Jeffery B. Klauda

Department of Chemical and Biomolecular Engineering
University of Maryland
College Park, MD 20742
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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

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
Assistant Professor – Chemical and Biomolecular Engineering **2007 – Present**
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
Assistant Professor – Chemical and Biomolecular Engineering **2007 – Present**
ENCH 468/648G (Statistics and Experimental Design: Spring 2008-11)
ENCH 610 (Graduate Thermodynamics: Fall 2008, 2010)
ENCH 468P/648P (Molecular Modeling Methods: Fall 2009)
ENCH 400 (Undergraduate Thermodynamics: Fall 2011)
Research advisor for three graduate students, research scholar, 13 undergraduates, and one high school student.

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 = 18**)

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. *JMB.* **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.* **Accepted** (2011).
35. Pandit, K.R. & J.B. Klauda. Membrane models of E. coli containing cyclic moieties in the aliphatic lipid chain. *Biophys. J*. **Accepted**. (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*. **Submitted** (2011).
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*. **Submitted** (2011).

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).

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).

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).

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).

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, Geophysical Research Letters, Industrial & Engineering Chemistry Research, Journal of Molecular Biology, Journal of Molecular Graphics and Modelling, Journal of Physical Chemistry, Journal of Physical Chemistry Letters, Journal of Computational Chemistry, Journal of Chemical Physics, Langmuir, Molecular Simulation, Polymers.

Grants: 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** (2008-2010)
2. M.S. Thesis Committees: 5
3. Ph.D. Dissertation Committees: 4

COMPUTER EXPERIENCE

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