Jeffery B. Klauda

Department of Chemical and Biomolecular Engineering
University of Maryland
4418 Stadium Dr.
College Park, MD 20742
301-405-1320
jbklauda@umd.edu
www.terpconnect.umd.edu/~jbklauda

EDUCATION

University of Delaware, Newark, DE
Ph.D. in Chemical Engineering **2003**
Dissertation: "From ab initio Intermolecular Potentials to Predictions of Macroscopic Thermodynamic Properties and the Global Distribution of Gas Hydrates"
Advisor: Stanley I. Sandler (National Academy of Engineering)

Rensselaer Polytechnic Institute, Troy, NY
B.S. in Chemical Engineering and B.S. in Applied Mathematics **1998**
Magna Cum Laude

AWARDS

NSF CAREER Award **2012 – 2017**
Minta Martin Award, University of Maryland **2008 – 2010**
IRTA Postdoctoral Fellow, National Institutes of Health **2003 – 2007**
Pigford Fellowship, University of Delaware **1998 – 1999**

POSITIONS

University of Maryland, College Park, MD
Associate Chair and Graduate Program Director **July 2015-Present**
Associate Professor – Chemical and Biomolecular Engineering **2014-Present**
Assistant Professor – Chemical and Biomolecular Engineering **2007 – 2014**
Biophysics Program
Affiliate of the University of Maryland Energy Research Center (UMERC)

National Institutes of Health, Bethesda, MD
IRTA Postdoctoral Fellow – NHLBI **2003 – 2007**
Advisor: Bernard R. Brooks
Co-Advisor: Richard W. Pastor

TEACHING AND ADVISING EXPERIENCE

University of Maryland, College Park, MD
ENCH 468/648G (Statistics and Experimental Design: Spring 2008-12) **2007 – Present**
ENCH 610 (Graduate Thermodynamics: Fall 2008, 2010)
ENCH 468P/648P (Molecular Modeling Methods: Fall 2009)
ENCH 400 (Undergraduate Thermodynamics: Fall 2011)
CHBE 410 (Statistics and Experimental Design: Fall 2012-2016)
ENCH 609 (Graduate Seminar: Fall 2012-2014)
CHBE 302 (Chemical Engineering Thermodynamics: Spring 2013, 2016, 2017)

CHBE476/ENCH648P ((Molecular Modeling Methods: Spring 2014 and 2015)

Research advisor for 8 graduate students, research scholar, 40 undergraduates, and 4 high school students.

National Institutes of Health, Bethesda, MD
IRTA Postdoctoral Fellow – NHLBI **2005 – 2007**
Advised an intern to develop a web interface for CHARMM and run molecular dynamics simulations of the Osh4 sterol binding protein

University of Melbourne, Melbourne, Australia
Visiting Scientist **2003**
Developed a senior project for studying sequestering CO_2 on the seafloor.

PUBLICATIONS (**h-index = 27**)

1. Klauda, J. B. & S.I. Sandler. A Fugacity Model for Gas Hydrate Phase Equilibria. *Ind. Eng. Chem. Res.* **39**, 3377-3386 (2000).
2. Klauda, J. B. & S.I. Sandler. Modeling Gas Hydrate Phase Equilibria in Laboratory and Natural Porous Media. *Ind. Eng. Chem. Res.* **40**, 4197-4208 (2001).
3. Klauda, J. B. & S.I. Sandler. Ab Initio Intermolecular Potentials for Gas Hydrates and Their Predictions. *J. Phys. Chem. B.* **106**, 5722-5732 (2002).
4. Klauda, J. B. & S.I. Sandler. Phase Behavior of Clathrate Hydrates: A Model for Single and Multiple Gas Component Hydrates. *Chem. Eng. Sci.* **58**, 27-41 (2003).
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). **Cover Article**
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).
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. *J. Phys. Chem. A*. **108**, 107-112 (2004).
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. *J. Phys. Chem. B.* **108**, 9842-9851 (2004).
9. Jiang, J., J.B. Klauda, & S.I. Sandler. Hierarchical Modeling Gas Adsorption in the C_{168} Schwarzite: From Quantum Mechanics to Molecular Simulation. *J. Phys. Chem. B.* **108**, 9852-9860 (2004).
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. *J. Phys. Chem. B.* **109**, 17267-17273 (2005).
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. *J. Phys. Chem. B.* **109**, 4731-4737 (2005).
12. Klauda, J. B. & S.I. Sandler. Global Distribution of Methane Hydrate in Ocean Sediment. *Energy & Fuels.* **19**, 469-470 (2005).
13. Klauda, J.B., R.W. Pastor, & B.R. Brooks. Adjacent Gauche Stabilization in Linear Alkanes: Implications for Lipid/Polymer Models. *J. Phys. Chem. B.* **109**, 15684-15686 (2005).
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. *J. Phys. Chem. B.* **109**, 5300-5311 (2005).
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. *Biophys. J.* **90**, 2796-2807 (2006).
16. Klauda, J.B., B.R. Brooks, & R.W. Pastor. Dynamical Motions of Lipids and a Finite Size Effect in Simulations of Bilayers. *J. Chem. Phys.* **125**, 144710 (2006).

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. *J. Phys. Chem. B.* **111**, 4393-43400 (2007).
18. Klauda, J.B. & B.R. Brooks. Sugar Binding in Lactose Permease: Anomeric State of a Disaccharide Influences Binding Structure. *J Mol. Biol.* **367**, 1523-1534 (2007).
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. *J. Phys. Chem. B.* **112**, 5924-5929 (2008).
20. Klauda, J.B. & B.R. Brooks. CHARMM Force Field Parameters for Nitroalkanes and Nitroarenes. *J. Chem. Theory Comp.* **4**, 107-115 (2008).
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. *Biophys. J*. **94**, 3074-3083 (2008).
22. 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).
23. 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. *J. Chem. Info. Mod.* **48**, 1920-1929 (2008).
24. 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).
25. Jo, S.H., J.B. Lim, J.B. Klauda, & W. Im. CHARMM-GUI Membrane Builder for Mixed Bilayers and Its Application to Yeast Membranes. *Biophys. J.* **97**, 50-58 (2009).
26. 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. *J. Phys. Chem. B*. **114**, 7830-7843 (2010).
27. Jo, S.H., H. Rui, J.B. Lim, J.B. Klauda, & W. Im. Cholesterol Flip-Flop: Insights from Free Energy Simulation Studies. *J. Phys. Chem. B.* **114**, 13342-13348 (2010).
28. Rogaski, B., J.B. Lim, & J.B. Klauda. Sterol binding and membrane lipid attachment to the Osh4 protein of yeast. *J. Phys. Chem. B.* **114**, 13562-13573 (2010).
29. 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. *J. Mol. Bio.* **404**, 506-521 (2010). **Cover Article**
30. 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. *I&EC Research*. **50**, 148-157 (2011).
31. Lim, J.B. & J.B. Klauda. Branching at the Iso- and Anteiso- Positions in Complex Chlamydia Membranes: A Molecular Dynamics Study. *BBA-Membranes*. **1808**, 323-331 (2011).
32. 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. *J. Phys. Chem. B*. **115**, 6157-6165 (2011).
33. O'Connor, J.W. and J.B. Klauda. Lipid Membranes with a Majority of Cholesterol: Applications to the Ocular Lens and Aquaporin 0. *J. Phys. Chem. B.* **115**, 6455-5464 (2011).
34. Lim, J.B., B. Rogaski & J.B. Klauda. Update of the Cholesterol Force Field Parameters in CHARMM. *J. Phys. Chem. B.* **116**, 203-210 (2012).
35. Pandit, K.R. & J.B. Klauda. Membrane models of E. coli containing cyclic moieties in the aliphatic lipid chain. *Biophys. J*. **1818**, 1205-1210 (2012).
36. 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. *Biophys. J*. **102**, 1341-1351 (2012). **Cover Article**
37. Ezzeldin, H.M., J.B. Klauda, & S.D. Solares. Modeling of the Major Gas Vesicle Protein, GvpA: from Protein Sequence to Vesicle Wall Structure. *J. Struct. Biol*. **179**, 18-28 (2012).
38. Klauda, J.B., V. Monje, T. Kim, and W. Im. Improving the CHARMM Force Field for Polyunsaturated Fatty Acid Chains. *J. Phys. Chem. B*. **116**, 9424-9431 (2012). **Cover Article**
39. Rogaski, B. and J.B. Klauda. Membrane-binding Mechanism of a Peripheral Membrane Protein through Microsecond Molecular Dynamics Simulations. *J. Mol. Bio*. **423**, 847-861 (2012).
40. Subramanian, D., J.B. Klauda, J. Leys, and M.A. Anisimov. Thermodynamic Anomalies and Structural Fluctuations in Aqueous Solutions of Tertiary Butyl Alcohol. *Herald of St. Petersburg University (Вестник*

СПбГУ). **4**, 140-153 (2013)

41. Cheng, X., S.H. Jo, J.B. Klauda, and W. Im. CHARMM-GUI Micelle Builder for Pure/Mixed Micelle and Protein/Micelle Complex Systems. *J. Chemical Information and Modeling*. **53**, 2171-2180 (2013).
42. 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. *Biophys. J.* **105**, 1444-1455 (2013).
43. Villanueva, D.Y., J.B. Lim, & J.B. Klauda. Influence of Ester-modified Lipids on Bilayer Structure. Langmuir. **29**, 14196-14203 (2013).
44. 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).
45. Lee, S., A. Tran, M. Allsopp, J.B. Lim, J. Hénin, & J.B. Klauda. CHARMM36 United-Atom Chain Model for Lipids and Surfactants. *J. Phys. Chem. B.* **118**: 547-556 (2014).
46. 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. *J. of Comp. Chem*. **35**: 957-963 (2014).
47. 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. *Biophys. J.* **106**: 2493–2502 (2014). **Cover Article**
48. 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. *J. Phys. Chem. B*. **118**: 4315-4325 (2014).
49. Subramanian, D. J.B. Klauda, and M.A. Anisimov. Mesoscale Phenomena in Ternary Solutions of Tertiary Butyl Alcohol, Water, and Propylene Oxide. *J. Phys. Chem. B*. **118**: 5994-6006 (2014).
50. Zhuang, X., J.R. Makover, W. Im, & J.B. Klauda. A Systematic Molecular Dynamics Simulation Study of Temperature Dependent Bilayer Structural Properties. *BBA-Biomemb*. **1838**: 2520-2529 (2014).
51. 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. *Biophys. J*. **107**: 134-145 (2014).
52. 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. *J. of Comp. Chem*. **35**: 1997-2004 (2014).
53. 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. *Biophys. J.* **107**: 1885-1895 (2014).
54. 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).
55. Kang, H & J.B. Klauda. Molecular Dynamics Simulations of Palmitoyloleoyl-phosphatidylglycerol Bilayers. *Molecular Simulation*. **41**: 948-954 (2015).
56. Park, S., A.H. Beaven, J.B. Klauda and W. Im. How Tolerant are Membrane Simulations with Mimatch in Area per Lipid between Leaflets? J. Chem. Theor. Comp. **11**: 3466-3477 (2015).
57. Khakbaz, P. and J.B. Klauda. Probing the Importance of Lipid Diversity in Cell Membranes via Molecular Simulation. *Chem. Phys. Lipids*. **192**: 12-22 (2015). **Invited**
58. 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. *J. Phys. Chem. B*. **119**: 13134-13141 (2015).
59. 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. *Biophys. J.* **109**: 2012-2022 (2015).
60. Monje-Galvan, V. and J.B. Klauda. Modeling Yeast Organelle Membranes and How Lipid Diversity Influences Bilayer Properties. *Biochem.* **54**: 6852-6861 (2015).
61. 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. *Biophys. J.* **109**: 2090-2100 (2015).
62. 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. *J. Chem. Phys.* **143**, 243144 (2015).

63. 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. *J. Chem. Theor. Comp.* **12**, 405-413 (2016).
64. Choudhary, R. and J.B. Klauda. The Simultaneous Mass and Energy Evaporation (SM2E) Model. *J. of Occupational & Environmental Hygiene*. **13**, 247-257 (2016).
65. Monje-Galvan, V. and J.B. Klauda. Peripheral Membrane Proteins: Tying the Knot between Experiment and Computation. *BBA-Biomemb.* **1858**, 1584-1593 (2016). **Invited**
66. Zhuang, X., and J.B. Klauda. Modeling Structural Transitions from the Periplasmic-open State of Lactose Permease and Interpretations of Spin Label Experiments. *BBA-Biomemb.* **1858**, 1541-1552 (2016).
67. 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. *Biophys. J.* **111**, 1750-1760 (2016).
68. 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. *Biochem*. **55**, 4928-4938 (2016).
69. 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. *J. Phys. Chem. C*. **120**, 23692-23697 (2016).
70. 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. *BBA-Biomemb*. **1858**, 3093-3104 (2016).
71. Qi, Y., J.B. Klauda and W. Im. Effects of Spin-labels on Membrane Burial Depth of MARCKS-ED Residues. *Biophys. J.* **111**, 1600-1603 (2016).
72. 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. *Biophys. J.* **111**, 1987-1999 (2016).
73. Boughter, C.T., V. Monje-Galvan, W. Im and J.B. Klauda. Influence of Cholesterol on Phospholipid Bilayer Structure and Dynamics. *J. Phys. Chem. B.* **120**, 11761-11772 (2016).
74. 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).
75. 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. *J. Chem. Theor. Comp.* **38**, 1114-1124 (2017).
76. Bera, I. and J.B. Klauda. Molecular Simulations of Mixed Lipid Bilayers with Sphingomyelin, Glycerophospholipids and Cholesterol. *J. Phys. Chem. B.* **121**, 5197-5208 (2017).
77. Wang, E. and J.B. Klauda. An Examination of Mixtures Containing Sphingomyelin and Cholesterol by Molecular Dynamics Simulations. *J. Phys. Chem. B.* **121**, 4833-4844 (2017).
78. Zhuang, X, A. Ou, and J.B. Klauda. Simulations of simple Linoleic acid-containing Lipid Membranes and Models for the Soybean Plasma Membranes. *J. Chem. Phys.* **Accepted**. (2017).

INVITED SEMINARS/TALKS

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).
8. “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).
9. “Structure and Dynamics of Lipids, Model Cellular Membranes, and Membrane Proteins”, *University of Kansas*, Center for Bioinformatics, Lawrence (2008).
10. “Understanding the Structure and Dynamics of Biomembranes and Their Components”, *National Taiwan University*, Department of Chemical Engineering, Taipei (2009)
11. “Predicting the Locations and Amounts of Seafloor Methane Hydrates”, *Central Geological Survey of Taiwan*, Taipei (2009).
12. “Gas Hydrates: A Significant but Relatively Untapped Alternate Source of Natural Gas”, *National Capitol Section of AIChE*, College Park, MD (2009).
13. “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).
14. “Multi-scale Modeling of Gas Hydrates Reserves in the Seafloor Sediment”, *Petroleum Institute*, Department of Chemical Engineering, Abu Dhabi, UAE (2011).
15. “Molecular Modeling of Cellular Membranes and Associated Proteins”, *University of Maryland*, Special Joint ChBE/Chemistry & Biochemistry Seminar (2011).
16. “Molecular simulations of certain model human membranes and secondary active transport proteins”, *National Institutes of Health*, NHLBI, Laboratory of Computational Biology (2011).
17. “Diversity of Lipids in Organisms and their Organelles: Is this Required to Accurately Model Real Membranes?”, *Biological Membranes and Membrane Proteins*, Snowmass, CO (2011).
18. “Modeling Bacterial Membrane Structure to Membrane Protein Dynamics at an Atomic Level”, *Univeristy of Virginia*, Department of Chemical Engineering (2011).
19. “All-atom Molecular Simulations to Probe Structure and Dynamics of Bacterial Membranes and Membrane-associated Proteins”. *NIST Center for Neutron Research* (2012).
20. “Simulation Studies on Biological Membranes with High Performance Computing” *Enabling Discovery with HPC*, Baltimore, MD (2012).
21. “Modeling Plasma Membranes and Proteins that Transport Small Molecules and Membrane Components”, *Georgia Institute of Technology*, Department of Chemical and Biomolecular Engineering (2013).
22. “Modeling Plasma Membranes and Proteins that Transport Small Molecules and Membrane Components”, *Temple University*, Institute for Computational Molecular Science (2013).
23. “E. coli Plasma Membrane Modeling and Membrane-associated Transport Proteins”, *University of Maryland*, Department of Bioengineering (2013).
24. “Modeling Lipid Bilayer and Microsecond Simulations of a Peripheral Membrane Protein”, *Biological Membranes and Membrane Proteins*, Snowmass, CO (2013).
25. “Force Field Development and Molecular Simulations of Model Lipid Membranes” *Satellite Meeting of ICMS2013*. Nagoya University, Japan (2013).
26. “Simulations of Biomembranes: Importance of Lipid Diversity and Structural Changes of Membrane Transport Proteins” *3rd International Conference on Molecular Simulation (ICMS)*. Kobe, Japan (2013).
27. “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).

28. "Molecular Simulations of Pore-forming Membranes and Membrane-associated Proteins" *Rensselaer Polytechnic Institute*, Department of Chemical and Biological Engineering (2014).
29. "Lipid Bilayer Simulations: Force fields, Simulation and Analysis" *Computational Modeling Workshop and Mini-Symposium*. University of Chicago (2014).
30. "Probing the Transport Cycle of Secondary Active Transporters with Atomistic Simulations" *Computational Modeling Workshop and Mini-Symposium*. University of Chicago (2014).
31. "Lipid Force Fields: Current Approaches to Force Field Development and their Accuracy" *2nd Molecular Simulations Summer School*. University of Calgary (2014).
32. "Simulations of Cell Membranes: Developing Accurate Lipid Force Fields and Probing Conformational Changes in Membrane Transporters" *University of Maryland*, Biophysics Program (2014).
33. "Probing Small Molecule Self-assembly, Lipid Membranes and Membrane-associated Proteins" *Lehigh University*, Department of Chemical and Biomolecular Engineering (2014).
34. "Molecular Modeling of Biomolecules: How can GPUs Advance Research?" *GPU Summit*, University of Maryland, Institute for Advanced Computing (2014).
35. "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).
36. "Binding of a Curvature-sensing Peptide to Model Organelle Membranes of Yeast", *Biological Membranes and Membrane Proteins*, Telluride, CO (2015)
37. "Molecular Simulations of Hydrotropes, Lipid Membranes and a Peripheral Membrane Protein" *West Virginia University*, Morgantown, WV (2015).
38. "Developing Quantum Mechanically-based Force Field Parameters from Gas Hydrates to Biology", *AIChE Annual Meeting,* Prof. Sandler Symposium (2015).
39. "Modeling Yeast Organelle Membranes and a Curvature Sensing Peptide." *4th International Conference on Molecular Simulation (ICMS)*. Shanghai, China (2016).
40. "The Influence of Alcohols on the Oil/Water Interface and Cell Membrane." *National Taiwan University,* Department of Chemical Engineering (2016).
41. "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).
42. "Improving the Tolerance of Organisms to Biofuels and Intracellular Transport of Lipids." *North Carolina State University*, Department of Chemical Engineering, Raleigh, NC (2017).

MENTORED PRESENTATIONS

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." *Biophsyical Society* (2011).
17. Rogaski, B. & J.B. Klauda. "Phosphoplipid Binding and Membrane Attachment of the Osh4 Protein." *Biophsyical Society* (2011).
18. Pandit, K & J.B. Klauda. "In Silico Model Escherichia Coli Membranes: Simulating a Lipid with a Cyclopropane Ring." *Biophsyical Society* (2011).
19. Pendse, P.Y & J.B. Klauda. "Mechanistic and Thermodyanmic Insights into the Transport Cycle of Lactose Permease." *Biophsyical 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)

PRESENTATIONS

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).
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. Klauda, J.B. “Lipid Diversity: Is It Important in Modeling Organism and Organelle Membranes?” *AIChE Annual Meeting* (2012).
33. Klauda, J.B. “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[o], & **J.B. Klauda**. "PSimulations of Linoleoyl-containing Pure Lipid Bilayer and Soybean Plasma Membranes." *Biophysical Society* (2017).

AWARDED COMPUTATIONAL ALLOCATIONS

1. TeraGrid (Startup Allocation): "Computational Studies on Membranes and Associated Proteins" Awarded 50,000 SU (1/2010-12/2010).
2. Anton (NRBSC special call for all-atom simulations): "Simulations of a Sterol Transport Protein (Osh4) that Tethers Membranes of the Endoplasmic Reticulum and Plasma Membrane" Awarded. 25,000 CPU hours (4/1/2011~9/30/2011).
3. TeraGrid (TRAC Allocation): "Molecular Simulations of Transmembrane and Membrane-associated Proteins". Awarded 1,074,000 SU (10/1/2010-9/30/2011) on Kraken Cray XT5.
4. XSEDE: "Molecular Simulations of Transmembrane and Membrane-associated Proteins". Awarded 450,154 SU (10/1/2011-9/30/2012).
5. "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).
6. "Molecular Simulations of Transmembrane and Membrane-associated Proteins" XSEDE Grant Number: TG-MCB100139 SU: 994,807 node hours (10/1/2012-9/30/2013).
7. "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).
8. "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).
9. "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).
10. "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).
11. "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.
12. "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).
13. "Molecular Simulations of Transmembrane and Membrane-associated Proteins" XSEDE Grant Number: TG-MCB100139 SU: 4,068,000 node hours (10/1/2015-9/30/2016). *Value of awarded resources:* $184,040.

14. Ligand Effects on the Biological Function of the Serotonin Receptor in model Raft-forming Membraness" **Anton2** hosted by the National Resource for Biomedical Supercomputing (NRBSC) at the Pittsburgh Supercomputing Center (PSC). Grant Number: PSCA16007P. SU: 460,000 Anton node hours. (12/1/2016-11/30/2017).

RESEARCH FUNDING

1. NSF CAREER (BIO/MCB): "Secondary Active Membrane Transporters: Determining Protein Structure and Transport Mechanisms with a New Hybrid Simulation" (PI, 8/1/2012-7/31/2018, $668,313)
2. NSF (BIO/DBI): "Development and Application of Graphical User Interfaces for System Building and Analysis of Membrane Simulations" (co-PI, 6/1/2012-5/31/2015, $125,081).
3. NIST: "Sensing Biological & Non-biological Polymers with a Nanopore" (PI, 2/1/2015-1/31/2018, $216,953).
4. NSF (ENGR/CBET): "Collaborative Research: Mechanism for Cell Membrane Damage during Production of Biorenewable Fuels" (PI, 9/1/2016-8/31/2019, collaborative with Dr. Laura Jarboe at Iowa State University, $200,000).

MEMBERSHIPS

American Chemical Society, American Institute of Chemical Engineers, and Biophysical Society

REFEREE

Journals: AIChE Journal, BBA-Biomembranes, Biochemistry, Biophysical Journal, Chemical Physics Letters, Energies, Fluid Phase Equilibria, Geophysical Research Letters, Industrial & Engineering Chemistry Research, Journal of the American Chemical Society, Journal of Molecular Biology, Journal of Molecular Graphics and Modelling, Journal of Physical Chemistry (A/B/C), Journal of Physical Chemistry Letters, Journal of Computational Chemistry, Journal of Chemical Physics, Journal of Chemical Information and Modeling, Langmuir, Molecular Simulation, Polymers, PLoS One.

Grants: NIH, NSF, ACS Petroleum Research Fund, Qatar National Research Fund

PROFESSIONAL SERVICE

1. Chair/Co-Chair of Session: Thermodynamics and Transport in Lipid Bilayers, **AIChE National Meeting** (2008-2011)
2. Chair/Co-Chair of Session: Model Development for Biomolecular Systems, **AIChE National Meeting** (2012-2013)
3. M.S. Thesis Committees: 9
4. Ph.D. Dissertation Committees: 23

COMPUTER EXPERIENCE

UNIX, LINUX, Windows, C, FORTRAN, AMBER, GAUSSIAN 98/03, GROMACS, CHARMM, MATLAB, NAMD, National Computing Centers, and Superuser of LINUX Cluster