Q2	33	0
Journal of Physical Chemistry A	2.6417	Q2	1	0
Macromolecular Chemistry and Physics	2.622	Q2	1	0
Chemistry and Physics of Lipids	2.536	Q2-Biophys	1	1
Fluid Phase Equilibria	2.514	Q2-Chem. Eng.	1	0
Living Journal of Computational Molecular Science	New	N/A	1	1
Proteins-Structure Function and Bioinformatics	2.501	Q3	1	0
Molecular Simulation	1.782	Q3	3	0

InCites Web of Science Publication Metrics (as of June 27, 2023)



InCites Web of Science Publication Metrics (as of June 27, 2023)

	All	without self
Citations	11,557	10,733
Citing Articles	7,257	7,133
h-index	42	

Google Scholar Publication Metrics (as of June 27, 2023)

	All	Since 2018
Citations	16,355	10,805
h-index	49	41
i10-index†	105	92

†i10-index being the number of papers with 10 or more citations

Publication List (**Cite=Total Citations based on the Web of Science as of June 27, 2023**)

1. **Klauda, J. B.** & S.I. Sandler. A Fugacity Model for Gas Hydrate Phase Equilibria. *Industrial & Engineering Chemistry Research.* **39**, 3377-3386 (2000). **(Cit.=221)**
2. **Klauda, J. B.** & S.I. Sandler. Modeling Gas Hydrate Phase Equilibria in Laboratory and Natural Porous Media. *Industrial & Engineering Chemistry Research.* **40**, 4197-4208 (2001). **(Cit.=83)**
3. **Klauda, J. B.** & S.I. Sandler. Ab Initio Intermolecular Potentials for Gas Hydrates and Their Predictions. *Journal of Physical Chemistry B.* **106**, 5722-5732 (2002). **(Cit.=72)**
4. **Klauda, J. B.** & S.I. Sandler. Phase Behavior of Clathrate Hydrates: A Model for Single and Multiple Gas Component Hydrates. *Chemical Engineering Science.* **58**, 27-41 (2003). **(Cit.=141)**
5. Jiang, J., **J.B. Klauda**, & S.I. Sandler. Monte Carlo Simulation of O_2 and N_2 Adsorption in Nanoporous Carbon (C_{168} Schwarzite). *Langmuir.* **19**, 3512-3518 (2003). **(Cit.=38)**
6. **Klauda, J. B.** & S.I. Sandler. Predictions of Gas Hydrate Phase Equilibria and Amounts in Natural Sediment Porous Media. *Marine Petroleum Geology.* **20**, 459-470 (2003). **(Cit.=66)**
7. **Klauda, J.B.**, S.L. Garrison, G. Arora, J. Jiang, & S.I. Sandler. HM-IE: A Quantum Chemical Hybrid Method for Accurate Interaction Energies. *Journal of Physical Chemistry A*. **108**, 107-112 (2004). **(Cit.=45)**
8. **Klauda, J.B.,** J. Jiang, & S.I. Sandler. An Ab Initio Study on the Effect of Carbon Surface Curvature and Ring Structure on N_2(O_2)-Carbon Intermolecular Potentials. *Journal of Physical Chemistry B.* **108**, 9842-9851 (2004). **(Cit.=33)**
9. Jiang, J., **J.B. Klauda,** & S.I. Sandler. Hierarchical Modeling Gas Adsorption in the C_{168} Schwarzite: From Quantum Mechanics to Molecular Simulation. *Journal of Physical Chemistry B.* **108**, 9852-9860 (2004). **(Cit.=17)**
10. Arora, G., **J.B. Klauda**, & S.I. Sandler. A Comparative Study of Nitrogen Physisorption on Different C_{70} Crystal Structures Using an Ab Initio Based Potential. *Journal of Physical Chemistry B.* **109**, 17267-17273 (2005). **(Cit.=4)**
11. Jiang, J., **J.B. Klauda**, & S.I. Sandler. Hierarchical Modeling N_2 Adsorption on the Outer Surface of and within a C_{60} Crystal: From Quantum Mechanics to Molecular Simulation. *Journal of Physical Chemistry B.* **109**, 4731-4737 (2005). **(Cit.=16)**
12. **Klauda, J. B.** & S.I. Sandler. Global Distribution of Methane Hydrate in Ocean Sediment. *Energy & Fuels.* **19**, 469-470 (2005). **(Cit.=391)**
13. **Klauda, J.B.**, R.W. Pastor, & B.R. Brooks. Adjacent Gauche Stabilization in Linear Alkanes: Implications for Lipid/Polymer Models. *Journal of Physical Chemistry B.* **109**, 15684-15686 (2005). **(Cit.=49)**
14. **Klauda, J.B.**, B.R. Brooks, A.D. MacKerell, R.M. Venable, & R.W. Pastor. An Ab Initio Study on the Torsional Surface of Alkanes and its Effect on Molecular Simulations of Alkanes and DPPC Bilayers. *Journal of Physical Chemistry B.* **109**, 5300-5311 (2005). **(Cit.=272)**

15. **Klauda, J.B.**, N. Kučerka, B.R. Brooks, R.W. Pastor, & J.F. Nagle. Simulation-based Methods for Interpreting X-ray Data from Lipid Bilayers. *Biophysical J.* **90**, 2796-2807 (2006). **(Cit.=187)**
16. **Klauda, J.B.**, B.R. Brooks, & R.W. Pastor. Dynamical Motions of Lipids and a Finite Size Effect in Simulations of Bilayers. *Journal of Chemical Physics.* **125**, 144710 (2006). **(Cit.=111)**
17. **Klauda, J.B.**, X. Wu, R.W. Pastor, & B.R. Brooks. Long-range Lennard-Jones and Electrostatic Interactions in Interfaces: Application of the Isotropic Periodic Sum Method. *Journal of Physical Chemistry B.* **111**, 4393-43400 (2007). **(Cit.=73)**
18. **Klauda, J.B.*** & B.R. Brooks. Sugar Binding in Lactose Permease: Anomeric State of a Disaccharide Influences Binding Structure. *Journal of Molecular Biology.* **367**, 1523-1534 (2007). **(Cit.=28)**
19. **Klauda, J.B.**, N.V. Eldho, K. Gawrisch, B.R. Brooks, & R.W. Pastor. Collective and Noncollective Models of NMR Relaxation in Lipid Vesicles and Multilayers. *Journal of Physical Chemistry B.* **112**, 5924-5929 (2008). **(Cit.=29)**
20. **Klauda, J.B.*** & B.R. Brooks. CHARMM Force Field Parameters for Nitroalkanes and Nitroarenes. *Journal of Chemical Theory and Computation.* **4**, 107-115 (2008). **(Cit.=11)**
21. **Klauda, J.B.,** M.F. Roberts, A.G. Redfield, B.R. Brooks, & R.W. Pastor. Rotation of Lipids in Membranes: MD Simulation, ^{31}P Spin-Lattice Relaxation, and Rigid-Body Dynamics. *Biophysical J.* **94**, 3074-3083 (2008). **(Cit.=82)**
22. Miller, T., R.P. Singh, **J.B. Klauda**, M. Hodošček, B.R. Brooks, & H.L. Woodcock III. CHARMMing: A New, Flexible, Web-based front-end to CHARMM. *Journal of Chemical Information and Modeling.* **48**, 1920-1929 (2008). **(Cit.=104)**

Articles Published or Submitted Based on Work at UMD

23. Singh, R.P., B.R. Brooks, & **J.B. Klauda***. Binding and Release of Cholesterol in the Osh4 Protein of Yeast. *Proteins: Structure, Function, and Bioinformatics*. **75**, 468-477 (2009). **(Cit.=28)**
24. Jo, S.H., J.B. Lim†, **J.B. Klauda**, & W. Im. CHARMM-GUI Membrane Builder for Mixed Bilayers and Its Application to Yeast Membranes. *Biophysical Journal.* **97**, 50-58 (2009). **(Cit.=996)**
25. **Klauda, J.B.**, R.M. Venable, J.A. Freites, J.W. O'Connor†, D.J. Tobias, C. Mondragon-Ramirez, I. Vorobyov, A.D. MacKerell, Jr., & R.W. Pastor. Update of the CHARMM all-atom additive force field for lipids: Validation on six lipid types. *Journal of Physical Chemistry B*. **114**, 7830-7843 (2010). **(Cit.=2816)**
26. Jo, S.H., H. Rui, J.B. Lim†, **J.B. Klauda**, & W. Im. Cholesterol Flip-Flop: Insights from Free Energy Simulation Studies. *Journal of Physical Chemistry B.* **114**, 13342-13348 (2010). **(Cit.=100)**

27. Pendse, P.Y. ‡, B.R. Brooks & **J.B. Klauda***. Probing the Periplasmic-open State of Lactose Permease in Response to Sugar Binding and Proton Translocation. *Journal of Molecular Biology.* **404**, 506-521 (2010). **(Cit.=26)**

28. Rogaski, B. ‡, J.B. Lim†, & **J.B. Klauda***. Sterol Binding and Membrane Lipid Attachment to the Osh4 Protein of Yeast, Osh4. *Journal of Physical Chemistry B.* **114**, 13562-13573 (2010). **(Cit.=4)**

29. Bandyopadhyay, A.A. † & **J.B. Klauda***. Gas Hydrate Structure and Pressure Predictions based on an Updated Fugacity-based Model with the PSRK Equation of State. *Industrial & Engineering Chemistry Research*. **50**, 148-147 (2011). **(Cit.=36)**

30. Lim, J.B. † & **J.B. Klauda***. Lipid chain branching at the Iso- and Anteiso-Positions in Complex Chlamydia Membranes: A Molecular Dynamics Study. *Biochimica et Biophysica Acta-Biomembranes*. **1808**, 323-331 (2011). **(Cit.=40)**

31. Song, K.C., P.W. Livanec, **J.B. Klauda**, K. Kuczera, R.C. Dunn, & W. Im. Orientation of Fluorescent Lipid Analog BODIPY-PC to Probe Lipid Membrane Properties: Insights from Molecular Dynamics Simulations. *Journal of Physical Chemistry B*. **115**, 6157-5165 (2011). **(Cit.=24)**

32. O'Connor, J.W† & **J.B. Klauda***. Lipid Membranes with a Majority of Cholesterol: Applications to the Ocular Lens and Aquaporin 0. *Journal of Physical Chemistry B.* **115,** 6455-5464 (2011). **(Cit.=37)**

33. Lim, J.B. †, B. Rogaski‡ & **J.B. Klauda***. Update of the Cholesterol Force Field Parameters in CHARMM. *Journal of Physical Chemistry B.* **116,** 203-210 (2012). **(Cit.=156)**

34. Pandit, K.R. ‡ & **J.B. Klauda***. Membrane models of E. coli containing cyclic moieties in the aliphatic lipid chain. *Biochimica et Biophysica Acta-Biomembranes.* **1818**, 1205-1210. (2012). **(Cit.=72)**

35. Kwon, T.K., B. Roux, SW Jo, **J.B. Klauda**, A.L. Harris, & T.A. Bargiello. Molecular Dynamics Simulations of the Cx26 Hemichannel: Insights into voltage-dependent loop-gating. *Biophysical J.* **102**, 1341-1351 (2012). **(Cit.=31)**

36. Ezzeldin, H.M., **J.B. Klauda**, & S.D. Solares. Modeling of the Major Gas Vesicle Protein, GvpA: from Protein Sequence to Vesicle Wall Structure. *Journal of Structural Biology.* **179**, 18-28 (2012). **(Cit.=14)**

37. **Klauda, J.B.***, V. Monje,† T. Kim, and W. Im. Improving the CHARMM Force Field for Polyunsaturated Fatty Acid Chains. *Journal of Physical Chemistry B.* **116**, 9424-9431 (2012). **(Cit.=116)**

38. Rogaski, B‡ & **J.B. Klauda***. Membrane-binding Mechanism of a Peripheral Membrane Protein through Microsecond Molecular Dynamics Simulations. *Journal of Molecular Biology.* **423**, 847-861 (2012). **(Cit.=30)**

39. Cheng, X., S.H. Jo, **J.B. Klauda**, and W. Im. CHARMM-GUI Micelle Builder for Pure/Mixed Micelle and Protein/Micelle Complex Systems. *Journal of Chemical Information and Modeling*. **53**, 2171-2180 (2013). **(Cit.=70)**

40. Wu, E.L., O. Engström, S. Jo, D, Stuhlsatz, MS Yeom, **J.B. Klauda**, G. Widmalm, and W. Im. Molecular Dynamics and NMR Spectroscopy Studies of E. coli Lipopolysaccharide Structure and Dynamics. *Biophysical J.* **105**, 1444-1455 (2013). **(Cit.=132)**

41. Villanueva, D.Y.,[†] J.B. Lim[†], & **J.B. Klauda**[*]. Influence of Ester-modified Lipids on Bilayer Structure. *Langmuir.* **29**, 14196-14203 (2013). **(Cit.=13)**

42. Subramanian, D., C.T. Boughter[†], **J.B. Klauda**, B. Hammouda, and M.A. Anisimov. Mesoscale inhomogeneities in aqueous solutions of small amphiphilic molecules. *Faraday Discuss.* **167**: 217-238 (2013). **(Cit.=55)**

Articles Published Based on Post-tenure Work at UMD

43. Lee, S.,[†] A. Tran,[†] M. Allsopp,[†] J.B. Lim,[†] J. Hénin, & **J.B. Klauda**[*]. CHARMM36 United-Atom Chain Model for Lipids and Surfactants. *Journal of Physical Chemistry B.* **118**: 547-556 (2014). **(Cit.=102)**

44. Jeong, J.C., S. Jo, E.L. Wu, Y. Qi, V. Monje,[‡] M.S. Yeom, L. Gorenstein, F. Chen, **J.B. Klauda**, & W. Im. ST-analyzer: A Web-based User Interface for Simulation Trajectory Analysis. *Journal of Computational Chemistry*. **35**: 957-963 (2014). **(Cit.=11)**

45. Wu, E.L., P.J. Fleming, M.S. Yeom, G. Widmalm, **J.B. Klauda**, K.G. Fleming & W. Im. E. coli Outer Membrane and Interactions with OmpLA. *Biophysical J.* **106**: 2493–2502 (2014). **(Cit.=101)**

46. Wu, E.L., Y. Qi, K.C. Song, **J.B. Klauda**, & W. Im. Preferred Orientations of Phosphoinositides in Bilayers and Their Implications in Protein Recognition Mechanisms. *Journal of Physical Chemistry B.* **118**: 4315-4325 (2014). **(Cit.=28)**

47. Subramanian, D. **J.B. Klauda**, and M.A. Anisimov. Mesoscale Phenomena in Ternary Solutions of Tertiary Butyl Alcohol, Water, and Propylene Oxide. *Journal of Physical Chemistry B.* **118**: 5994-6006 (2014). **(Cit.=32)**

48. Zhuang, X.,[‡] J.R. Makover,[†] W. Im, & **J.B. Klauda**. A Systematic Molecular Dynamics Simulation Study of Temperature Dependent Bilayer Structural Properties. *Biochimica et Biophysica Acta-Biomembranes.* **1838**: 2520-2529 (2014). **(Cit.=71)**

49. Venable, R.M., A.J. Sodt, B. Rogaski, H. Rui, E. Hatcher, A.D. MacKerell, Jr., R.W. Pastor, and **J.B. Klauda**[*]. CHARMM All-Atom Additive Force Field for Sphingomyelin: Elucidation of Hydrogen Bonding and of Positive Curvature. *Biophysical J.* **107**: 134-145 (2014). **(Cit.=158)**

50. Wu, E., X. Cheng, S. Jo, H. Rui, K.C. Song, E.M. Dávila-Contreras, Y. Qi, J. Lee, V. Monje-Galvan,[‡] R.M. Venable, **J.B. Klauda**, and W. Im. CHARMM-GUI Membrane Builder Toward Realistic Biological Membrane Simulations. *Journal of Computational Chemistry.* **35**: 1997-2004 (2014). **(Cit.=1223)**

51. Kern, N.R, H.S. Lee, E.L. Wu, K. Vanommeslaeghe, A.D MacKerell, Jr., **J.B. Klauda**, S. Jo, and W. Im. Lipid-Linked Oligosaccharides in Membranes Sample Conformations

that Facilitate Binding to Oligosaccharyltransferase. *Biophysical J.* **107**: 1885-1895 (2014). **(Cit.=19)**

52. Kang, H[†] & **J.B. Klauda**[*]. Molecular Dynamics Simulations of Palmitoyloleoyl-phosphatidylglycerol Bilayers. *Molecular Simulation*. **41**: 948-954 (2015). **(Cit.=7)**
53. Park, S., A.H. Beaven, **J.B. Klauda** and W. Im. How Tolerant are Membrane Simulations with Mismatch in Area per Lipid between Leaflets? *Journal of Chemical Theory and Computation.* **11**: 3466-3477 (2015). **(Cit.=48)**
54. Khakbaz, P.[‡] and **J.B. Klauda**[*]. Probing the Importance of Lipid Diversity in Cell Membranes via Molecular Simulation. *Chemical Physics of Lipids.* **192**: 12-22 (2015). **Invited (Cit.=45)**
55. Konas, R.M.,[†] J.L. Daristotle,[†] N.B. Harbor,[†] and **J.B. Klauda**[*]. Biophysical Changes of Lipid Membranes in the Presence of Ethanol at Varying Concentrations. *Journal of Physical Chemistry B.* **119**: 13134-13141 (2015). **(Cit.=13)**
56. Qi, Y., X. Cheng, J. Lee, J. Vermaas, T.V. Pogorelov, E. Tajkhorshid, S. Park, **J.B. Klauda**, and Wonpil Im. CHARMM-GUI HMMM Builder for Membrane Simulations with the Highly Mobile Membrane-Mimetic Model. *Biophysical Journal.* **109**: 2012-2022 (2015). **(Cit.=63)**
57. Monje-Galvan, V.[‡] and **J.B. Klauda**[*]. Modeling Yeast Organelle Membranes and How Lipid Diversity Influences Bilayer Properties. *Biochemistry.* **54**: 6852-6861 (2015). **(Cit.=44)**
58. Wu, E., Y. Qi, S. Park, S.S. Mallajosyula, A.D. MacKerell, Jr., **J.B. Klauda**, and W. Im. Insight into Early-Stage Unfolding of GPI-Anchored Human Prion Protein. *Biophysical J.* **109**: 2090-2100 (2015). **(Cit.=17)**
59. MacDermaid, C.M., H.K. Kashyap, R.H. DeVane, W. Shinoda, **J.B. Klauda**, M.L. Klein, and G. Fiorin. Molecular Dynamics Simulations of Cholesterol-rich Membranes using a Coarse-grained Force Field for Cyclic Alkanes. *Journal of Chemical Physics.* **143**, 243144 (2015). **(Cit.=42)**
60. Lee, J., X. Cheng, J. Swails, M.S. Yeom, P. Eastman, J. Lemkul, S. Wei, J. Buckner, J.C. Jeong, Y. Qi, S. Jo, V.S. Pande, D.A. Case, C.L. Brooks III, A.D. MacKerell Jr, **J.B. Klauda**, and W. Im CHARMM-GUI Input Generator for NAMD, GROMACS, AMBER, OpenMM, and CHARMM/OpenMM Simulations using the CHARMM36 Additive Force Field. *Journal of Chemical Theory and Computation.* **12**, 405-413 (2016). **(Cit.=1166)**
61. Choudhary, R.[‡] and **J.B. Klauda**[*]. The Simultaneous Mass and Energy Evaporation (SM2E) Model. *Journal of Occupational & Environmental Hygiene*. **13**, 247-257 (2016). **(Cit.=1)**
62. Monje-Galvan, V.[‡] and **J.B. Klauda**[*]. Peripheral Membrane Proteins: Tying the Knot between Experiment and Computation. *Biochimica et Biophysica Acta-Biomembranes.* **1858**, 1584-1593 (2016) **Invited**. **(Cit.=33)**

63. Zhuang, X., ‡ and **J.B. Klauda***. Modeling Structural Transitions from the Periplasmic-open State of Lactose Permease and Interpretations of Spin Label Experiments. *Biochimica et Biophysica Acta-Biomembranes.* **1858**, 1541-1552 (2016). **(Cit.=5)**

64. Kim, S., D. Patel, S. Park, J. Slusky, **J.B. Klauda**, G. Widmalm, and W. Im. Bilayer Properties of Lipid A from Various Gram-negative Bacteria. *Biophysical Journal.* **111**, 1750-1760 (2016). **(Cit.=72)**

65. Barton, R. P. Khakbaz,‡ I. Bera,| **J.B. Klauda**, M.K. Iovine, and B.W. Berger. Interplay of specific trans- and juxtamembrane interfaces in Plexin A3 dimerization and signal transduction. *Biochemistry*. **55**, 4928-4938 (2016). **(Cit.=1)**

66. Adhikari, A., S. Re, W. Nishima, M. Ahmed, S. Nihonyanagi, **J.B. Klauda**, Y. Sugita, and T. Tahra. Water Orientation at Ceramide / Water Interfaces Studied by Heterodyne-Detected Vibrational Sum Frequency Generation Spectroscopy and Molecular Dynamics Simulation. *Journal of Physical Chemistry C*. **120**, 23692-23697 (2016). **(Cit.=12)**

67. Zhuang, X,‡ E.M. Dávila-Contreras, A.H. Beaven, W. Im, and **J.B. Klauda***, An Extensive Simulation Study of Lipid Bilayer Properties with Different Head Groups, Acyl Chain Lengths, and Chain Saturations. *Biochimica et Biophysica Acta-Biomembranes*. **1858**, 3093-3104 (2016). **(Cit.=38)**

68. Qi, Y., **J.B. Klauda** and W. Im. Effects of Spin-labels on Membrane Burial Depth of MARCKS-ED Residues. *Biophysical Journal.* **111**, 1600-1603 (2016).

69. Patel, D.S., S. Park, E.L. Wu, M.S. Yeom, G. Widmalm, **J.B. Klauda*** and W. Im. Influence of Ganglioside GM1 Concentration on Lipid Clustering and Membrane Properties and Curvature. *Biophysical Journal.* **111**, 1987-1999 (2016). **(Cit.=34)**

70. Boughter, C.T.,† V. Monje-Galvan‡, W. Im and **J.B. Klauda***. Influence of Cholesterol on Phospholipid Bilayer Structure and Dynamics. *Journal of Physical Chemistry B.* **120**, 11761-11772 (2016). **(Cit.=43)**

71. Jo, S., X. Cheng, J. Lee, S. Kim, S.-J. Park, D.S. Patel, A.H. Beaven, K.I. Lee, H. Rui, B. Roux, A.D. MacKerell, Jr., **J.B. Klauda**, Y.. Qi, and W. Im. CHARMM-GUI 10 Years for Biomolecular Modeling and Simulation. *Journal of Chemical Theory and Computation.* **38**, 1114-1124 (2017). **(Cit.=134)**

72. Bera, I.| and **J.B. Klauda***. Molecular Simulations of Mixed Lipid Bilayers with Sphingomyelin, Glycerophospholipids and Cholesterol. *Journal of Physical Chemistry B.* **121**, 5197-5208 (2017). **(Cit.=42)**

73. Wang, E.† and **J.B. Klauda***. Examination of Mixtures Containing Sphingomyelin and Cholesterol by Molecular Dynamics Simulations. *Journal of Physical Chemistry B.* **121**, 4833-4844 (2017). **(Cit.=37)**

74. Zhuang, X,‡ A. Ou,º and **J.B. Klauda***. Simulations of simple Linoleic acid-containing Lipid Membranes and Models for the Soybean Plasma Membranes. *Journal of Chemical Physics.* **146**, 215103 (2017). **(Cit.=18)**

75. Monje-Galvan, V. ‡ and **J.B. Klauda***. Two sterols, two bilayers: insights on membrane structure from molecular dynamics. *Molecular Simulation.* **43**, 1179-1188 (2017). **(Cit.=7)**

76. Novikov, A.A., A.P. Semenov, V. Monje-Galvan,[‡] V.N. Kuryakov, **J.B. Klauda**, and M.A. Anisimov. Dual Action of Hydrotropes at the Water/Oil Interface. *Journal of Physical Chemistry C.* **121**, 16423-16431 (2017). **(Cit.=19)**

77. Tan, Z., P. Khakbaz,[‡] Y. Chen, J. Lombardo, J.M. Yoon, J.V. Shanks, **J.B. Klauda**, and L.R. Jarboe. Engineering *Escherichia coli* Membrane Phospholipid Head Distribution Improves Tolerance and Production of Biorenewables. *Metabolic Engineering*. **44**, 1-12 (2017). **(Cit.=70)**

78. Wang, E.[†] and **J.B. Klauda***. Molecular Dynamics Simulations of Ceramide and Ceramide-Phosphatidylcholine Bilayer Mixtures. *Journal of Physical Chemistry B.* **121**, 10091-10104 (2017). **(Cit.=26)**

79. Leonard, A.N.,[‡] A.C. Simmonett, F.C. Pickard, IV, J. Huang, R.M. Venable, **J.B. Klauda**, B.R. Brooks, and R.W. Pastor. Comparison of Additive and Polarizable Models with Explicit Treatment of Long-Range Lennard-Jones Interactions Using Alkane Simulations. *Journal of Chemical Theory Computation.* **14**, 948-958 (2018). **(Cit.=39)**

80. Wang, E.[†] and **J.B. Klauda***. Simulations of Pure Ceramide and Ternary Lipid Mixtures as Simple Interior *Stratum Corneum* Models. *Journal of Physical Chemistry B.* **122**, 2757-2768 (2018). **(Cit.=28)**

81. Gavrilenko, L[†] and **J.B. Klauda***. Aggregation of Modified Hexabenzocoronenes as Models for early-stage Asphaltene Self-Assembly. *Molecular Simulation*. **44**, 992-1003 (2018). **(Cit.=2)**

82. Khakbaz, P. [‡] and **J.B. Klauda***. Investigation of Phase Transitions of Saturated Phosphocholine Lipid Bilayers via Molecular Dynamics Simulations. *Biochimica et Biophysica Acta-Biomembranes*. **1860**, 1489-1501 (2018). **(Cit.=44)**

83. Leonard, A.N.,[‡] R.W. Pastor, and **J.B. Klauda***. Parameterization of the CHARMM All-Atom Force Field for Ether Lipids and Model Linear Ethers. *Journal of Physical Chemistry B.* **122**, 6744-6754 (2018). **(Cit.=19)**

84. Adams, M.[†] E. Wang[†], X. Zhuang[‡] and **J.B. Klauda***. Simulations of Simple Bovine and Homo sapiens Outer Cortex Ocular Lens Membrane Models with a Majority Concentration of Cholesterol. *Biochimica et Biophysica Acta-Biomembranes*. **1860**: 2134-2144 (2018). **Invited (Cit.=14)**

85. Bera, I.[‖] and **J.B. Klauda***. Structural events in a bacterial uniporter leading to translocation of glucose to the cytosol. *Journal of Molecular Biology*. **430**, 3337-3352 (2018). **(Cit.=6)**

86. Guros, N.B.,[‡] A. Balijepalli, and **J.B. Klauda***. The Role of Lipid Interactions in Accurate Simulations of the *alpha-hemolysin* Transporter. *Biophysical Journal.* **115**, 1720-1730 (2018). **(Cit.=8)**

87. Monje-Galvan, V.[‡] and **J.B. Klauda***. Preferred binding mechanism of Osh4's ALPS motif, insights from molecular dynamics. *Journal of Physical Chemistry B*. **122**, 9713-9723 (2018). **(Cit.=13)**

88. Yu, Y.[‡] and **J.B. Klauda**[*]. Modeling Pseudomonas Aeruginosa Inner Plasma Membrane in Planktonic and Biofilm Modes. *Journal of Chemical Physics*. **149**, 215102 (2018). **(Cit.=6)**

89. **J.B. Klauda**[*]. Perspective: Computational Modelling of Accurate Cellular Membranes with Molecular Resolution. *Journal of Chemical Physics*. **149**, 220901 (2018). **Invited-Perspectives Article (Cit.=15)**

90. Wang, E.[†] and **J.B. Klauda**[*]. Models for the Stratum Corneum Lipid Matrix: Effects of Ceramide Concentration, Ceramide Hydroxylation, and Free Fatty Acid Protonation. *Journal of Physical Chemistry B*. **122**, 11996-12008 (2018). **(Cit.=17)**

91. Smith, D.J., **J.B. Klauda**[*], A.J. Sodt. Simulation Best Practices for Lipid Membranes: v1.0. *Living Journal of Computational Molecular Science*. **1**, 5966 (2019). **Invited**

92. Qi, Y., J. Lee, **J.B. Klauda**, and W. Im. CHARMM-GUI Nanodisc Builder for Modeling and Simulation of Various Nanodisc Systems. *Journal of Computational Chemistry.* **40**, 893-899 (2019). **(Cit.=36)**

93. Lee, J., D.S. Patel, J. Ståhle, S.-J. Park, N.R. Kern, S. Kim, J. Lee, X. Cheng, M.A. Valvano, O. Holst, Y.A. Knirel, Y. Qi, S. Jo, **J.B. Klauda**, G. Widmalmn and W. Im. CHARMM-GUI Membrane Builder for Complex Biological Membrane Simulations with Glycolipids and Lipoglycans. *Journal of Chemical Theory and Computation*. **15**, 775-786 (2018). **(Cit.=218)**

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95. Wildermuth, K.D.,[†] V. Monje-Galvan[‡], L.M. Warburton,[†] and **J.B. Klauda**[*]. Effect of membrane lipid packing on stable binding of the ALPS peptide. *Journal of Chemical Theory and Computation*. **15**, 1418-1429 (2019). **(Cit.=15)**

96. A.N. Leonard,[‡] **J.B. Klauda**,[*] and S. Sukharev. Isothermal Titration Calorimetry of Be^{2+} with Phosphatidylserine Models Guides All-Atom Force Field Development for Lipid-Ion Interactions. *Journal of Physical Chemistry B.* **123**, 1554-1565 (2019). **(Cit.=1)**

97. Wang, E.[†] and **J.B. Klauda**[*]. Structure and Permeability of Ceramide Bilayers and Multilayers. *Journal of Physical Chemistry B*. **123**, 2525-2535 (2019). **(Cit.=17)**

98. Hughes, A.V., D.S. Patel, G. Widmalm, **J.B. Klauda**, L.A. Clifton, and W. Im. Physical Properties of Gram-negative Bacterial Outer Membranes: Neutron Reflectometry and Molecular Simulation. *Biophysical Journal* **116**, 1095-1104 (2019). **(Cit.=23)**

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101. Wong, S,[†] J. Condon,[†] E.L. Eckersley, B.W. Berger[*], and **J.B. Klauda**[*]. Probing the pH effects on Sugar Binding to a Polysaccharide Lyase. *Journal of Physical Chemistry B*. **123**, 7123-7136 (2019). **(Cit.=6)**

102. Lee, S.T., N.B. Guros,[‡] R.C. Bruce, A. Cardone, N.D. Amin, S. Zhang, **J.B. Klauda**, H.C. Pant, C.A. Richter, A. Balijepalli. Quantum Capacitance-limited MoS_2 Biosensors Enable Label-Free Enzyme Measurements. *Nanoscale.* **11**: 15622-15632 (2019). **(Cit.=10)**

103. Wang, E.[†] and **J.B. Klauda**[*]. Molecular Structure of the Long Periodicity Phase in the Stratum Corneum. *Journal of the American Chemical Society*. **141**: 16930-16943 (2019). **(Cit.=24)**

104. Guros, N.B, [‡] A. Balijepalli, and **J.B. Klauda**[*]. Microsecond Timescale Simulations Demonstrate 5-HT mediated Pre-activation of the 5-HT_{3A} Serotonin Receptor. *Proceedings of the National Academy of Sciences. U.S.A*. **117**: 405-414 (2020). **(Cit.=17)**

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108. Yu, Y. [‡] and **J.B. Klauda**[*]. Update of the CHARMM36 United Atom Chain Model for Hydrocarbons and Phospholipids. *Journal of Physical Chemistry B*. **124**: 6797-6812 (2020). **(Cit.=8)**

109. Krämer, A, A. Ghysels, E. Wang,[†] R.M. Venable, **J.B. Klauda**, B.R. Brooks, and R.W. Pastor. Membrane Permeability of Small Molecules from Unbiased Molecular Dynamics Simulations. *Journal of Chemical Physics.* **153**: 124107 (2020). **(Cit.=23)**

110. Ghorbani, M.,[‡] E. Wang,[†] A. Krämer, and **J.B. Klauda**[*]. Molecular Dynamics Simulations of Ethanol Permeation through Single and Double-Lipid Bilayers. *Journal of Chemical Physics.* **153**: 125101 (2020). **(Cit.=10)**

111. Ghorbani, M.,[‡] B.R. Brooks, and **J.B. Klauda**[*]. Critical Sequence Hot-spots for Binding of nCOV-2019 to ACE2 as Evaluated by Molecular Simulations. *Journal of Physical Chemistry B*. **124**: 10034–10047 (2020). **(Cit.=34)**

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Lipid Force Field to Include Explicit Treatment of Long-Range Dispersion. *Journal of Chemical Theory and Computation*. **17**: 1562-1580 (2021). **(Cit.=23)**

114. Yu, Y.[‡], A. Krämer, R.M. Venable, B.R. Brooks, **J.B. Klauda**[*], and R.W. Pastor[*]. CHARMM36 Lipid Force Field with Explicit Treatment of Long-Range Dispersion: Parametrization and Validation for Phosphatidylethanolamine, Phosphatidylglycerol, and Ether Lipids. *Journal of Chemical Theory and Computation*. **17**: 1581-1595 (2021). **(Cit.=25)**

115. Feng, S., R. Wang,[‡] R.W. Pastor, **J.B. Klauda***, and W. Im. Location and Conformational Ensemble of Menaquinone and Menaquinol, and Protein–Lipid Modulations in Archaeal Membranes. *Journal of Physical Chemistry B*. **125**: 4714-4725 (2021). **(Cit.=5)**

116. Gao, Y., J. Lee, I.P.S. Smith, H. Lee, S. Kim, Y. Qi, **J.B. Klauda**, G. Widmalm, S. Khalid, and W. Im. CHARMM-GUI Supports Hydrogen Mass Repartitioning and Different Protonation States of Phosphates in LPS. *Journal of Chemical Information and Modeling*. **61**: 831-839 (2021).

117. Allsopp, R.J.[‡] and **J.B. Klauda**[*]. Impact of PIP2 Lipids and Force Field Parameters on the Binding of Osh4's α_6-α_7 Domain. *Journal of Physical Chemistry B*. **125**: 5293-5308 (2021).

118. Ghorbani, M.,[‡] B.R. Brooks, and **J.B. Klauda**[*]. A replica exchange umbrella sampling (REUS) approach to predict host-guest binding free energies in SAMPL8 challenge. *Journal of Computer-Aided Molecular Design*. **35**: 667-677 (2021). **(Cit.=2)**

119. Ghorbani, M.,[‡] B.R. Brooks, and **J.B. Klauda**[*]. Exploring dynamics and network analysis of spike glycoprotein of SARS-COV-2. *Biophysical Journal*. **120**: 2902–2913 (2021). **(Cit.=14)**

120. **Klauda, J.B.** Virtual Issue on Docking. *Journal of Physical Chemistry B*. **125**: 5455-5457 (2021). **Invited Editorial**

121. **Klauda, J.B**. Considerations of Recent All-Atom Lipid Force Field Development. *Journal of Physical Chemistry B.* **125**: 5676-5682 (2021). **Invited Perspectives (Cit.=4)**

122. Yuan, Y.,[†] Y. Yu, [‡] and **J.B. Klauda**[*]. Simulations of Diabetic and Non-Diabetic Peripheral Nerve Myelin Lipid Bilayers. *Journal of Physical Chemistry B*. **125**: 6201-6213 (2021). **(Cit.=2)**

123. Yu, Y. [‡] and **J.B. Klauda**[*]. Symmetric and Asymmetric Models for the Arabidopsis thaliana Plasma Membrane: A Simulation Study. *Journal of Physical Chemistry B*. **125**: 11418-11431 (2021). **(Cit.=2)**

124. Ghorbani, M.,[‡] S. Prasad, **J.B. Klauda**, and B.R. Brooks. Variational embedding of protein folding simulations using Gaussian mixture variational autoencoders. *Journal of Chemical Physics.* **155:** 194108 (2021). **(Cit.=4)**

125. Hsieh, M.-K.,[‖] Y. Yu,[‡] and **J.B. Klauda**[*]. All-atom Modeling of Complex Cellular Membranes. *Langmuir*. **38**: 317 (2022). **Invited (Cit.=4)**

126. Hsieh, M.-K.,[‖] and **J.B. Klauda**[*]. Leaflet Asymmetry Modeling in Lipid Composition of Escherichia coli Cytoplasmic Membrane. *Journal of Physical Chemistry B.* **126**: 184-196 (2022). **(Cit.=1)**

127. Karmakar, S.[‖] and **J.B. Klauda**[*]. Modeling the Membrane Binding Mechanism of a Lipid Transport Protein Osh4 to Single Membranes. *Biophysical Journal*. **121**: 1560-1575 (2022).

128. Ghorbani, M.,[‡] S. Prasad, **J.B. Klauda**, and B.R. Brooks. GraphVAMPNet, using graph neural networks and variational approach to Markov processes for dynamical modeling of biomolecules. *Journal of Chemical Physics.* **156**: 184103 (2022). **(Cit.=6)**

129. Tammareddy, T. [‡] W. Keyrouz, R.D. Sriram, H.C. Pant, A. Cardone, **J.B. Klauda***. Computational Study of the Allosteric Effects of p5 on the CDK5-p25 Hyperactivity as Alternate Inhibitory Mechanisms in Neurodegeneration. *Journal of Physical Chemistry B*. **126**: 5033-5044 (2022).

130. Banerjee, A. D. Li, Y. Guo, Z. Mei, C. Lau, K. Chen, J. Westwick, **J.B. Klauda**, A.G. Schrum, E. Lazear, A. Krupnick. A Re-Engineered Common Chain Cytokine Augments $CD8^+$ T Cell-Dependent. *Journal of Clinical Investigation Insight*. **7**: e158889 (2022).

131. Fernandes, J.[†] Y. Yu,[‡] **J.B. Klauda***. Molecular Dynamics Simulations of the Human Ocular Lens with Age and Cataract. *Biochimica et Biophysica Acta-Biomembranes*. **1864**: 184025 (2022).

132. Allsopp, R.J, [‡] A. Pavlova, T. Cline,[‡] A.M. Salyapongse, R.E Gillilan, Y.P. Di, B. Deslouches, **J.B. Klauda**, J. C. Gumbart, and S.A, Tristram-Nagle. Antimicrobial peptide mechanisms revealed with scattering-guided molecular dynamics simulation. *Journal of Physical Chemistry B*. **126**: 6922-6935 (2022). **(Cit.=1)**

133. Mann, M.M, M.-K. Hsieh,[‖] J.D. Tang, W.S. Hart, M.J. Lazzara, **J.B. Klauda***, and B.W. Berger*. Understanding how transmembrane domains regulate interactions between human BST-2 and the SARS-CoV-2 accessory protein ORF7a. *Biochimica et Biophysica Acta-Biomembranes*. **1865**: 184174 (2023).

134. Yu, Y., [‡] R.M. Venable, J. Thirman, P. Chatterjee, A. Kumar, R.W. Pastor, B. Roux, A.D. MacKerell, Jr., and **J.B. Klauda**[*]. Drude Polarizable Lipid Force Field with Explicit Treatment of Long-Range Dispersion: Parametrization and Validation for Saturated and Monounsaturated Zwitterionic Lipids. *Journal of Chemical Theory and Computation*. **19**: 2590-2605 (2023).

135. Ghorbani, M.,[‡], B.R. Brooks, and **J.B. Klauda**. Conformational Fluctuations in β2-Microglubulin using Markov State Modeling and Molecular dynamics. *Journal of Physical Chemistry B.* **127**: 6887-6895 (2023).

136. Niu, Y.[†] and **J.B. Klauda***. Simulations of naïve and KLA-activated macrophage plasma membrane models. *Biochimica et Biophysica Acta-Biomembranes*. **1866**: 184242 (2024).

137. Wang, Z.-J., M. Ghorbani,[‡] X. Chen, C. Thomas, P.B. Tiwari, **J.B. Klauda**,[*] and T.I. Brelidze.[*] Molecular Mechanism of EAG1 Channel Inhibition by Imipramine Binding to the PAS domain. *Journal of Biological Chemistry*. **299**: 105391 (2023).

138. Hsieh, M.-K.[!] and **J.B. Klauda**. Multi-scale Molecular Dynamics Simulations of the Homodimer Accessory Protein ORF7b of SARS-CoV-2. *Journal of Physical Chemistry* B. **128**: 150-162 (2024) **Invited**.

139. Kio, M.[!] and J.B. Klauda. Advances in Emerging Hydrogel Fouling-release Coatings for Marine Applications. *Journal of Coatings Technology Research*. **21**: 827-856 (2024).

140. Lucker, J.,[‡] M. Kio,[!] and **J.B. Klauda***. Expanding the CHARMM36 United Atom Chain Model for the Inclusion of Sphingolipids. *Journal of Physical Chemistry B.* **128**: 4428-4439 (2024). **Invited**

141. Allsopp, R.J.[‡] and **J.B. Klauda***. Understanding Folding of bFGF and Potential Cellular Protective Mechanisms of Neural Cells. *Biohemistry*. **Submitted** (2024).

142. Wang, H., M.-K. Hsieh,[!] K. Noroozi, Y, Chen, M.C. Santoscoy, **J.B. Klauda**, L.R. Jarboe. Escherichia coli species variation of membrane composition and properties with evolution towards a unified membrane fluidity. *Journal of Industrial Microbiology and Biotechnology*. **Submitted** (2023).

143. Karmakar, S.[!] and **J.B. Klauda***. Proposed Dual Membrane Contact with Full-Length Osh4. *Biochimica et Biophysica Acta-Biomembranes*. **Submitted** (2024).

144. Tammareddy, T. [‡] W. Keyrouz, R.D. Sriram, H.C. Pant, A. Cardone, and **J.B. Klauda***. Investigation of the effect of peptide p5 targeting CDK5-p25 hyperactivity on Munc18-1 (P67) regulating neuronal exocytosis using molecular simulations. *Biochemistry*. **Submitted** (2024).

145. Bodosa, J.[‡] and **J.B. Klauda***. Metadynamics study of lipid mediated antibacterial toxin binding to the EmrE multi-efflux protein. *Journal of Physical Chemistry B.* **Submitted**. (2024). **Invited**

II.E. Conferences, Workshops and Talks.

II.E.2 Invited Talks

Listed below are invited talks with a title to delineate talks given after starting at UMD.

1. "Phase Behavior of Gas Hydrates and Global Predictions for Methane Hydrate Seafloor Reserves" *The University of Melbourne*–Department of Chemical & Biomolecular Engineering (2003).
2. "Structure of Lipid Membranes and Improving the Head Group Force Field" *eChemInfo*, Philadelphia (2005).
3. "Structure, Dynamics, and Small Molecule Transport through Cell Membranes: How can Simulations Aid Experiments?" *University of Kentucky*, Lexington (2007).
4. "Structure, Dynamics, and Small Molecule Transport through Cell Membranes: How can Simulations Aid Experiments?" *University of Pennsylvania*, Philadelphia (2007).
5. "Structure, Dynamics, and Small Molecule Transport through Cell Membranes: How can Simulations Aid Experiments?" *University of South Carolina*, Columbia (2007).
6. "Structure, Dynamics, and Small Molecule Transport through Cell Membranes: How can Simulations Aid Experiments?" *University of Maryland*, College Park (2007).

7. "Pure Lipid Membranes and Active Transport of Sugars through the Cytoplasmic Membrane via Lactose Permease" *Biological Membranes: Emerging Challenges at the Interface between Theory, Computer Simulation, and Experiment*, Park City, UT (2007).

Invited talks when at UMD

Talks to National and International Universities

8. "Structure and Dynamics of Lipids, Model Cellular Membranes, and Membrane Proteins", *University of Kansas*, Center for Bioinformatics, Lawrence (2008).
9. "Understanding the Structure and Dynamics of Biomembranes and Their Components", *National Taiwan University*, Department of Chemical Engineering, Taipei (2009).
10. "Model Biomembranes of Single-Celled Organisms and a Protein that Controls Substrate Transport in *E. coli*", *Advanced Materials Research*, Central Michigan University, Mt. Pleasant, MI (2010).
11. "Multi-scale Modeling of Gas Hydrates Reserves in the Seafloor Sediment", *Petroleum Institute*, Department of Chemical Engineering, Abu Dhabi, UAE (2011).
12. "Molecular Modeling of Cellular Membranes and Associated Proteins", *University of Maryland*, Special Joint ChBE/Chemistry & Biochemistry Seminar (2011).
13. "Modeling Bacterial Membrane Structure to Membrane Protein Dynamics at an Atomic Level", *University of Virginia*, Department of Chemical Engineering (2011).
14. "Modeling Plasma Membranes and Proteins that Transport Small Molecules and Membrane Components", *Georgia Institute of Technology*, Department of Chemical and Biomolecular Engineering (2013).
15. "Modeling Plasma Membranes and Proteins that Transport Small Molecules and Membrane Components", *Temple University*, Institute for Computational Molecular Science (2013).
16. "*E. coli* Plasma Membrane Modeling and Membrane-associated Transport Proteins", *University of Maryland*, Department of Bioengineering (2013).
17. "Force Field Development and Molecular Simulations of Model Lipid Membranes" Satellite Meeting of ICMS2013. *Nagoya University,* Japan (2013).
18. "Molecular Simulations of Pore-forming Membranes and Membrane-associated Proteins" *Rensselaer Polytechnic Institute*, Department of Chemical and Biological Engineering (2014).
19. "Simulations of Cell Membranes: Developing Accurate Lipid Force Fields and Probing Conformational Changes in Membrane Transporters" *University of Maryland*, Biophysics Program (2014).
20. "Probing Small Molecule Self-assembly, Lipid Membranes and Membrane-associated Proteins" *Lehigh University*, Department of Chemical and Biomolecular Engineering (2014).

21. "Molecular Simulations of Hydrotropes, Lipid Membranes and a Peripheral Membrane Protein" *West Virginia University*, Morgantown, WV (2015).
22. "The Influence of Alcohols on the Oil/Water Interface and Cell Membrane." *National Taiwan University,* Department of Chemical Engineering (2016).
23. "Molecular Modeling of a Curvature-Sensing Peptide and Structural Changes in a Secondary Active Transporter." *National Chiao Tung University*, Institute of Bioinformatics and Systems Biology (2016).
24. "Improving the Tolerance of Organisms to Biofuels and Intracellular Transport of Lipids." *North Carolina State University*, Department of Chemical Engineering, Raleigh, NC (2017).
25. "New Developments in the CHARMM Lipid Force Field and Applications to Membrane-associated Proteins" *University of Illinois at Urbana-Champaign*, Theoretical & Computational Biophysics Group, Urbana, IL (2018).
26. "Permeation of Membranes: Research on Improving the Tolerance of Organisms to Biofuels and Modeling the Skin Barrier." *Howard University*, Department of Chemical Engineering, Washington, DC (2018).
27. "Probing the Mechanism of a Peripheral Membrane Protein and Modeling the Skin Barrier." *University of Fribourg,* Department of Biology, Switzerland (2018).
28. "Modeling the Stratum Corneum and its Permeation and a Protein involved in Intracellular Lipid Transport" *University of New England*, Department of Pharmaceutical Sciences, Portland, ME (2019).
29. "Modeling Lipid Membranes: Developing an Improved Interaction Potential to Probing Accessory Proteins of SARS-CoV-2" *Johns Hopkins University*, Department of Material Science, Baltimore, MD (2021).
30. "Modeling Gas Hydrate Growth in the Seafloor and Molecular Simulations to Understand SARS-CoV-2." Kuwait University, Department of Chemical Engineering. Virtual (2021).
31. "Molecular Simulations to Probe Intracellular Lipid Transport and an Accessory Protein of SARS-CoV-2" Carnegie Mellon University/U. Pittsburgh, Molecular Biophysics + Structural Biology Program, Pittsburgh, PA (2022).
32. "Force Field Development for Lipids in Membranes and Applications to Intracellular Lipid Transport" IISC-Bangalore, Molecular Biophysics, Integrative Modelling in Biophysics Seminar. Virtual (2022).
33. "Probing Intracellular Lipid Transport and the Function of an Accessory Protein of SARS-CoV-2" University of Buffalo, Department of Chemical and Biomolecular Engineering, Buffalo, NY (2022).
34. "Modelling Natural Cell Membranes and their Lipid Asymmetry" Big10 Lipid Symposium 2023, University of Iowa, Iowa City, IA (2023).

Talks to National and International Laboratories

35. "Improving the Lipid Force Field from ab Initio Methods and the Sugar Transporter of E. coli" *mini-Carbohydate Symposium*. National Institutes of Health, Bethesda (2008).
36. "Predicting the Locations and Amounts of Seafloor Methane Hydrates", *Central Geological Survey of Taiwan*, Taipei (2009).
37. "Molecular simulations of certain model human membranes and secondary active transport proteins" *National Institutes of Health,* NHLBI, Laboratory of Computational Biology (2011).
38. "All-atom Molecular Simulations to Probe Structure and Dynamics of Bacterial Membranes and Membrane-associated Proteins", *NIST Center for Neutron Research* (2012).
39. "Interpreting Experimental Studies of Self-Assembly and Transmembrane Proteins with Molecular Simulation", *National Institute of Standards and Technology*, Gaithersburg, MD, Software and Systems Division (2014).

Talks to National and International Conferences

40. "Gas Hydrates: A Significant but Relatively Untapped Alternate Source of Natural Gas", *National Capitol Section of AIChE*, College Park, MD (2009).
41. "Diversity of Lipids in Organisms and their Organelles: Is this Required to Accurately Model Real Membranes?", *Biological Membranes and Membrane Proteins*, Snowmass, CO (2011).
42. "Simulation Studies on Biological Membranes with High Performance Computing" Enabling Discovery with HPC, Baltimore, MD (2012).
43. "Modeling Lipid Bilayer and Microsecond Simulations of a Peripheral Membrane Protein", *Biological Membranes and Membrane Proteins*, Snowmass, CO (2013).
44. "Simulations of Biomembranes: Importance of Lipid Diversity and Structural Changes of Membrane Transport Proteins" *3rd International Conference on Molecular Simulation (ICMS)*. Kobe, Japan (2013).
45. "Probing the Transport Cycle of Secondary Active Transporters with Atomistic Simulations" *Computational Modeling Workshop and Mini-Symposium*. University of Chicago (2014).
46. "Molecular Modeling of Biomolecules: How can GPUs Advance Research?" *GPU Summit*, University of Maryland, Institute for Advanced Computing (2014).
47. "Binding of a Curvature-sensing Peptide to Model Organelle Membranes of Yeast", *Biological Membranes and Membrane Proteins*, Telluride, CO (2015)
48. "Developing Quantum Mechanically-based Force Field Parameters from Gas Hydrates to Biology", *AIChE Annual Meeting,* Prof. Sandler Symposium (2015).
49. "Modeling Yeast Organelle Membranes and a Curvature Sensing Peptide." *4th International Conference on Molecular Simulation (ICMS)*. Shanghai, China (2016).

50. "Modeling Yeast Asymmetric Membranes and Dimerization of a Plexin Protein in the Membrane", *Biological Membranes and Membrane Proteins*, Santa Fe, NM (2017).
51. "Probing the Mechanism of a Peripheral Membrane Protein and Influence of the Lipid Environment on the Function of α-hemolysin" *Delaware Membrane Protein Symposium,* Newark, DE (2018).
52. "Studies of a Peripheral Membrane Protein in Yeast (Osh4) and its Peptide that Senses Lipid Packing" *ACS Spring National Meeting*, Orlando, FL (2019).
53. "Modeling the Stratum Corneum Lipid Matrix and Plasmalogen Lipids for Neuronal Membranes", *Biological Membranes and Membrane Proteins*, Santa Fe, NM (2019).
54. "Studies of a Peripheral Membrane Protein in Yeast that Exchanges Lipids at Membrane Contact Sites", 19th KIAS Conference on Protein Structure and Function, KIAS, Seoul, Korea (2019).
55. "Improving the CHARMM Force Field Parameters for Lipid-ion and Plasmalogen Lipids" *ACS Spring National Meeting*, Philadelphia, PA (2020).
56. "Oligomerization of COVID19 Accessory Proteins: Structure, Specificity and Signal Transduction" *ACS Fall National Meeting*. Virtual (2020).
57. "Reoptimization of the CHARMM Lipid Force Field for Inclusion of Long-Range Dispersion" *ACS Spring National Meeting*. Virtual (2021).
58. "Accessory Proteins of SARS-CoV-2: A Study of the Dimerization of ORF7a and ORF7b" *ACS Spring National Meeting*. Virtual (2021).
59. "Updating the CHARMM Lipid Force Field and Modeling Membrane Leaflet Composition Asymmetry" *Middle Atlantic Regional Meeting (MARM) of ACS*. June (2021).
60. "Receptor binding and glycan dynamics in spike protein of SARS-COV-2 as unraveled by MD simulations" *ACS Fall National Meeting.* Virtual (2021).
61. "Nearing the Final Stage in the Ongoing Saga of Pairwise Additive and Polarizable Lipid Force Field Development in CHARMM" *Biological Membranes and Membrane Proteins*, Santa Fe, NM (2022).
62. "Modelling Natural Cell Membranes and How Lipid Asymmetry Influences Structure" *Biophysical Society National Meeting*, San Diego, CA (2023).

II.E.3 Refereed Presentations

This section is divided into two sections with mentored presentations given by students a postdocs and presentations given by Dr. Klauda.

Mentored Conference Talks

1. Lim, J.B.† & **J.B. Klauda**. "The Application of Molecular Dynamics Simulations to Sterols and Lipid Bilayers" *UMD Bioscience Day* (2008).

2. Lim, J.B.[†], S. Jo, W. Im, & **J.B. Klauda** "Molecular Dynamics Simulations of Complex Mixed Lipid Bilayers to Model Yeast Membranes" *Chemistry and Biology Interface Symposium*, Baltimore (2009).
3. Pendse, P.Y.[‡] & **J.B. Klauda** "Structural Changes and Sugar Binding in Lactose Permease of *E. coli*" *Chemistry and Biology Interface Symposium*, Baltimore (2009).
4. Lim, J.B.[†] & **J.B. Klauda** "Molecular Dynamics Simulations of Complex Mixed Lipid Bilayers to Model Yeast Membranes" *ACS National Fall Meeting* (2009).
5. Pendse, P.Y.[‡] & **J.B. Klauda** "Structural Changes and Quantification of Ligand Affinity in Lactose Permease of Escherichia coli." *ACS National Fall Meeting* (2009).
6. Lim, J.B.[†] & **J.B. Klauda** "Molecular Dynamics Simulations of Complex Mixed Lipid Bilayers to Model Yeast Membranes" *AIChE Annual Meeting* (2009).
7. Pendse, P.Y.[‡] & **J.B. Klauda** "Structural Changes and Quantification of Ligand Binding Affinity in Membrane Transport Proteins." *AIChE Annual Meeting* (2009).
8. Pendse, P.Y.[‡], B.R. Brooks, & **J.B. Klauda**. "An Atomic-level Model for the Periplasmic Open State of Lactose Permease." *Biophysical Society* (2010).
9. Rogaski, B.[‡] & **J.B. Klauda**. "Binding of a Natural Sterol to the Osh4 Protein of Yeast and Membrane Attachment." *Biophysical Society* (2010).
10. Pendse, P.Y.[‡], B.R. Brooks, & **J.B. Klauda**. "An Atomic-level Model for the Periplasmic Open State of Lactose Permease." *Chemistry and Biology Interface Symposium*, Baltimore (2010).
11. Rogaski, B.[‡] & **J.B. Klauda**. "Binding of A Natural Sterol to the Osh4 Protein of Yeast and Membrane Attachment." *Chemistry and Biology Interface Symposium*, Baltimore (2010).
12. Noon, M.S.[†] & **J.B. Klauda**. "Structure Prediction of the Major Outer Membrane Protein of Chlamydia." *Chemistry and Biology Interface Symposium*, Baltimore (2010).
13. Lim, J.B.[†] & **J.B. Klauda**. "Branching at the Iso- and Anteiso- Positions in Complex Chlamydia Membranes: A Molecular Dynamics Study." *Chemistry and Biology Interface Symposium*, Baltimore (2010).
14. Pendse, P.Y.[‡] & **J.B. Klauda**. "Binding Free Energy Calculations to Understand the Mechanism of Sugar Binding to Lactose Permease of E. Coli." *AIChE Annual Meeting* (2010).
15. Rogaski, B.[‡] & **J.B. Klauda**. "PIP Binding and Membrane Attachment of a Protein Involved in Intracellular Transport of Sterols." *AIChE Annual Meeting* (2010).
16. Noon, M.S.[†] J.B. Lim[†], A.D.. MacKerell Jr., **J.B. Klauda**. "Structure Prediction and Simulations of the Major Outer Membrane Protein of Chlamydia." *Biophysical Society* (2011).
17. Rogaski, B.[‡] & **J.B. Klauda**. "Phosphoplipid Binding and Membrane Attachment of the Osh4 Protein." *Biophysical Society* (2011).

18. Pandit, K‡ & **J.B. Klauda**. "*In Silico* Model *Escherichia Coli* Membranes: Simulating a Lipid with a Cyclopropane Ring." *Biophysical Society* (2011).
19. Pendse, P.Y‡ & **J.B. Klauda**. "Mechanistic and Thermodyanmic Insights into the Transport Cycle of Lactose Permease." *Biophysical Society* (2011).
20. Villanueva, D.Y.† & **J.B. Klauda**. "Lipid Bilayers of Ester-modified Lipids." *Biophsyical Society* (2011).
21. Rogaski, B.‡ & **J.B. Klauda**. "Phosphoplipid Binding and Membrane Attachment of the Osh4 Protein." *ACS Spring National Meeting* (2011).
22. Pendse, P.Y‡ & **J.B. Klauda**. "Quantification of binding affinity in lactose permease of E. coli to understand the anomeric binding phenomenon." *ACS Spring National Meeting* (2011).
23. Pandit, K‡ & **J.B. Klauda**. "*In Silico* Model *Escherichia Coli* Membranes: Simulating a Lipid with a Cyclopropane Ring." *AIChE Annual Meeting* (2011).
24. Pendse, P.Y.‡ & **J.B. Klauda.** "Study of Ligand Binding Thermodynamics and Proton Translocation in Lactose Permease of Escherichia Coli." *ACS Spring National Meeting* (2012).
25. Pendse, P.Y.‡ & **J.B. Klauda**. "Investigation of the Proton Translocation Mechanism in Lactose Permease of E. Coli by a Hybrid QM/MM Approach." *AIChE Annual Meeting* (2012).
26. Monje, V.,‡ T. Kim, W. Im, & **J.B. Klauda**. "Improved CHARMM Force Field for Polyunsaturated Fatty Acid Chains, A Study on DAPC Membranes" *Biophysical Society* (2013).
27. Monje, V.,‡ & **J.B. Klauda**. "Simulation studies on organelle-specific yeast membrane models and amphipathic lipid packing sensor (ALPS) motif binding mechanism" *AIChE Annual Meeting* (2013).
28. Monje, V.‡ & **J.B. Klauda**. "Molecular Dynamics of Yeast Membranes & Preliminary studies of ALPS-motif binding mechanism" *Biophysical Society* (2014).
29. Khakbaz, P.‡ & **J.B. Klauda**. "Studying Conformational Changes of Mhp1 using Unbiased All-atom Molecular Simulations" *Biophysical Society* (2014).
30. Zhuang, X.‡ J.R. Makover† & **J.B. Klauda**. "Temperature Dependence of Bilayer Structural Properties Studied with Molecular Dynamics Simulations" *Biophysical Society* (2014).
31. Monje, V.‡ & **J.B. Klauda.** "Molecular dynamics of yeast membrane models and binding of the ALPS-like motif" *Computational/Theory Washington/Baltimore Symposium at NIH* (2014).
32. Khakbaz, P.‡ & **J.B. Klauda**. "Studying Conformational Changes of Mhp1 Using All-atom Simulations." *Computational/Theory Washington/Baltimore Symposium at NIH* (2014).

33. Zhuang, X.[‡] J.R. Makover[†] & **J.B. Klauda**. "Investigating the accuracy of C36 for lipid at various temperatures." *Computational/Theory Washington/Baltimore Symposium at NIH* (2014).

34. Khakbaz, P.[‡] & **J.B. Klauda**. "Studying Conformational Changes of Mhp1 using Unbiased All-atom Molecular Simulations." *AIChE Annual Meeting* (2014).

35. Zhuang, X.[‡] & **J.B. Klauda**. "Molecular Dynamics Simulations on the Periplasmic-Open State Lactose Permease." *AIChE Annual Meeting* (2014).

36. Monje-Galvan, V.[‡] & **J.B. Klauda.** "Membrane Binding of the Osh4 Curvature-Sensing Peptide" *Quitel Conference in Ecuador* (2014).

37. Konas, R.M.,[†] J.L. Daristotle,[†] N.B. Harbor[†] & **J.B. Klauda.** "How does Ethanol Affect the Stability of Simple Model Yeast Membranes?" *Biophysical Society* (2015).

38. Kang, H.[†] & **J.B. Klauda.** "Molecular Dynamics Simulations of Sphingomyelin-Cholesterol Bilayers." *Biophysical Society* (2015).

39. Boughter, C.T,[†] V. Monje-Galvan,[‡] & **J.B. Klauda.** "Influence of Cholesterol on Phospholipid Bilayer Dynamics." *Biophysical Society* (2015).

40. Zhuang, X.[‡] & **J.B. Klauda**. "Molecular Dynamics Simulations on the Periplasmic-Open State Lactose Permease." *Biophysical Society* (2015).

41. Khakbaz, P.[‡] & **J.B. Klauda**. "Investigating Lipid Phase Changes from Liquid Crystalline to Ripple to Gel Phases with All-atom Molecular Dynamics Simulations." *Biophysical Society* (2015).

42. Monje-Galvan, V.[‡] & **J.B. Klauda.** "Membrane Binding of the Osh4 Curvature-Sensing Peptide" *Biophysical Society* (2015).

43. Monje-Galvan, V.[‡] & **J.B. Klauda.** "Binding Studies of a *Saccharomyces Cerevisiae* Peripheral Protein Osh4" *ACS Spring National Meeting* (2015).

44. Zhuang, X.[‡] & **J.B. Klauda**. "Molecular Dynamics Simulations on the Periplasmic-Open State Lactose Permease." *ACS Spring National Meeting* (2015).

45. Khakbaz, P.[‡] & **J.B. Klauda**. "Investigating Lipid Phase Changes from Liquid Crystalline to Ripple to Gel Phases with All-atom Molecular Dynamics Simulations." *ACS Spring National Meeting* (2015).

46. Zhuang, X.[‡] & **J.B. Klauda**. "Molecular Dynamics Simulations on the Periplasmic-Open State Lactose Permease." *Delaware Membrane Protein Symposium* (2015).

47. Monje-Galvan, V.[‡] & **J.B. Klauda.** "Membrane Binding of the Osh4 Curvature-Sensing Peptide" *Delaware Membrane Protein Symposium* (2015).

48. Khakbaz, P.[‡] & **J.B. Klauda**. "Probing the Ripple Phase of Bilayers using Molecular Dynamics Simulations." *Biophysical Society* (2016).

49. Zhuang, X.[‡] & **J.B. Klauda**. "Probing Conformational Changes of Secondary Active Transporters." *Biophysical Society* (2016).

50. Guros, N.,[‡] A. Balijepalli, & **J.B. Klauda**. "Characterizing Nanopore-Polymer and Cyc-loop Protein Receptor Gating." *Biophysical Society* (2016).

51. Monje-Galvan, V.‡ & **J.B. Klauda.** "Lo/Ld Phase Coexistence and Interaction in Model Membranes with IPC Lipids." *Biophysical Society* (2016).
52. Monje-Galvan, V.‡ & **J.B. Klauda.** "Lo/Ld Phase Coexistence and Interaction in Model Membranes with IPC Lipids." *Delaware Membrane Protein Symposium* (2016).
53. Guros, N.,‡ A. Balijepalli, & **J.B. Klauda**. "Characterizing Nanopore-Polymer and Cyc-loop Protein Receptor Gating." *Delaware Membrane Protein Symposium* (2016).
54. Zhuang, X.‡ & **J.B. Klauda**. "Probing Conformational Changes of Secondary Active Transporters." *Delaware Membrane Protein Symposium* (2016).
55. Khakbaz, P.‡ & **J.B. Klauda**. "Probing the Ripple Phase of Bilayers using Molecular Dynamics Simulations." *Delaware Membrane Protein Symposium* (2016).
56. Zhuang, X.‡ & **J.B. Klauda**. "Simulation study on the interpretations of spin label experiments and conformational changes of lactose permease." *4th International Conference on Molecular Simulation (ICMS)*. Shanghai, China (2016).
57. Guros, N.‡, A. Balijepalli, & **J.B. Klauda**. "Analyzing the Effects of Lipid Type on the α-Hemolysin Nanopore and 5HT3 Receptor Structure and Gating using Molecular Dynamics Simulations." *4th International Conference on Molecular Simulation (ICMS)*. Shanghai, China (2016). **Poster Award Winner**
58. Monje-Galvan, V.‡ & **J.B. Klauda.** "Asymmetric membrane models for the PM and TGN of yeast, an all-atom molecular dynamics study." *Biophysical Society* (2017).
59. Guros, N.‡, A. Balijepalli, & **J.B. Klauda**. "Analyzing the Effects of Lipid Type on the α-Hemolysin Nanopore and 5HT3 Receptor Structure and Gating using Molecular Dynamics Simulations." *Biophysical Society* (2017).
60. Khakbaz, P.‡ & **J.B. Klauda**. "Simulations Provide Insight into Improving the Tolerance of the E. coli membrane." *Biophysical Society* (2017).
61. Leonard, A.‡ & **J.B. Klauda**. "Modeling Ethers with Molecular Dynamics." *Biophysical Society* (2017).
62. Monje-Galvan, V.‡ & **J.B. Klauda.** "Asymmetric membrane models for the PM and TGN of yeast, an all-atom molecular dynamics study." *Delaware Membrane Protein Symposium* (2017).
63. Guros, N.‡, A. Balijepalli, & **J.B. Klauda**. "Analyzing the Effects of Lipid Type on the α-Hemolysin Nanopore and 5HT3 Receptor Structure and Gating using Molecular Dynamics Simulations." *Delaware Membrane Protein Symposium* (2017).
64. Leonard, A.‡ & **J.B. Klauda**. "Modeling Ethers with Molecular Dynamics." *Delaware Membrane Protein Symposium* (2017).
65. Bera, I.‖ & **J.B. Klauda**. "Studying conformational changes facilitating sugar transport in a semi-SWEET transporter." *Delaware Membrane Protein Symposium* (2017).

66. Wang, E.[†] & **J.B. Klauda**. "Examination of lipid bilayer mixtures containing sphingomyelin and cholesterol by molecular dynamics simulation." *American Chemical Society-Fall Meeting* (2017).
67. Bera, I.[ǁ] & **J.B. Klauda**. "All-atom simulation studies on lipid bilayers, composed of sphingomyelin, glycerophospholipids and cholesterol." *American Chemical Society-Fall Meeting* (2017).
68. Monje-Galvan, V.[‡] & **J.B. Klauda.** "Asymmetric models for the trans-Golgi Network and plasma membranes of S. cerevisiae, insights from molecular dynamics." *American Chemical Society-Fall Meeting* (2017).
69. Novikov, A.A., A.P. Semenov, V. Monje-Galvan,[‡] V.N. Kuryakov, **J.B. Klauda**, and M.A. Anisimov. "Interfacial behavior of hydrotropes in aqueous solutions" *American Chemical Society-Fall Meeting* (2017).
70. Leonard, A. [‡] & **J.B. Klauda**. "Isothermal Titration Calorimetry of Be2+ and Ca2+ with phosphatidylserine models guides all-atom force field development for lipid-ion interactions." *Biophysical Society* (2018).
71. Bera, I.[ǁ] & **J.B. Klauda**. "Structural events in a bacterial uniporter leading to translocation of glucose inside the cytosol." *Biophysical Society* (2018).
72. Guros, N.[‡], A. Balijepalli, & **J.B. Klauda**. "Analyzing the effects of membrane lipid type on transmembrane proteins (αHL and 5-HT3) using molecular dynamics simulations." *Biophysical Society* (2018).
73. Wang, E.[†] & **J.B. Klauda**. "Molecular dynamics simulations of stratum corneum model membranes." *Biophysical Society* (2018).
74. Leonard, A. [‡] & **J.B. Klauda**. "Isothermal Titration Calorimetry of Be2+ and Ca2+ with phosphatidylserine models guides all-atom force field development for lipid-ion interactions." *Delaware Membrane Protein Symposium* (2018).
75. Bera, I.[ǁ] & **J.B. Klauda**. "Structural events in a bacterial uniporter leading to translocation of glucose inside the cytosol." *Delaware Membrane Protein Symposium* (2018).
76. Guros, N.[‡], A. Balijepalli, & **J.B. Klauda**. "Analyzing the effects of membrane lipid type on transmembrane proteins (αHL and 5-HT3) using molecular dynamics simulations." *Delaware Membrane Protein Symposium* (2018).
77. Wang, E.[†] & **J.B. Klauda**. "Atomistic Models of the Lipid Matrix in the Stratum Corneum." *American Chemical Society-Fall Meeting* (2018).
78. Leonard, A. [‡] R.W. Pastor & **J.B. Klauda**. "Parameterization of the CHARMM Force Field for Ether Lipids and Model Linear Ethers." *Biophysical Society* (2019).
79. Ghorbani, M.,[‡] E. Wang[†] & **J.B. Klauda**. "Calculating Ethanol Permeability of Membranes through Molecular Dynamics Simulations." *Biophysical Society* (2019).
80. Guros, N., [‡] A. Balijepalli, & **J.B. Klauda**. "Microsecond-scale Molecular Dynamics Simulations Reveal Desensitized Behavior of 5HT3." *Biophysical Society* (2019).

81. Yu, Y. ‡ and **J.B. Klauda**. "Modeling *Pseudomonas aeruginosa* Inner Plasma Membrane in Planktonic and Biofilm Modes." *Biophysical Society* (2019).
82. Adhikari, S.,‡ M. Ghorbani,‡ K. Dura, **J.B. Klauda** & A.J. Karlsson. "Translocation of CPP-cargo Protein Fusions into *Candida Albicans* Cells and Designing for Enhanced Translocation with Simulations." *Biophysical Society* (2019).
83. Wang, E.† & **J.B. Klauda**. "Molecular Structure of the Long Periodicity Phase in the Stratum Corneum." *Biophysical Society* (2019).
84. Tammareddy, T., ‡ A. Cardone, S. Hassan, H. Pant, M. Brady, R. Sriram, & **J.B. Klauda.** Investigation of Allosteric Inhibition Mechanisms by the Peptide p6 on the Alzheimer's Disease (AD) Pathological Complex Cdk5-p26 through Molecular Dynamics Simulations. *Biophysical Society* (2020).
85. Ghorbani, M.,‡ **J.B. Klauda** & B.R. Brooks. "Mechanism of Degradation of Histatin-5 Peptide by Secreted Aspartic Proteases (SAPS) of *C. albicans*." *Biophysical Society* (2020).
86. Yu, Y. ‡, A. Krämer, **J.B. Klauda** & R.W. Pastor. "Modifying the CHARMM36 Lipid Force field for LJ-PME Simulations." *Biophysical Society* (2020).
87. Karmakar, S.‖ and **J.B. Klauda**. "Molecular Dynamics Study of Membrane Binding Mechanism of a Peripheral Membrane Protein Osh4." *Biophysical Society* (2021).
88. Hsieh, M.-K.‖ and **J.B. Klauda**. "Investigating SARS-CoV-2 ORF7b Homodimerization by Molecular Dynamics Simulations." *Biophysical Society* (2021).
89. Ghorbani, M., ‡ B.R. Brooks, and **J.B. Klauda**. "An Integrative MD Simulation and Network Analysis Approach to study glycosylation of spike in SARS-COV-2." *Biophysical Society* (2021).
90. Allsopp, R., ‡ and **J.B. Klauda**. "Peripheral Membrane Binding Characteristics of Osh α_6–α_7 Helices and the Effect of the Presence of PIP_2 Lipids and Force Field Parameters." *Biophysical Society* (2021).
91. Yu, Y. ‡, A. Krämer, A. MacKerell, J.R., B. Roux, **J.B. Klauda** & R.W. Pastor. "Recent Updates to the CHARMM Lipid Force Fields." *Biophysical Society* (2021).
92. Kheradmand-Hajibashi, M, S. Adhikari, M. Ghorbani,‡ **J. B. Klauda**, & A. J. Karlsson. Orientation of Cargo attachment affects Translocation of Cell-Penetrating Peptides. *Biophysical Society* (2022).
93. R. Allsopp,‡ D. Konakbayeva, A.J. Karlsson, **J.B. Klauda**. Computational Study of Membrane Binding and Free Energy of Amphipathic Helix (ALPS) on Osh4 to Varied Bilayers. *Biophysical Society* (2022).
94. D. Konakbayeva, R. Allsopp,‡ Ella Mihailescu, **J.B. Klauda**, A.J. Karlsson. Experimental Investigation of the Mechanism of Lipid-Binding of the ALPS-like Motif of Osh4 Protein. *Biophysical Society* (2022).
95. M. Ghorbani, ‡ S. Prasad, B.R. Brooks, **J.B. Klauda**. Unraveling the Allosteric Activation of GPCR Metadynamics and Deep Learning. *Biophysical Society* (2022).

96. Y. Yu, ‡ J. Thirman, A.D. MacKerell, B. Roux, **J.B. Klauda**, R.W. Pastor. New Parameterization of the Drude Polarizable Lipid Force Field. *Biophysical Society* (2022).
97. T. Tammareddy,‡ A. Cardone, S.A. Hassan, H.C. Pant, M. Brady, W. Keyrouz, R. Sriram, **J.B. Klauda**. In silico Study on the Selective Inhibition of Alzheimer's Disease (AD) Pathological Complex CDK5-P25 by Peptide P5 in Presence of MUNC 18 (P67). *Biophysical Society* (2022).
98. R. Allsopp‡ and **J.B. Klauda**. Conotoxin GVIIIA: Binding to 5HT3A with Microsecond Simulations and Docking of Diverse Structures. *Biophysical Society* (2023).
99. T. Tammareddy,‡ A. Cardone, S.A. Hassan, H.C. Pant, M. Brady, W. Keyrouz, R. Sriram, **J.B. Klauda**. Investigation of the potential off-target effects on Munc 18 (p67) involved in synaptic vesical transport due to the interaction with peptide p5. *Biophysical Society* (2023).
100. Karmakar, S.‖ and **J.B. Klauda**. Mechanism for Membrane Contact Formation with Full-Length Osh4 in Dual-Membrane Environment. *Biophysical Society* (2023).
101. Min, J.‡ M. Britt, S. Sukharev, B.R. Brooks, and **J.B. Klauda**. CHARMM36m Force Field for Arginine-Phosphate Interactions. *Biophysical Society* (2023).
102. Lucker, J. ‡ and **J.B. Klauda**. A United-atom Representation for Sphingolipids in the CHARMM Force Field. *Biophysical Society* (2023).
103. Bodosa, J. ‡ and **J.B. Klauda**. Metadynamics Study of Benzyltrimethylammonium Binding Free Energy to EmrE Protein in All-atom Molecular Dynamics Simulations. *Biophysical Society* (2023).

Conference Talks as Speaker

1. **Klauda, J.B.** & S.I. Sandler. "Predictions of Gas Hydrate Phase Equilibria in Laboratory and Natural Sediment Porous Media" *AIChE Annual Meeting* (2001).
2. **Klauda, J.B.** & S.I. Sandler. "Intermolecular Potentials for Gas-Hydrates Obtained from *Ab Initio* Quantum Mechanics" *ACS National Fall Meeting* (2002).
3. **Klauda, J.B.** & S.I. Sandler. "Phase Behavior of Clathrate Hydrates: A Model for Single and Multiple Gas Component Hydrates" *AIChE Annual Meeting* (2002).
4. **Klauda, J.B.** & S.I. Sandler. "*Ab Initio* Intermolecular Potentials of Absorbents in Nanoporous Carbon Schwartzite Structures" *AIChE Annual Meeting* (2002).
5. **Klauda, J.B.** & S.I. Sandler. "A Quantum Chemical Hybrid Method (HM-IE) for Calculating Interaction Energies Used to Develop Accurate Intermolecular Potentials" *AIChE Annual Meeting* (2003).
6. **Klauda, J.B.** & B.R. Brooks. "A Self-guided Langevin Dynamic Study of β-Hairpin Folding with Explicit Solvent: Computational Efficiency and Folding Pathways" *AIChE Annual Meeting* (2004).

7. **Klauda, J.B.**, R.W. Pastor, & B.R. Brooks. "An Ab Initio Study on the Torsional Surface of Alkanes and its Effect on Molecular Simulations of Alkanes and DPPC Bilayers" *AIChE Annual Meeting* (2004).
8. **Klauda, J.B.**, R.W. Pastor, & B.R. Brooks. "Lipid Bilayers: Structural and Dynamical Properties with an Improved Forcefield Fit to Ab Initio Quantum Mechanics" *Biophysical Society* (2005).
9. **Klauda, J.B.**, R.W. Pastor, & B.R. Brooks. "Refining the Structure of Lipid Bilayers with Insight from Molecular Dynamics Simulations" *ACS National Fall Meeting* (2005).
10. **Klauda, J.B.**, R.W. Pastor, & B.R. Brooks. "Structure and Dynamics of Lipid Membranes: How can Simulations Aid Experiments?" *AIChE Annual Meeting* (2005).
11. **Klauda, J.B.**, R.W. Pastor, & B.R. Brooks. "Importance of Including Long-range Interactions in Simulations of Biologically Relevant 2D Surfaces" *AIChE Annual Meeting* (2005).
12. **Klauda, J.B.** & B.R. Brooks. "Lactose Permease-Sugar Interactions: The Anomeric State of a Disaccharide Determines its Binding Structure" *Symposium of Protein Society* (2006).
13. **Klauda, J.B.** & B.R. Brooks. "Disaccharide Binding in Lactose Permease of E. coli: Sugar Structure Influences Binding" *AIChE Annual Meeting* (2006).
14. **Klauda, J.B.**, R.W. Pastor, & B.R. Brooks. "Dynamical Motions of Lipids and a Finite Size Effect of Bilayers" *AIChE Annual Meeting* (2006).
15. **Klauda, J.B.** & B.R. Brooks. "Structural Changes in Lactose Permease and How Sugar-Type Effects Binding Structure" *Biophysical Society* (2007).

Conference Talks as Faculty at UMD

16. **Klauda, J.B.** & B.R. Brooks. "Determining the Outward-Facing Structure and Sugar Binding in Lactose Permease of *E. coli*" *AIChE Annual Meeting* (2007).
17. **Klauda, J.B.**, R.W. Pastor, & B.R. Brooks. "Long-range Lennard-Jones and Electrostatic Interactions in Interfaces: Application and Development of the Isotropic Periodic Sum Method" *AIChE Annual Meeting* (2007).
18. **Klauda, J.B.**, R.P. Singh, & B.R. Brooks. "Binding and Release of Cholesterol in the Osh4 Protein of Yeast" *ACS National Fall Meeting* (2008).
19. **Klauda, J.B.**, R.P. Singh, & B.R. Brooks. "Binding and Release of Cholesterol in the Osh4 Protein of Yeast" *AIChE Annual Meeting* (2008).
20. **Klauda, J.B.**, P.Y. Pendse‡, & B.R. Brooks. "An Atomic-level Model for the Periplasmic Open State of Lactose Permease" *Biophysical Society* (2009).
21. **Klauda, J.B.**, R.W. Pastor, & B.R. Brooks. "Improving the lipid force field of CHARMM: A quantum mechanical and experimental approach" *ACS National Fall Meeting* (2009).

22. **Klauda, J.B.**, R.W. Pastor, & B.R. Brooks. "Improving the lipid force field of CHARMM: A quantum mechanical and experimental approach" *AIChE Annual Meeting* (2009).
23. **Klauda, J.B.**, J.B. Lim†, R.M. Venable, & R.W. Pastor. "A Modified Lipid Force Field for CHARMM: Development and Application to Single-Celled Organism Membranes" *Biophysical Society* (2010).
24. Lim, J.B.† & **J.B. Klauda**. "Refining and Testing CHARMM Lipid Parameters for Biologically Important Membranes" *Biophysical Society* (2011).
25. Lim, J.B.†, J.W. O'Connor† & **J.B. Klauda**. "Molecular simulations of model bacterial and ocular lens lipid membranes with the CHARMM36 force field" *ACS National Spring Meeting* (2011).
26. **Klauda, J.B.** "Gas hydrates: Where and how much is trapped in this alternative source of natural gas" *ACS National Spring Meeting* (2011).
27. **Klauda, J.B.** "New all-atom method to probe unknown conformations and substrate transport of secondary active membrane transport proteins" *ACS National Spring Meeting* (2011).
28. Rogaski, B.,‡ V. Monje† & **Klauda, J.B.** "Extending the CHARMM Force Field to Sphingolipids and Lipids with Polyunsaturated Chains" *AIChE Annual Meeting* (2011).
29. Pendse, P.Y‡ & **Klauda, J.B.** "Quantification of Sugar Binding Affinity and Study of Proton Translocation in Lactose Permease of *Escherichia Coli*" *AIChE Annual Spring Meeting* (2011).
30. Pendse, P.Y. ‡ K.R. Pandit, ‡ & **J.B. Klauda**. "Atomic-level Simulations to Probe Conformational Changes of Secondary Active Transport Proteins" *Biophysical Society* (2012).
31. Rogaski, B.‡ & **J.B. Klauda**. "Osh4 Membrane Binding Through Molecular Dynamics" *Biophysical Society* (2012).
32. **J.B. Klauda** "Lipid Diversity: Is It Important in Modeling Organism and Organelle Membranes?" *AIChE Annual Meeting* (2012).
33. **J.B. Klauda** "Developing CHARMM-compatible Lipid Parameters for Ceramides and United Atom Chains" *Biophysical Society* (2013).
34. **J.B. Klauda** "What can we Learn From Microsecond Simulations of a Peripheral Membrane Protein of Yeast?" *ACS National Spring Meeting* (2013).
35. **J.B. Klauda.** "CHARMM-Compatible Lipid Parameters for Ceramides and United Atom Chains" *AIChE Annual Meeting* (2013).
36. Daristotle, J.L.,† R. Konas† & **J.B. Klauda**. "Probing the Toxicity of Ethanol to Biological Membranes with Application to Biofuels Production." *AIChE Annual Meeting* (2014).
37. Wong, S.Y.† & **J.B. Klauda**. "Probing the Dependence of pH on Sugar Binding and Protein Structure in a Polysaccharide Lyase." *Biophysical Society* (2015).

38. Khakbaz, P.,‡ I. Bera, & **J.B. Klauda**. PlexinA3 Trans- and Juxtamembrane Dimer Helix Association. *Biophysical Society* (2016).
39. Zhuang, X. ‡, A. Oou°, & **J.B. Klauda**. "Simulations of Linoleoyl-containing Pure Lipid Bilayer and Soybean Plasma Membranes." *Biophysical Society* (2017).
40. Khakbaz, P.,‡ I. Bera, & **J.B. Klauda**. PROBING PLEXIN A3 DIMERIZATION AND THE IMPORTANCE OF THE NEAR MEMBRANE EXTRACELLULAR RESIDUES. *Biophysical Society* (2018).
41. Phakbaz, P.,‡ & **J.B. Klauda**. Ripple and Gel Phases of Saturated Phosphocholine Bilayers Investigated with Simulations. *Biophysical Society* (2019).
42. Yu, Y.,‡ & **J.B. Klauda**. Update of the CHARMM36 United Atom Chain Model for Lipids. *Biophysical Society* (2020).
43. Hsieh, M.-K.‖ & **J.B. Klauda**. Investigating SARS-COV-2 ORF7A and BST-2 Heterodimerization by Molecular Dynamics Simulations. *Biophysical Society* (2022).

II.E.14 Workshops

1. "Mechanisms for a novel pore-forming lipid and lipid binding to a peripheral membrane protein" *Workshop on Molecular Simulations of Biophysics and Biochemistry*. RIKEN AICS in Kobe, Japan (2013).
2. "Lipid Bilayer Simulations: Force fields, Simulation and Analysis" *Computational Modeling Workshop and Mini-Symposium.* University of Chicago *(2014).*
3. "Lipid Force Fields: Current Approaches to Force Field Development and their Accuracy" *2nd Molecular Simulations Summer School*. University of Calgary (2014).
4. "Development of the All-atom CHARMM Lipid Force Field and Asymmetric Membrane Models for the PM and TGN of Yeast" *CECAM Workshop: The future of biomembrane simulations: hidden pitfalls and future challenges*, Lyon, France (2017).
5. "Molecular Mechanics and Force Fields" CHARMM-GUI School, *CECAM Workshop*, Lausanne, Switzerland (2018).
6. "Lipid Membrane Simulations" CHARMM-GUI School, *CECAM Workshop*, Lausanne, Switzerland (2018).
7. "Molecular Mechanics and Force Fields" KIAS CHARMM-GUI School, *KIAS*, Seoul, Korea (2019).
8. "Minimization & Molecular Dynamics" KIAS CHARMM-GUI School, *KIAS*, Seoul, Korea (2019).
9. "Lipid Membrane Simulations" KIAS CHARMM-GUI School, *KIAS*, Seoul, Korea (2019).
10. "Molecular Mechanics and Force Fields" CHARMM-GUI School, *CECAM Workshop*, Lausanne, Switzerland (2021).

11. "Lipid Membrane Simulations" CHARMM-GUI School, *CECAM Workshop*, Lausanne, Switzerland (2021).
12. "CHARMM United Atom Model for Lipids (C36UAr)" Tinker Developer Workshop, Bethesda, MD (2022).
13. "Machine Learning for Analyzing Simulation Trajectories" Tinker Developer Workshop, Bethesda, MD (2022).

II.J. Sponsored Research Programs – Administered by the Office of Research Administration (ORA)

II.J.1. Grants

Current

Dates	Grant Title	PI	Co-PI	Funding Agency	Total Amount	JBK Share
4/2021-3/2025	*Functional Mechanisms and Therapeutic Potential of EAG Channel Regulators*	Tinatin Brelidze (Georgtown)	Klauda (sub-award)	NIH	$62,300	$62,300
6/2020-5/2022	*EAGER: Collaborative Research: Design of Inhibitors for ORF7a and ORF7b Oligomerization in COVID-19*	Klauda	B. Berger (UVA)	NSF/MPS/CHE	$150,000	$150,000
6/2020-5/2021	*CDK5 investigating drug targets*	Klauda		NIST-PREP	$60,513	$60,513
2/2020-1/2023	*Studies on the Protein-assisted Mechanism for Intracellular Membrane Contact Sites*	Klauda	Karlsson (UMD)	NSF/BIO/MCB	$983,837	$590,302
8/2020-7/2023	*The Mechanism of Polyvalent Ion Competition with Membranes and Membrane-Associated Proteins*	Klauda	S. Sukharev (UMD/Biology)	NSF/MPS/CHE	$646,000	312,845
10/2018-9/2021	*GAANN: UMD GROW (Generating a Research Outstanding Workforce)*	A. Asa-Awuku (UMD)	Klauda P. Kofinas (UMD)	Department of Education	$447,750	$0
				Total	$2,350,400	$1,175,960

Previous

Dates	Grant Title	PI	Co-PI	Funding Agency	Total Amount	JBK Share
6/2012-5/2015	*Collaborative Research: Development and Application of a Web-based Graphical User Interface for Membrane System Building and Analysis*	W. Im (U. Kansas)	Klauda	NSF/BIO/DBI	$125,081	$125,081
8/2012-7/2017	***CAREER:*** *Secondary Active Membrane Transporters: Determining Protein Structure and Transport Mechanisms with a New Hybrid Simulation Method*	Klauda		NSF/BIO/MCB	$668,313	$668,313
2/2015-1/2018	*Sensing Biological & Non-biological Polymers with a Nanopore*	Klauda		NIST	$216,953	$216,953
9/2016-8/2019	*Collaborative Research: Mechanisms for Cell Membrane Damage during Production of Biorenewable Fuels*	Klauda L. Jarboe (Iowa State U.)		NSF/ENG/CBET	$200,000	$200,000
7/2018-5/2020	*Measuring Biomolecular Interactions with Field Effect Transistors and Simulations*	Klauda		NIST	$233,327	$233,327
12/2019-5/2020	*CDK5 investigating drug targets*	Klauda		NIST-PREP	$25,532	$25,532
7/2020-12/2020	*I-Corps: Development of a Fouling Release Coating Formulation*	Klauda		NSF/IIP	$50,000	$50,000
				Total	$1,519,206	$1,519,206

II.K. Gifts and Funded Research not administered by ORA

II.K.4. Other

Listed below are two sections for funding of students intramurally at NIH and computational resources awarded through competitive grants and estimated value of award is listed when given.

NIH Support of Graduate Students

1. Support for a Graduate Student (Brent Rogaski) from Dr. Richard Pastor's Lab at NIH/NHLBI. Period (8/2010-8/2011)
2. Support for Graduate Student (Alison Leonard) from Dr. Richard Pastor's Lab at NIH/NHLBI. Period (1/2016-7/2019)
3. Support for Graduate Student (Yalun Yu) from Dr. Richard Pastor's Lab at NIH/NHLBI. Period (9/2018-8/2022)
4. Support for Graduate Student (Mahdi Ghorbani) from Dr. Bernie Brooks' lab at NIH/NHLBI. Period (6/2019-8/2022)
5. Support for Graduate Student (Anthony Pane) from Dr. Richard Pastor's Lab at NIH/NHLBI. Period (6/2022-current)

Computational Award/Time (Reviewed Proposals)

1. "Simulations of a Sterol Transport Protein (Osh4) that Tethers Membranes of the Endoplasmic Reticulum and Plasma Membrane". **Anton** hosted by the National Resource for Biomedical Supercomputing (NRBSC) at the Pittsburgh Supercomputing Center (PSC). Grant Number: PSCA00009P. SU: 25,000 Anton node hours. (4/1/2011-9/30/2011).
2. "Molecular Simulations of Transmembrane and Membrane-associated Proteins" TeraGrid Grant Number: TG-MCB100139 SU: 1,074,000 node hours (10/1/2010-9/30/2011)
3. "Molecular Simulations of Transmembrane and Membrane-associated Proteins" XSEDE Grant Number: TG-MCB100139 SU: 450,154 node hours (10/1/2011-9/30/2012)
4. "Conformational changes in lactose permease of E. coli to understand spin label dynamics and helix movements". **Anton** hosted by the National Resource for Biomedical Supercomputing (NRBSC) at the Pittsburgh Supercomputing Center (PSC). Grant Number: PSCA12035P. SU: 50,000 Anton node hours. (11/1/2012-7/31/2013).
5. "Molecular Simulations of Transmembrane and Membrane-associated Proteins" XSEDE Grant Number: TG-MCB100139 SU: 994,807 node hours (10/1/2012-9/30/2013).
6. "Molecular Simulations of Transmembrane and Membrane-associated Proteins" XSEDE Grant Number: TG-MCB100139 SU: 2,311,419 node hours (10/1/2013-9/30/2014).
7. "Simulations of a Peripheral Membrane Protein Binding Mechanism to Yeast Organelle Membranes and Forming Membrane Contact Sites" **Anton** hosted by the National Resource for Biomedical Supercomputing (NRBSC) at the Pittsburgh Supercomputing Center (PSC). Grant Number: PSCA13048P. SU: 90,000 Anton node hours. (11/1/2013-7/31/2014).

8. "Molecular Simulations of Transmembrane and Membrane-associated Proteins" XSEDE Grant Number: TG-MCB100139 SU: 3,033,692 node hours (10/1/2014-9/30/2015). **Value of awarded resources:** $104,978.
9. "Yeast membrane Simulations with Inositol Phosphoceramide with Applications to Lateral Organization and binding of a Peripheral Membrane Protein" **Anton** hosted by the National Resource for Biomedical Supercomputing (NRBSC) at the Pittsburgh Supercomputing Center (PSC). Grant Number: PSCA14030P. SU: 100,000 Anton node hours. (10/20/2014-7/31/2015).
10. "Molecular Simulations of Transmembrane and Membrane-associated Proteins" XSEDE Grant Number: TG-MCB100139 SU: 5,912,434 node hours (10/1/2015-9/30/2016). **Value of awarded resources:** $212,168.
11. "Phase Separation of Long-chained Inositol Phosphoceramide in Model Yeast Membranes" **Anton** hosted by the National Resource for Biomedical Supercomputing (NRBSC) at the Pittsburgh Supercomputing Center (PSC). Grant Number: PSCA15043P. SU: 100,000 Anton node hours. (11/1/2015-7/31/2016).
12. "Molecular Simulations of Transmembrane and Membrane-associated Proteins" XSEDE Grant Number: TG-MCB100139 SU: 4,067,999 node hours (10/1/2016-9/30/2017). **Value of awarded resources:** $184,040.
13. "Ligand effects on the biological function of the serotonin receptor in model raft-forming membranes" **Anton2** hosted by the National Resource for Biomedical Supercomputing (NRBSC) at the Pittsburgh Supercomputing Center (PSC). Grant Number: PSCA16007P. SU: 760,000 Anton2 node hours. (12/1/2016-11/30/2017).
14. "Molecular Simulations of Transmembrane and Membrane-associated Proteins" XSEDE Grant Number: TG-MCB100139 SU: 4,204,234 node hours (10/1/2017-9/30/2018). **Value of awarded resources:** $276,114.
15. "Antagonist and Glycosylation Effects on the Biological Function of the Serotonin Receptor" **Anton2** hosted by the National Resource for Biomedical Supercomputing (NRBSC) at the Pittsburgh Supercomputing Center (PSC). Grant Number: PSCA17009P. SU: 395,025 Anton2 node hours. (12/7/2017-11/30/2018).
16. "Molecular Simulations of Transmembrane and Membrane-associated Proteins" XSEDE Grant Number: TG-MCB100139 SU: 1,110,246 CPU hours and 180,000 Node hours (1/1/2019-1/31/2019). **Value of awarded resources:** $60,269.
17. "Unraveling the Structure-Function Relationship of the Serotonin Receptor (5HT3)" **Anton2** hosted by the National Resource for Biomedical Supercomputing (NRBSC) at the Pittsburgh Supercomputing Center (PSC). Grant Number: PSCA18011P. SU: 230,000 Anton2 node hours. (12/1/2018-11/30/2019).
18. "Modeling the Intracellular and Transmembrane Structure of the Active Dimer of PlexinA1" **Anton2** hosted by the National Resource for Biomedical Supercomputing (NRBSC) at the Pittsburgh Supercomputing Center (PSC). Grant Number: MCB110012P. SU: 460,000 Anton2 node hours. (12/1/2019-11/30/2020).
19. "Molecular Simulations of Transmembrane and Membrane-associated Proteins" XSEDE Grant Number: TG-MCB100139 SU: 2,660,000 CPU hours and 160,000 Node hours

(1/1/2020-12/31/2020). **Value of awarded resources:** $75,986.

20. "Structural study of active and inactive dimerization of the plexinA1 intracellular domain" **Anton2** hosted by the National Resource for Biomedical Supercomputing (NRBSC) at the Pittsburgh Supercomputing Center (PSC). Grant Number: MCB110012P. SU: 460,000 Anton2 node hours. (12/1/2020-11/30/2021).
21. "Molecular Simulations of Transmembrane and Membrane-associated Proteins" XSEDE Grant Number: TG-MCB100139 SU: 3,750,000 CPU hours and 30,000 GPU node hours (7/1/2021-6/30/2022).
22. "Studies of Transmembrane Proteins: PlexinA1 intracellular dimerization and toxin deactivation of 5-HT3" **Anton2** hosted by the National Resource for Biomedical Supercomputing (NRBSC) at the Pittsburgh Supercomputing Center (PSC). Grant Number: MCB110012P. SU: 230,000 Anton2 node hours. (12/1/2021-11/30/2022).
23. "Molecular Simulations of Transmembrane and Membrane-associated Proteins" XSEDE Grant Number: TG-MCB100139 SU: 5,800,000 CPU hours and 33,000 GPU node hours (7/1/2022-6/30/2023). **Value of awarded resources:** $48,695.

II.P. Research Fellowships, Prizes, and Awards.

1. Pigford Fellowship (1998-1999): University of Delaware
2. IRTA Postdoctoral Fellow (2003-2007): National Institutes of Health
3. Minta Martin Award (2008-2010) $60,000
4. NSF CAREER (2012-2017)
5. Omega Chi Epsilon Award from the Chi Chapter (UMD)
6. University System of Maryland's PROMISE AGEP Outstanding Faculty Mentor (2015)
7. *Biochimica et Biophysica Acta – Biomembranes*: Editorial Board (2019-current)
8. *Journal of Physical Chemistry B*: Editorial Advisory Board (2020-current)
9. Graduate Student Mentorship Award (2023): For developing a Mentorship Plan and fostering strong mentorship in CHBE. Monetary award for grad student activities.

III. Teaching, Extension, Mentoring, and Advising

III.A. Courses Taught

Listed in the table below are the courses taught with their semester and enrollment numbers.

Course	Semester/Year	Enrollment
ENCH476: Statistics and Experimental Design	Spring/2008	26
ENCH648G: Statistics and Experimental Design	Spring/2008	6
ENCH610: Chemical Engineering Thermodynamics	Fall/2008	20
ENCH476: Statistics and Experimental Design	Spring/2009	29
ENCH648G: Statistics and Experimental Design	Spring/2009	5
ENCH648P: Molecular Modeling Methods	Fall/2009	12
ENCH476: Statistics and Experimental Design	Spring/2010	24
ENCH648G: Statistics and Experimental Design	Spring/2010	1
ENCH610: Chemical Engineering Thermodynamics	Fall/2010	14

ENCH476: Statistics and Experimental Design	Spring/2011	47
ENCH648G: Statistics and Experimental Design	Spring/2011	2
ENCH400: Chemical Engineering Thermodynamics	Fall/2011	69
ENCH476: Statistics and Experimental Design	Spring/2012	31
ENCH648G: Statistics and Experimental Design	Spring/2012	1
CHBE410: Statistics and Experimental Design	Fall/2012	100
CHBE302: Chemical Engineering Thermodynamics	Spring/2013	85
CHBE410: Statistics and Experimental Design	Fall/2013	80
CHBE476: Molecular Modeling Methods	Spring/2014	26
ENCH648P: Molecular Modeling Methods	Spring/2014	6
CHBE410: Statistics and Experimental Design	Fall/2014	93
CHBE476: Molecular Modeling Methods	Spring/2015	10
ENCH648P: Molecular Modeling Methods	Spring/2015	4
CHBE410: Statistics and Experimental Design	Fall/2015	94
CHBE302: Chemical and Biomolecular Engineering Thermodynamics II	Spring/2016	113
CHBE410: Statistics and Experimental Design	Fall/2016	116
CHBE302: Chemical and Biomolecular Engineering Thermodynamics II	Spring/2017	85
CHBE301: Chemical and Biomolecular Engineering Thermodynamics I	Fall/2017	69
CHBE302: Chemical and Biomolecular Engineering Thermodynamics II	Spring/2018	72
CHBE301: Chemical and Biomolecular Engineering Thermodynamics I	Fall/2018	46
CHBE302: Chemical and Biomolecular Engineering Thermodynamics II	Spring/2019	80
CHBE301: Chemical and Biomolecular Engineering Thermodynamics I	Fall/2019	59
CHBE302: Chemical and Biomolecular Engineering Thermodynamics II	Spring/2020	73
CHBE301: Chemical and Biomolecular Engineering Thermodynamics I	Fall/2020	57
CHBE302: Chemical and Biomolecular Engineering Thermodynamics II	Spring/2021	72
CHBE301: Chemical and Biomolecular Engineering Thermodynamics I	Fall/2021	42
CHBE302: Chemical and Biomolecular Engineering Thermodynamics II	Spring/2022	58
CHBE610: Chemical Engineering Thermodynamics	Fall/2022	11
CHBE302: Chemical and Biomolecular Engineering Thermodynamics II	Spring/2023	49
CHBE610: Chemical Engineering Thermodynamics	Fall/2023	11
CHBE302: Chemical and Biomolecular Engineering Thermodynamics II	Spring/2024	48

III.B. Teaching Innovations

III.B.6. Course or Curriculum Development.

Listed below are courses in which I developed course material from scratch.

Course	Semester/Year
ENCH476: Statistics and Experimental Design	Spring/2008
ENCH648G: Statistics and Experimental Design	Spring/2008
ENCH610: Chemical Engineering Thermodynamics	Fall/2008
ENCH648P: Molecular Modeling Methods	Fall/2009
ENCH400: Chemical Engineering Thermodynamics	Fall/2011
CHBE302: Chemical and Biomolecular Engineering Thermodynamics II	Spring/2016 (new book and organization)
CHBE301: Chemical and Biomolecular Engineering Thermodynamics I	Fall/2017

III.C. Advising: Research or Clinical

Current Active Group

Level	Students	# of researchers
High School	None	0
Undergrad	Edward Niu, Erin Jackson, Pavan Bhat, Dai-Bao Van, Dylan Mendes, Joe Kutza, Sasha Cotes-Park, Shyam Patel, Sriya Pragada, Taran Mehta, Vincent Zhao, Sukrit Mangla, Nicholas Dadzie, Nida Shah, Tanya Budhiraja, Paige Wells, Yash Porwal	17
Graduate – M.S.	Joshua Lucker	1
Graduate – Ph.D.	Tejaswi Tammareddy, Robert Allsopp, Jessica Bodosa, Anthony Pane, Joshua Lucker, Kinjal Mondal	6
Postdoc	Min-Kang Hsieh, Sharmistha Kamakar	2

III.C.1. Undergraduate

Listed below are undergraduates that have worked in my lab researching on various projects. In total, there have been **80+ undergraduate/high students** that have worked under my direction. Also listed in the table are any awards and placement of these students.

#	Student	Time Period	Project &Awards	Graduation & Placement
1	Joseph Lim	S2008-Su2010	Various Lipid Membrane Studies and Osh4 Protein *Awards* • ASPIRE Program (2008) • UMD Bioscience Day (2008) best poster (Biochem/Biophys) • HHMI Undergrad	B.S. 2010 MIT/ChE (PhD)

			Fellowship (2009-2010) • NSF Graduate Fellowship	
2	Marcus Hadley	Su2008-S2009	POPE membranes	B.S. 2010
3	Glen Guglietta	Su2008	Hydrates for Hydrogen Storage	B.S. 2009 Drexel Univ./ChE (PhD)
4	Joe O'Connor	F2008-Su2010	Ocular Lens Membrane Models and AQP0	B.S. 2010 PSU/ChE (PhD)
5	Krishan Parikh	F2009-S2010	Hydrates: Data collection	
6	Diana Villanueva	S2010-Su2011, F2012-	Lipid membrane studies *Awards* • Travel award to the ACC "Meeting of Minds" Research Conference (2011)	B.S. 2013 GSK (Rockville, MD)
7	Mike Harris	Su2010-S2011	MOMP Protein	University of Minnesota/ChE (PhD)
8	Sabrina Wanys	Su2010-Su2011	Gulf of Mexico Hydrate Modeling	
9	Viviana Monje	F2010-Su2012	PUFA Lipids *Awards* • LSAMP Student (2010-12)	UMD/ChBE (M.S.)
10	Ivy Muregi	S2011-S2012	Aggregation of asphaltenes	Accenture then 2013 UPitt/ChE (PhD)
11	Andy Do (Chemistry)	S2011-F2012	AQP0 and Lens	
12	Alan Tran (Chemistry)	S2012-F2013	Lipid Membrane Studies	B.S. 2014
13	Sarah Lee (Chemistry)	S2012-S2014	Lipid Membrane Studies	B.S. 2014 Pharmacy School
14	Christopher Boughter (Physics)	S2012-S2015	Hydrotropes and Lipid membranes with cholesterol *Awards* ChBE Undergrad Research Award (2015)	B.S. 2015 U. Chicago/ Biophysics (PhD)
15	Judah Makeover	F2012-F2013	Temperature Dependence of Lipid Properties	B.S. 2015 Israeli Army
16	Matthew Allsopp	F2012-S2014	Micelle Formation with UA Models	B.S. 2014

17	Tae Yang	W2013-S2013	Aggregation of asphaltenes	B.S. 2013
18	Rob Pullen	W2013-Su2013	Toxic molecules from biofuels research (effects on membranes)	B.S. 2013 U. Tenn/ChE (PhD)
19	David Weglein	W2013-Su2014	ALPS-like motif of Osh4 with membranes	B.S. 2014
20	Jacob Hebert	S2013-F2014	Alkane-water surface tension Aggregation of asphaltenes	B.S. 2015
21	Sylvia Kang (Computer Sci.)	Su2013-F2016	Lipid Membrane and Educational Website Design	B.S. 2016
22	John Daristotle	Su2013-S2014	Toxic molecules from biofuels research (effects on membranes)	B.S. 2014 UMD/BioE (PhD)
23	Mengesteab Adera	Su2013-S2014	Gas Hydrates and Water Model Testing	B.S. 2014/ Schreiber Foods
24	Ryan Konas	Su2013-Su2015	Toxic molecules from biofuels research (effects on membranes)	B.S. 2015
25	Ndubuisi (Ben) Harbor	Su2013-S2014	Toxic molecules from biofuels research (effects on membranes)	B.S. 2014/U. Toronto
26	Sook Wong	F2013-S2015	Polysaccharide Lysases	B.S. 2014
27	Francis Bacarisas (BioE)	S2014-F2015	Ceramide bilayers	B.S. 2016/ Consulting Firm
28	Connor Welch	S2014-S2016	Ice formation Bilayer gel Formation	B.S. 2016 / Deloitte Consulting
29	Rui Ponte	F2014-S2016	CHARMM36UA testing	B.S. 2017
30	Mark Adams	F2014-S2016	CHARMM36UA testing	B.S. 2016
31	Joshua Condon	F2014-S2015	Polysaccharide Lyases	B.S. 2015 UD/ChE (PhD)
32	Ky Wildermuth	Su2015-Su2017	Drude Testing and Osh4-ALPS with HMMM *Award* OXE Poster Award (2016)	B.S. 2017
33	Tylar Clark	S2015-S2016	Drude Testing on DMPC bilayer *Award (at JHU)* NSF GRF (2019)	B.S. 2018 JHU/Phys. Chem (PhD)
34	Monica Chu (BioE)	S2015-S2017	PE/PG bilayers and drug binding	B.S. 2018
35	Lidiya Gavrilenko	Su2015-	Aggregation of asphaltenes	B.S. 2016

		F2016	*Award* OXE Poster Award (2015)	
36	Lenny Fobe	Su2015-S2018	Buffer interaction with lipids and FF development. Ceramide pore formation	B.S. 2018 U. Colorado – Boulder (PhD)
37	Nao Rho (Computer Science)	Su2015-F2016	PE/PG bilayers and manual development	
38	Samuel Guo	S2016	Gas Hydrate (CO_2 Sequester) GoM depth map	
39	Yusuf Khan	Su2016-S2017	Ceramide bilayers	B.S. 2017
40	Nebeyu Mesfin	Su2016-F2017	Cell membrane damage during biofuels/chemical production	B.S. 2019
41	Eric Wang (BioE)	Su2016-Su2019	Sphingolipid mixtures with cholesterol, ocular lens membranes and skin membranes *Awards* • HHMI Undergraduate Research Fellow (2017) • Jeffry Madura Outstanding Research Award at ACS Fall 2017 Meeting (COMP Poster Session) • Goldwater Scholarship AY2018 • Churchill Scholarship • NSF GRF (2019)	M.S. University of Cambridge (2019-2020) Ph.D. Harvard-MIT (2020-), Biomedical Engineering
42	Kirellos Elsaad	F2016-S2018	Gas Hydrate simulations of benzene/cyclohexane growth	B.S. 2018
43	Annika Vaerst	F2016-S2016	Ocular Lens	
44	Linnea Warburton (ME)	S2016-Su2019	AMP Peptides and membranes *Awards* • NSF GRF (2020)	B.S. MechE (2020), Ph.D. ME program at UC Berkeley
45	Chris Hiner (BioE)	F2017-S2019	CDK5 structure and electrostatics	B.S. 2019 Albert Einstein College of Medicine Ph.D. in Biomedical

				Sciences (2019-)
46	Emma Moore (BioE)	F2017-S2018	Neurological Membranes	B.S. 2020
47	Lauren Moyer (BioE)	F2017-S2018	AMP peptides	B.S. 2020
48	Leonard Unger (Math)	F2017-F2022	Lyme Bacterial Membrane Models	Transfer to Brown
49	Tyler Cline	Su2017-S2018	AMP work with Stephanie Nagle at CMU *Awards* • BS/MS ChBE program	MS. 2019
50	Juan Correa	Su2018-S2019	Gas hydrates for separation with MD simulations	
51	Niayesh Razi (Chemistry)	Su2018-F2019	Drug-membrane interactions and partitioning	
52	Marc Harron	Su2018-F2019	Biofuels project and interaction with membranes	B.S. 2020
53	Nidhi Kalaria (BioE)	Su2018-F2018	Membranes	
54	Owen Roy (BioE)	Su2018-Su2019	AMPs with skin (β-defensin)	
55	Tyla Holoman	Su2018-Su2021	AMPs with skin *Awards* • LSAMP URP	B.S. 2021 Ph.D. at UT-Austin (ChE)
56	Josh Fernandes	Su2018-Su2021	Ocular Lens Membranes	B.S. 2021 Ph.D. at UC Berkeley (ChE)
57	Kyle Pomykala	F2018-S2019	Ecophysics and Entropy	B.S. 2020
58	Yiding Yuan	S2019-F2021	Neurological Membranes	
59	Yueqi (Edward) Niu	S2019-	Immune Cell Modeling	
60	Erin Jackson	Su2019-F2023	Antimicrobials with Membranes *Awards* • LSAMP URP	
61	Jacob Olondo Kuba	F2019-Su2020	Statins and Cellular Membranes	NIH Postbac
62	Pavan Bhat	S2020-S2023	PUFA Lipids	Ph.D. BIOE, Northwester U.
63	Crystal Lin	Su2020-Su2021	QM of Reactions at Surfaces with DFT	
64	Sarah Browning	F2020	AMPS with membrane asymmetry	

65	Dai-Bao Van	F2020-	Archeal membrane with ether branched lipids	
66	Deepika Tripu	F2020-F2021	Metal ion binding	
67	Sasha Coats-Park	F2020-	Auxin binding to membranes	
68	Varunaa Sri Hemanth Kumar	F2020-F2021	AMPS	
69	Sriya Pothapragada	F2020-Su2023	Stereocilia membranes (ear hair cells) *Awards* • BIOE Honors	Ph.D. Clemson University
70	Abdul Butt	F2020-Su2021	Gas Hydrates in GoM	
71	Dylan Mendes	S2021-S2023	Antimicrobial peptides interaction with SC skin membrane models	
72	Jai Dadarwala	S2021-F2022	Proteins in Asymmetric Membranes	
73	Joseph Kuta	S2021-	Sugars binding to the TLR complex	
74	Shyam Patel	S2021-S2023	Sugars binding to the TLR complex	
75	Taran Mehta	S2021-S2023	Polysaccharide lyase simulations on SMLT1473	
76	Akhil Jayan	S2022-F2022	Advanced Neurological Membrane models	
77	Shane Saunders	S2022-F2022	Primordial Membrane Models	
78	Zach Teselko	S2022-F2022	SARS-CoV-2 ORF7b in asymmetric membranes	
79	Vincent Zhao	S2022-	Ladderdane Lipid Membranes	
80	Sukrit Mangla	S2023-	CDK5	
81	Nicholas Dadzie	F2022-	Lipid Membranes and FF development	
82	Nida Shah	S2022-	CDK5 *Awards* • BIOE Honors	
83	Tanya Budhiraja	F2022-	ORF7b dimerization of TGN vs. PM *Awards* • BIOE Honors	
84	Paige Wells	S2023-F2023	Lipid Membranes	
85	Yash Porwal	S2023-F2023	Lipid Membranes	
86	Anjola Akintoba	S2023-	Lipid Membranes	
87	Sho Sniderman Takeshita	S2023-S2024	Microglia Membrane Models for Alzheimer's Disease	Ph.D. Biophysics at

				JHU
88	Abhi Senthikumar	S2023-	Lipid Membranes and AMPs	
89	Emily Davies	F2023-	ML of Smlt1473	
90	Daniel Erickson	F2023-	Microglia Membrane Models for Alzheimer's Disease	
91	Neelay Sachdevan	F2023-	Microglia Membrane Models for Alzheimer's Disease	

Listed below are high school students, undergraduates or those with only undergraduate degrees who worked in my lab but were not students at UMD.

#	**Student**	**Time Period**	**Project**	**School & *Placement***
1	Muhammad Saad Noon	Su2009-Su2010	Protein Structure Prediction (Chlyamidia MOMP)	COMSATS Institute of Information Technology, Islamabad B.S. 2009 *Research Scholar at Alex MacKerell's Lab*
2	Arpan A. Bandyopadhyay	Su2010	Hydrate Modeling (with electrolytes)	IIT/Bombay *U. Minnesota-ChE (Ph.D.)*
3	Yubaraj Boro	Su2011	Hydrate Coding/MD simulations	IIT/Guwahati
4	Allen Chang	Su2010, Su2011	Hydrate GUI-code	Poolesville High School *MSE/UMD (B.S.)*
5	Joshua Nichols	F2012-S2013	Temperature Dependence of Lipid Properties	Eleanor Roosevelt High School *ChBE/UMD (B.S.)*
6	Michael Lu	F2013-S2014	Ceramide Bilayers	Eleanor Roosevelt High School *ChBE/UMD (B.S.)*
7	Anna Ou	Su2014-S2016	Lipids with two double bonds and peroxidation	Montgomery Blair High School *UC-Berkeley*
8	Edgar Sanchez	Su2016	Butanol simulations with an organic interface	Universidad Nacional

				Autónoma de México
9	Michelle Marsandi	F2016-S2017	Cell membrane damage during biofuels/chemical production	Eleanor Roosevelt High School
10	Muhamad Zakaria	Su2017-S2018	Cell membrane damage during biofuels/chemical production	Al-Huda School in College Park
11	Andrew Selvadoss	Su2017-F2017	Cell membrane damage during biofuels/chemical production (Dual bilayer models)	Poolesville High School *ChBE/UMD (B.S.)*
12	Alan Li	Su2018	Membrane effects on α-HL	Montgomery Blair High School
13	Leslie Wang	S2020-	Training and Membrane Projects	Marriotts Ridge High School
14	Afsa Khawar	F2020-F2021	Training and Membrane Projects	STEM program at North County High School

III.C.2. Master's

	Student	**Time Period**	**Thesis & Awards**	**Graduation & Placement**
1	Brent Rogaski	S2009-F2010	Computational Studies on the Binding and Dynamics of the Osh4 Protein of Yeast and a Model Yeast Membrane System	M.S. 2010 UMD/ChBE (PhD)
2	Kunal Pandit	S2010-F2011	Membrane Models of *E. coli* Containing Cyclic Moieties in the Aliphatic Lipid Chain *Awards* • Nominated by ChBE for the Dean's Masters Research Awards Competition	M.S. 2011-12 UMD/ChBE (PhD)
3	Viviana Monje	F2012-F2014	Computational Studies on Organelle-specific Yeast Membrane Models *Awards* • LSAMP Bridge to Doctorate Fellowship	M.S. 2014/ChBE (PhD)

4	Rehan Choudhary	Su2013-S2017	Modeling Liquid Evaporation and using Molecular Dynamics Simulations to estimate Diffusion Coefficients and Relative Solved Drying Times	M.S. 2017 DOE
5	Tyler Cline	Su2017-Su2019	Molecular Simulation of Antimicrobial Peptide WLBU2-MOD Binding with Gram-Negative Inner Membrane Mimics *Awards* • BS/MS ChBE program	MS. 2019
6	Tejaswi Tammareddy	Su2018-S2019	Effects of Lipid-Protein Interactions on the Conductance of the Transmembrane Protein Alpha-Hemolysin using Molecular Dynamics Simulations	M.S. 2019 Ph.D. Program
7	Joshua Lucker	S2022-S2023	A UNITED-ATOM REPRESENTATION FOR SPHINGOLIPIDS IN THE CHARMM MOLECULAR DYNAMICS FORCE FIELD	M.S. 2023 (Biophysics) Ph.D. Program
8	Omid Davoudi	Su2020-S2023	MODEL COMPOUNDS GUIDE AFFINITY MEASUREMENT OF BERYLLIUM AND CALCIUM INTERACTIONS WITH PHOSPHOLIPIDS Co-advised with Dr. Sukharev (BIO)	M.S. 2023

III.C.3. Doctoral

#	**Student**	**Time Period**	**Dissertation &Awards**	**Graduation & Placement**
1	Pushkar Pendse	S2008-S2013	Computational Studies on Lactose Permease of *E. coli* as a Model for Membrane Transport Proteins *Awards*	Postdoc at Dr. Michael Grabe's lab in collaboration with UCLA experiments

			• 2nd place at UMD's ResearchFest 2010 • 1st place poster at GRID's Modeling & Simulation Section • ACS/CSW travel award to 2012 Spring Meeting	(Dr. Abramson)
2	Brent Rogaski	F2010-S2012	*Awards* • ACS/CSW travel award to 2011 Spring Meeting	Left program early for Industrial Job at Power Plant Manufacturing (Western Services Corporation, Fredrick, MD)
3	Viviana Monje-Galvan	F2014-S2017	Computational Studies of Membrane Models and their Interaction with a Peripheral Protein in Yeast, and Disruption of the Water-oil Interface by a Hydrotrope *Awards* • ACS/CSW travel award to 2015 Spring Meeting • 2nd Place for TA of the Year award (2015) • Outstanding Graduate Assistant for AY 2015-16 • Anne Wiley Semester Fellowships AY 2015-16	Postdoc at U. Chicago in Dr. Greg Voth's lab. **U. Buffalo (SUNY) Faculty (S21-current)**
4	Pouyan Khakbaz	S2013-F2017	Computational Studies of Lipid Bilayers and Transmembrane Proteins	Postdoc at U. Illinois Urbana-Champaign (Dr. Diwakar Shukla)
5	Xiaohong Zhuang	S2013-F2016	Computational Simulations on Membranes and a Transmembrane Protein	Postdoc at Naval Research Lab
6	Nick Guros	S2015-Su2019	Advancements in Label-free Biosensing Using Field-Effect Transistors and Aided by Molecular Dynamics Simulations *Awards* • Poster Award at the 4th International Conference of Molecular Simulations	AstraZeneca/ MedImmune

			• Outstanding Graduate Assistant for AY 2018-19 • 2nd Place in the Clark's School PhD Dissertation Competition	
7	Allison Leonard	S2015-Su2019	Lipid Force Field Parameterization for Improved Modeling of Ion-Lipid Interactions and Ether Lipid, and Evaluation of the effects of Long-range Lennard-Jones Interactions on Alkanes *Awards* • Hockmeyer Scholarship AY 2016-17 (CMNS fellowship)	Postdoc at Ed Lyman's Lab (U. Delaware)
8	Qin Ni	S2016-F2020	Co-advised with Garyk Papoian (Chem/IPST)	Postdoc at JHU
9	Mahdi Ghorbani	S2018-Su2022	Molecular Dynamics Simulations and Machine Learning Study of Biological Processes	Postdoc with Prof. Michael Keiser (UC-San Francisco)
10	Yalun Yu	S2018-Su2022	Paramertization of the CHARMM Lipid Force Field and Applications to Membrane Modelling	Scientist at Schrödinger, Inc.
11	Ruixing Wang	F2018-S2021	Co-advised with Pratyush Tiwary (Chemistry PhD Student)	Dropped out due to visa and family reasons
12	Tejaswi Tammareddy	F2019-	Current student; co-advised with Antonio Cardone (NIST)	
13	Robert Allsopp	S2019-F2023	Study of Membrane Binding Proteins and Related Signaling Molecules	Postdoc with Dr. Curt Meuse (NIST)
14	Jiyeon Min	S2020	Current Student (Biophysics); co-advised by Bernie Brooks (NIH)	
15	Omid Davoudi	Su2020-Su2023	Co-advised with Dr. Sukharev (BIO)	Switched labs and then finished with M.S.
16	Jessica Bodosa	S2021-	Current Student (Biophysics) • Biophysics Excellence in Research Award (2024, pre-candidate)	
17	Anthony Pane	S2022-	Current Student (Biophysics)	
18	Kinjal Mondal	S2023-	Current Student (Biophysics)	

19	Joshua Lucker	S2023-	Current Student (Biophysics)	
20	Marlen Toktomamatov	S2024-	Current Student (Biochem)	

III.C.4. Post-doctoral

#	Student	Time Period	Research Area	Placement
1	Indrani Bera	S2015-F2019	Computational studies on membranes (PSM mixtures), signaling proteins (PlexinA3 with CGMD) and SAT proteins (SWEET family)	Postdoc at U. College at Dublin
2	Michael Kio	S2017-F2021	Computational Studies of Nanoparticle transport across membranes	Assistant Research Professor (UMD)
3	Min-Kang Hsieh	S2020-	Inner membrane of Gram Negative bacteria (Asymmetry effects)	Startup in San Francisco, CA
4	Sharmistha Karmakar	S2020-Su2024	Oxysterol Binding Protein Studies	

III.D. Mentorship

III.D.1. Junior Faculty

1. Prof. Taylor Woehl (Chemical and Biomolecular Engineering)
2. Prof. Chen Zhang (Chemical and Biomolecular Engineering)
3. Prof. Paul Albertus (Chemical and Biomolecular Engineering)
4. Prof. Hannah Zierden (Chemical and Biomolecular Engineering)

III.E. Advising: Other than Research Direction

III.E.1 Undergraduate

Listed below is the number of students whom I was an academic advisor for to aid in registration and other academic associated issues per each academic year.

1. 2007-2008: 11
2. 2008-2009: 27
3. 2009-2010: 27
4. 2010-2011: 25
5. 2011-2012: 24
6. 2012-2013: 32
7. 2013-2014: 30
8. 2014-2015: 28
9. 2015-2016: 28
10. 2016-2017: 10
11. 2017-2018: 5
12. 2018-2019: 6
13. 2019-2020: 5

14. 2020-2021: 5
15. 2021-2022: 5
16. 2022-2023: 5
17. 2023-2024: 5

IV. Service and Outreach

IV.A. Editorships, Editorial Boards, and Reviewing Activities

IV.A.2. Editorial Boards

1. *Biochimica et Biophysica Acta – Biomembranes*: Editorial Board (2019-current)
2. *Journal of Physical Chemistry B*: Editorial Advisory Board (2020-current)

IV.A.3 Reviewing Activities for Journals and Presses

Listed below is a table of journals which I have reviewed manuscripts and number of reviews and significant revision reviews.

Journal	**Year First Reviewed**	**# of Reviews**
AIChE Journal	2007	4
ACS Applied Biomaterials	2018	2
ACS Central Science	2019	4
ACS Chemical Neuroscience	2020	2
ACS Infectious Diseases	2018	2
ACS Omega	2019	6
Accounts of Chemical Research	2018	3
Advanced Theory and Simulations	2022	1
BBA-Advances	2023	1
BBA-Biomembranes	2014	49
Biochemistry	2010	11
Bioelectrochemistry	2021	1
Biophysical Chemistry	2016	4
Biophysical Journal	2007	57
Biophysical Reports	2021	1
BMC Biology	2020	1
Canadian Journal of Chemistry	2014	1
ChemBioChem	2021	1
Chemical Engineering Research and Design	2014	1
Chemical Engineering Science	2014	1
Chemistry and Physics of Lipids	2015	17
Chemical Physics Letters	2010	4
Chemical Reviews	2018	2
Chemical Science	2020	1
Colloids and Surfaces B	2019	1
Communications Biology	2018	2
Computational and Structural Biotechnology Journal	2017	3
Current Opinion in Structural Biology	2024	1
eLife	2021	1

EMBO	2023	1
Energies	2012	3
Energy & Fuels	2015	2
Environmental Geotechnics	2020	1
Experiment Eye Research	2018	2
FEBS Open Bio	2020	1
Fluid Phase Equilibria	2012	10
Frontiers Molecular Bioscience	2019	3
Geophysical Research Letters	2007	1
Industrial & Engineering Chemistry Research	2009	18
Journal of the American Chemical Society	2011	9
JACS-Au	2021	2
Journal of Biological Chemistry	2022	1
Journal of Biomolecular Structure & Dynamics	2019	4
Journal of Cell Science	2015	1
Journal of Chemical & Engineering Data	2013	3
Journal of Chemical Information and Modeling	2012	21
Journal of Chemical Physics	2009	11
Journal of Chemical Theory and Computation	2013	30
Journal of Computational Chemistry	2008	14
Journal of Lipid Research	2023	1
Journal of Medicinal Chemistry	2021	1
Journal of Membrane Biology	2015	4
Journal of Molecular Biology	2009	2
Journal of the Mexican Chemical Society	2016	1
Journal of Molecular Graphics and Modelling	2010	3
Journal of Physical Chemistry (A/B/C)	2007	95
Journal of Physical Chemistry Letters	2011	11
Journal of Physics: Conference Series	2017	1
Journal of the Royal Society Interface	2024	1
Journal of Scientific Research and Reports	2013	1
Journal of Structural Biology	2020	1
Langmuir	2008	21
Lipids	2020	1
Macromolecular Theory and Simulations	2022	1
Molecular Membrane Biology	2012	3
Molecular Pharmaceutics	2023	1
Molecular Simulation	2017	6
Nanoscale	2020	2
Nature Communications	2018	15
Nature Methods	2017	2
Nature Structural & Molecular Biology	2020	2
PeerJ	2018	2
Physical Chemistry Chemical Physics	2019	7
Phytochemistry	2023	1
Plant Science	2023	1
PLoS Computational Biology	2012	12

PLoS One	2012	11
Polymer	2010	1
Proceedings of the National Academy of Sciences	2014	4
Protein Science	2023	1
Proteins: Structure, Function, and Bioinformatics	2016	11
RSC Advances	2020	2
Royal Society Open Science	2020	1
Science	2022	2
Scientific Reports (Nature Pub)	2018	4
Soft Matter	2019	3
Trends in Biochemical Sciences	2019	1
Wire: Computational Molecular Science	2023	1
Wire: Systems Biology and Medicine	2016	2

IV.A.4 Reviewing Activities for Agencies and Foundations

1. NSF Grant Review Panel (2008): Directorate for Engineering
2. Qatar National Research Fund Grant Review Panel (2009)
3. Qatar National Research Fund Grant Review Panel (2010)
4. NSF External Grant Review: Directorate for Geosciences (2010)
5. NSF External Grant Review: Directorate for Mathematical and Physical Sciences (2011).
6. Canada Foundation for Innovation Grant Reviewer (2011)
7. Qatar National Research Fund Grant Review Panel (2011)
8. DOE SCGF (Graduate Fellowship) reviews (2012).
9. NSF External Grant Review: Directorate for Mathematical and Physical Sciences (2012)
10. Qatar National Research Fund Grant Review Panel (2012)
11. NSF External Grant Review: Directorate for Mathematical and Physical Sciences (2013)
12. Qatar National Research Fund Grant Review Panel (2013)
13. NSF External Grant Review: Directorate for Mathematical and Physical Sciences (2014)
14. NIH: Program Grant Review (2014)
15. NIH: *ad hoc* member to the Biochemistry and Biophysics Study Section (BBM) (June 2014).
16. NSF External Grant Reviewer (4 grants): Directorate for Biological Sciences (2014)
17. NSF External Grant Reviewer (2 grants): Directorate for Mathematical and Physical Sciences (2014)
18. NSF External Grant Reviewer (2 grants): Directorate for Biological Sciences (2015)
19. NSF External Grant Reviewer (1 grant): Directorate for Mathematical and Physical Sciences (2015)

20. DOE Mail-in Reviewer (1 grant): Office of Basic Energy Sciences (2015)
21. NSF External Grant Reviewer (1 grant): Directorate for Biological Sciences (2016)
22. NIH: Special Emphasis Panel R21/R01 Grant Reviews (April, 2016)
23. NIH: K99/R00 Applications to NIEHS (June, 2018)
24. FDA: Compositionally Different Topical Formulations RFA (July, 2018)
25. Independent Research Fund-Denmark: DFF-Starting Grant (July, 2018)
26. Czech Science Foundation: Standard Project (July, 2018)
27. ACS PRF: Grant Reviewer (March, 2019)
28. Czech Science Foundation: Standard Project (July, 2019)
29. Knowledge Foundation (Swedish Research Foundation): Grant Reviewer (October, 2019).
30. NSF Grant Reviewer (multiple grants/NSF wide) (2020)
31. NSF External Grant Reviewer (1 grant): Directorate of Mathematical and Physical Sciences (2020)
32. NSF External Grant Reviewer (1 grant): Directorate of Biological Sciences (2020)
33. NOW Domain Science – Klein (Netherlands) Grant Reviewer (1 grant, 2020)
34. Czech Science Foundation: Standard Project (July, 2020)
35. DOE Ad Hoc Review (2021)
36. F.R.S.-FNRS Proposal Review (Belgium) (2021)
37. National Science Center (Poland)-Proposal Review (2021)
38. NIH: Special Emphasis R01 Grant Review Panel (Feb 2022)
39. NSF Frontier's Graduate Fellowship Review (April 2023)
40. F.R.S.-FNRS Proposal Review (Belgium) (2023)
41. NSF Grant Reviewer: Division of Chemistry (S2024)

IV.B. Committees, Professional & Campus Service

IV.B.1 Campus Service – Departmental

Service from ChBE is unnoted; service for the Biophysics Program is noted. Departmental service committees listed first in blue then thesis defenses are listed here with date and advisor listed.

1. Faculty Assembly Committee (2008-2016, 2020-current)
2. Graduate Studies Committee (2010-current)
3. Omega Chi Epsilon Faculty Advisor (2013-current)
4. Salary Review Committee (2011-2014, 2016-17)
5. **Associate Chair and Graduate Director (July 2015-current)**
6. Biophysics Graduate Application Review Committee (2016-current)
7. Faculty Assembly Chair (2020-current)

8. **Co-Graduate Director of Biophysics Program (August 2020-current)**
9. M.S. Thesis Committee member: Maria del Pilar Leon (4/25/2008 – Adomaitis)
10. M.S. Thesis Committee member: Thomas C. Palathra (5/29/2008 – Adomaitis)
11. Ph.D. Proposal Committee member: Kunshan Sun (9/25/2008 – Raghavan)
12. M.S. Thesis Committee member: Sai Kishore Mamidi (12/4/2009 – Panos)
13. Ph.D. Defense Committee member: Patricia Castellanos (12/11/2009 – Ehrman)
14. Ph.D. Defense Committee member: Kunshan Sun (9/30/2009 – Raghavan)
15. Ph.D. Defense Committee member: Vivek Dwivedi (4/16/2010 – Adomaitis)
16. Ph.D. Proposal Committee member: David Arana-Chavez (6/28/2010 – Adomaitis)
17. Ph.D. Proposal Committee member: Szu-Ting Chou (10/21/2010 – Seog)
18. M.S. Thesis Chair of Committee: Brent Rogaski (10/29/2010)
19. Ph.D. Proposal Committee member: Deepa Subramanian (2/1/2011 – Anisimov)
20. Ph.D. Proposal Committee member: Daphne Fuentevilla (12/15/2011 – Anisimov)
21. Ph.D. Defense Committee member: Paul Shriner (12/19/2011 – N. Wang)
22. M.S. Thesis Chair of Committee: Kunal Pandit (12/20/2010)
23. Ph.D. Proposal Committee member: Curtisha Travis (1/24/2012 – Adomaitis)
24. Ph.D. Proposal Committee chair: Pushkar Pendse (3/13/2012)
25. Ph.D. Proposal Committee chain: Brent Rogaski (4/2012)
26. Ph.D. Defense Committee member: Deepa Subramanian (5/8/2012 – Anisimov)
27. M.S. Thesis Committee Member: Stephen Banik (8/3/2012 – Raghavan)
28. Ph.D. Defense Committee member: Daphne Fuentevilla (11/12/2012 – Anisimov)
29. Ph.D. Defense Chair of Committte: Pushkar Pendse (4/14/2013)
30. Ph.D. Proposal Committee member: Annie Lu (6/3/2013 – Raghavan)
31. M.S. Thesis Committee member: Kevin Diehn (1/21/2014 – Raghavan)
32. Ph.D. Defense Committee member: Szu-Ting Chou (2/3/2014 – Mixon)
33. M.S. Thesis Chair of Committee: Viviana Monje-Galvan (11/14/2014)
34. Ph.D. Defence Committee member: Annie Lu (5/18/2015 – Raghavan)
35. Ph.D. Proposal Committee Chair: Xiaohong Zhang (5/12/2015 - Klauda)
36. Ph.D. Dissertation Committee member: Annie Lu (5/18/2015 - Raghavan)
37. Ph.D. Dissertation Committee member: David Arana-Chavez (6/15/2015 - Adomaitis)
38. Ph.D. Proposal Committee Chair: Pouyan Khakbaz (6/22/2015 - Klauda)
39. M.S. Thesis Committee member (Biophysics): Brian Stock (7/31/2015 - Seog)
40. Ph.D. Proposal Committee member: Navadeep Boruah (8/27/2015 - Sriram)
41. M.S. Thesis Committee member: Nairui Zhou (12/3/2015 – Sriram)
42. Ph.D. Proposal Committee member: Svet Ikonomova (12/16/2015 – Karlsson)
43. Ph.D. Proposal Committee Chair: Viviana Monje-Galvan (1/14/2016 – Klauda)
44. Ph.D. Proposal Committee member: Zifan Gong (6/27/2016 – Karlsson)
45. Ph.D. Proposal Committee member: Abdollah Koolivand (11/10/2016 – Dimitrakopoulos)
46. Ph.D. Defense Committee Chair: Xiaohong Zhang (12/7/2016 - Klauda)
47. Ph.D. Defense Committee Chair: Viviana Monje-Galvan (3/23/2017 - Klauda)
48. M.S. Thesis Committee member: YiYang Wang (3/31/2017 – Dimitrakopoulos)
49. M.S. Thesis Committee member: Alan Uy (4/20/2017 – Adomaitis)
50. M.S. Thesis Committee member: Pompon Udipabu (5/30/2017 – Dimitrakopoulos)
51. Ph.D. Proposal Committee member: Sean Mack (6/14/2017 – Dwyer)

52. Ph.D. Defense Committee member: Zifan Gong (6/15/2017 – Karlsson)
53. Ph.D. Defense Committee member: Svet Ikonomova (7/15/2017 – Karlsson)
54. M.S. Thesis Committee member: Sayanee Adhikari (7/27/2017 – Karlsson)
55. M.S. Thesis Committee member: Ben Minnick (7/31/2017 – Calabrese)
56. Ph.D. Defense Committee member, Dean Rep (Biophysics): Yonathan Cwik (8/17/2017 – Thirmalai)
57. M.S. Thesis Committee member: James Liu (11/1/2017 – Raghavan)
58. Ph.D. Proposal Committee Chair: Nick Guros (12/1/2017 – Klauda)
59. Ph.D. Defense Committee Chair: Pouyan Khakbaz (12/13/2018 – Klauda)
60. Ph.D. Proposal Committee member: Najlaa Hassan (3/1/2018 – Al-Sheikhly)
61. Ph.D. Defense Committee member: Abdollah Koolivand (4/12/2018 – Dimitrakopoulos)
62. Ph.D. Proposal Committee member: Jung Kim (4/17/2018 – Calabrese)
63. Ph.D. Proposal Committee member: Qin Ni (6/1/2018 – Klauda/Papoian)
64. M.S. Defense Committee member: Thomas Deskins (7/13/2018 – Dimitrakopoulos)
65. Ph.D. Defense Committee member, Dean Rep (Biophysics): Hongcheng Xu (7/17/2019 – Matysiak)
66. Ph.D. Defense Committee member: Navadeep Boruah (9/10/2018 – Sriram)
67. Ph.D. Proposal Committee member: Niti Agrawal (12/13/2018 – Raghavan)
68. Ph.D. Defense Committee member: Najlaa Hassan (1/17/2019 – Al-Sheikhly)
69. Ph.D. Proposal Committee member: Sayanee Adikari (4/15/2019 – Karlsson)
70. Ph.D. Defense Committee member, Dean Rep (Biophysics): Guang Shi (5/17/2019 – Thirmalai)
71. Ph.D. Defense Committee Chair: Alison Leonard (6/18/2019 – Klauda/Biophys)
72. Ph.D. Defense Committee Chair: Nick Guros (6/26/2019 – Klauda)
73. M.S. Defense Committee Chair: Tyler Cline (7/10/2019 – Klauda)
74. Ph.D. Proposal Committee member: Salimeh Gharazi (8/8/2019 – Al-Sheikhly)
75. Ph.D. Proposal Committee member: Dan Lugar (8/15/2019 – Sriram)
76. Ph.D. Defense Committee member: Niti Agrawal (12/12/2019 – Raghavan)
77. Ph.D. Defense Committee member: Sean Mack (4/15/2020 – Dwyer)
78. Ph.D. Defense Committee member: Sayanee Adikari (5/28/2020 – Karlsson)
79. Ph.D. Proposal Committee Chair (Biophysics): Yalun Yu (11/30/2020)
80. Ph.D. Proposal Committee member (Biophysics): Abhilash Sahoo (1/6/2021 – Matysiak)
81. Ph.D. Proposal Committee Chair: Mahdi Ghorbani (2/1/2021)
82. M.S. Defense Committee member: Nathan Wong (4/16/2021 – Woehl)
83. Ph.D. Defense Committee Member: Dan Lugar (6/28/2021 – Sriram)
84. M.S. Defense Committee Member: Marzyeh Kheradmand-Hajibashi (7/13/2021 – Karlsson)
85. Ph.D. Proposal Committee member (Biophysics): Zachary Smith (9/20/2021 – Tiwary)
86. Ph.D. Proposal Committee member: Dinara Konakbayeva (1/24/2022 – Karlsson)
87. Ph.D. Proposal Committee Member: Makambi Wright (5/24/2022 – Karlsson)
88. Ph.D. Defense Committee Member (Deans Rep/Biophysics): Abhilash Sahoo (6/16/2022 – Matysiak)
89. Ph.D. Defense Committee Member (Deans Rep/Chemistry): Ryan Dykstra (7/8/2022

– Gutierrez)
90. Ph.D. Proposal Committee member (Biophysics): Madolyn Britt (7/13/2022 – Sukharev)
91. Ph.D. Defense Committee Member (Deans Rep/Chemical Physics): Pei-Yin Lee (10/7/2022 – Matysiak)
92. Ph.D. Defense Committee Member (Deans Rep/Biophyscs): Haoran Ni (12/2/2022 – Papoian)
93. Ph.D. Proposal Committee member: Faraz Burni (12/15/2022 – Raghavan)
94. Ph.D. Proposal Committee member (Biophysics): Riya Smanta (12/16/2022 – Matysiak)
95. Ph.D. Defense Committee Member: Kanishk Gohil (12/19/2022 – Asa-Awuku)
96. Ph.D. Defense Committee Member (Chemistry): Robert Martin (3/6/2023 – Gutierrez)
97. Ph.D. Defense Committee Member (Chemical Physics): Thomas Longo (3/6/2023 – Anisimov)
98. Ph.D. Defense Committee Member (Biochemistry): Wes Pawloski (4/18/2023 – Fushman)
99. Ph.D. Defense Committee Member: Jung Kim (5/2/2023 – Calabrese)
100. Ph.D. Proposal Committee member (Biophysics): Dedi Wang (5/8/2023 – Tiwary)
101. Ph.D. Defense Committee Member (Biophysics): Zachary Smith (5/19/2023 – Anisimov)
102. Ph.D. Proposal Committee member: Pompon Mputu Udipabu (6/12/2023 – Dimitrakopoulos)
103. Ph.D. Proposal Committee Chair (Biophysics): Jiyeon Min (12/12/2023 – Klauda)
104. Ph.D. Defense Committee Chair: Robert Allsopp (12/14/2023 – Klauda)
105. Ph.D. Proposal Committee member: Nahin Ferdousi-Rokib (2/21/2024 – Asa-Awuku)
106. Ph.D. Defense Committee Member: Wright Makambi (3/14/2024 – Karlsson)
107. Ph.D. Committee member (Biophysics): Madolyn Britt (3/25/2024 – Sukarev)
108. Ph.D. Committee member (Biophysics): Riya Smanta (4/1/2024 – Matysiak)
109. Ph.D. Committee member (Biophysics): Dedi Wang (4/4/2024 – Tiwary)
110. Ph.D. Defense Committee Member: Dinara Konakbayeva (4/11/2024 – Karlsson)
111. Ph.D. Proposal Committee member (Biophysics): Elissa Moller (4/30/2024 – Sukharev)
112. M.S. Scholar Paper (Chemical Physics): Yuanpeng Hou (5/13/2024 – Hill)
113. Ph.D. Proposal Committee member (Biophysics): Shams Mehdi (5/30/2024 – Tiwary)

IV.B.2 Campus Service – College

College committees are listed first in blue then thesis defenses.

1. APT Committee (July 2014-June 2017)
2. Engineering HPC Allocation Committee (June 2014-current)
3. **Engineering HPC Allocation Committee Chair (August 2015-current)**
4. **IPST (CHPH/BIPH Program Coordinator Search, Chair 2023)**

5. Ph.D. Proposal Committee member: Christina Kyrtsos (12/1/2009 – BioE)
6. Ph.D. Proposal Committee member: Mohammad Alizadeh (11/7/2012 – MechE)
7. Ph.D. Defense Committee member: Mohammad Alizadeh (7/21/2014 – MechE)
8. Ph.D. Dissertation Defense: Sai Ganesan (4/11/2016 – Matysiak)
9. Ph.D. Dissertation Defense member: Haiqing Zhao (3/30/2018 – Papoian/Biophys)
10. Ph.D. Dissertation Defense member: Greg Custer (4/6/2018 – Matysiak/BioE)
11. Ph.D. Dissertation Defense Deans Rep: Krystina Hess (7/25/2018 – Jewell/BioE)
12. Ph.D. Dissertation Defense Deans Rep: Hongcheng Xu (7/17/2018 – Matysiak/BioE)
13. Ph.D. Defense Committee Deans Rep: Teddy Baker (12/18/2019 – Weeks/ChemPhys)
14. Ph.D. Candidacy Committee member (CHPH): Thomos Longo (2/2/2021 – Anisimov)
15. Ph.D. Dissertation Defense, Deans Rep (CHEM): Mary Pitman (4/30/2021 – Papoian/CHEM)
16. Ph.D. Dissertation Defense, Deans Rep (CHEM): Sam Cohen (7/12/2021 – Fourkas)
17. Ph.D. Defense Committee Member, Deans Rep (CHPH): Sun Ting Tsai (5/5/2022 – Tiwary)

IV.B.3 Campus Service – University

1. Allocations and Advisory Committee (AAC) for DIT's High Performance Computational Cluster (2008-current)
2. Packard Fellow Review (2023)
3. **Chair of AAC (Fall 2017-current)**
4. **Chair of IT Council (F2022-current)**
5. **Graduate Council** (F2016-S2020, **F2023-current**)
6. Research Technology Work Governance Group of the UM IT Council (Senate associated work group, 2016-2021): advise IT on how to support campus-wide research computing
7. HPC Committee of Provost for financial sustainability (Su2021)
8. Chair of the Research Technology Work Governance Group (Fall 2019-S2021)
9. Member of the IT Council (Fall 2019-S2021, F2022-current)
10. Deepthought3 Evaluation Committee (2020, 2021)
11. Scientific Management Committee for MARCC a joint JHU/UMD resource (Spring 2018-2021)
12. Vice Chair of the Research Technology Work Governance Group (Fall 2016-Spring 2019)
13. High performance Computing Committee for DIT (2010-2015): Future directions for HPC at UMD
14. Academic Honor Council Boards (2013-2015): 1-2 per semester
15. Senator in the University Senate (5/2013-5/2016)
16. HPC Lecture Series Committee for OIT (2014): Help organize and setup speakers to this lecture series
17. RTWG Sub-committee on Supercomputing (Fall 2017-Spring 2018)
18. Graduate PCC Committee (Fall 2018-Spring 2019)
19. Enabling Research Work Group of the UM IT Council (Senate associated work group, 2014-2016): advise IT on how to support campus-wide research computing

IV.B.8 Leadership Roles in Meetings and Conferences

1. Co-Chair 2008 AIChE National Meeting Session titled “Thermodynamics and Transport in Lipid Bilayers”
2. Co-Chair 2009 AIChE National Meeting Session titled “Thermodynamics and Transport in Lipid Bilayers”
3. Chair 2010 AIChE National Meeting Session titled “Thermodynamics and Transport in Lipid Bilayers”
4. Co-Chair 2010 AIChE National Meeting Session titled “In Honor of Stanley Sandler's 70th Birthday II”
5. Chair 2011 AIChE National Meeting Session titled “Thermodynamics and Transport in Lipid Bilayers”
6. Co-Chair 2012 AIChE National Meeting Session titled “Model Development for Biomolecular Systems”
7. Chair 2013 AIChE National Meeting Session titled “Model Development for Biomolecular Systems”
8. Chair 2015 AIChE National Meeting Session titled “In Honor of Stanley Sandler II”

IV.F Community & Other Service

1. Review Panel for TOSHIBA/NSTA ExploraVision science competition for K-12 Students (2/2016)
2. Review Panel for TOSHIBA/NSTA ExploraVision science competition for K-12 Students (2/2017)