

# Jeffery B. Klauda

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

## Current Position

Assistant Professor at the University of Maryland

## Education

1998–2003 University of Delaware Newark, DE  
Ph.D., Chemical Engineering, June 2003

1994–1998 Rensselaer Polytechnic Institute Troy, NY  
B.S. Degrees, Chemical Engineering and Applied Mathematics  
Graduated Magna Cum Laude: 3.72/4.00

## Research Experience

2007–Current University of Maryland College Park, MD

### Assistant Professor

Structural changes of the membrane protein lactose permease of *E. coli*.  
Cholesterol transport between cellular membranes with *Osh4* protein  
Gas hydrate stability in sediment, methods of extraction, and molecular hydrogen storage

2003–2007 National Institute of Health Bethesda, MD  
**NIH IRTA Postdoctoral Fellow** *Advisor: Dr. Bernard Brooks*

MD evaluation of the substrate transport mechanism for the membrane protein lactose permease of *E. coli*.

Aid experimentalists with MD simulations on lipid structure and dynamics  
Improvement of lipid force field parameters from quantum mechanical studies  
Molecular simulations of  $\beta$ -hairpin peptide folding and misfolding to study precursors to amyloid formation

1998–2003 University of Delaware Newark, DE

**Ph.D. Thesis** (*Advisor: Prof. Stanley I. Sandler, National Academy of Engineering*):  
From *ab initio* Intermolecular Potentials to Predictions of Macroscopic Thermodynamic Properties and the Global Distribution of Gas Hydrates

*Ab initio* intermolecular potentials for absorbents in gas hydrates and nanoporous carbons used in MC/MD simulation

Developed a model to accurately predict hydrate equilibrium pressures in the bulk and porous media

Estimated regional and global amounts of CH<sub>4</sub> hydrates in ocean sediment

## Teaching Experience

2007–Current University of Maryland College Park, MD

Instructor: ENCH 468/648G (Stat. and Experimental Design, Spring 2008–9)

Instructor: ENCH 610 (Graduate Thermodynamics, Fall 2008)

Instructor: ENCH 468P/648P (Molecular Modeling Methods, Fall 2009)

Research advisor for two graduate students, research scholar, and four undergraduates

2005–2007 National Institutes of Health Bethesda, MD

Advised an intern to develop a web interface for CHARMM and run molecular dynamics simulations of the *Osh4* sterol binding protein

2003 University of Melbourne Melbourne, Australia  
Developed a senior project for studying sequestering CO<sub>2</sub> on the seafloor

2000-2002 University of Delaware Newark, DE  
**T.A. Graduate and Undergraduate Thermodynamics (3 semesters)**  
Graded homework, papers, computer projects, and exams  
Lectured, prepared exam problems, and developed course webpages

#### Work Experience

1995-1998 (Summers) Stiefel Laboratories, Inc. Oak Hill, NY  
**Assistant Engineer-Pharmaceuticals**  
Added to existing batch monitoring program to monitor an additional machine  
Prepared eight equipment qualification protocols for future FDA approval  
Process validation and control (manufacturing, packaging, and cleaning)

#### Referee

Biophysical Journal, Journal of Molecular Biology, BBA-Biomembranes, Journal of Physical Chemistry, AIChE Journal, Langmuir, Journal of Computational Chemistry, Journal of Chemical Physics, Molecular Simulation. **Grants:** NSF and ACS-PRF

#### Computer Experience

UNIX, LINUX, Windows, C, FORTRAN, GAUSSIAN 98, CHARMM, MATLAB, National Computing Centers, and Superuser of LINUX Cluster

#### Awards

RPI Medal and Deans List, National Deans List, Pigford Fellowship, NIH IRTA Fellow, Minta Martin Award (2008)

#### Society Memberships

ACS, AIChE, and Biophysical Society

#### Invited Talks/Seminars

2003-Current

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-Carbohydrate 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).

## Presentations

### 2001-Current

1. "Predictions of Gas Hydrate Phase Equilibria in Laboratory and Natural Sediment Porous Media" AIChE Annual Meeting (2001).
2. "Intermolecular Potentials for Gas-Hydrates Obtained from *Ab Initio* Quantum Mechanics" ACS National Fall Meeting (2002).
3. "Phase Behavior of Clathrate Hydrates: A Model for Single and Multiple Gas Component Hydrates" AIChE Annual Meeting (2002).
4. "*Ab Initio* Intermolecular Potentials of Absorbents in Nanoporous Carbon Schwartzite Structures" AIChE Annual Meeting (2002).
5. "A Quantum Chemical Hybrid Method (HM-IE) for Calculating Interaction Energies Used to Develop Accurate Intermolecular Potentials" AIChE Annual Meeting (2003).
6. "A Self-guided Langevin Dynamic Study of  $\alpha$ -Hairpin Folding with Explicit Solvent: Computational Efficiency and Folding Pathways" AIChE Annual Meeting (2004).
7. "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. "Lipid Bilayers: Structural and Dynamical Properties with an Improved Forcefield Fit to *Ab Initio* Quantum Mechanics" Biophysical Society (2005).
9. "Refining the Structure of Lipid Bilayers with Insight from Molecular Dynamics Simulations" ACS National Fall Meeting (2005).
10. "Structure and Dynamics of Lipid Membranes: How can Simulations Aid Experiments?" AIChE Annual Meeting (2005).
11. "Importance of Including Long-range Interactions in Simulations of Biologically Relevant 2D Surfaces" AIChE Annual Meeting (2005).
12. "Lactose Permease-Sugar Interactions: The Anomeric State of a Disaccharide Determines its Binding Structure" Symposium of Protein

Society (2006).

13. "Disaccharide Binding in Lactose Permease of *E. coli*: Sugar Structure Influences Binding" AIChE Annual Meeting (2006).
14. "Dynamical Motions of Lipids and a Finite Size Effect of Bilayers" AIChE Annual Meeting (2006).
15. "Structural Changes in Lactose Permease and How Sugar-Type Effects Binding Structure" Biophysical Society (2007).
16. "Determining the Outward-Facing Structure and Sugar Binding in Lactose Permease of *E. coli*" AIChE Annual Meeting (2007).
17. "Long-range Lennard-Jones and Electrostatic Interactions in Interfaces: Application and Development of the Isotropic Periodic Sum Method" AIChE Annual Meeting (2007).
18. "Binding and Release of Cholesterol in the Osh4 Protein of Yeast" ACS National Fall Meeting (2008).
19. "Binding and Release of Cholesterol in the Osh4 Protein of Yeast" AIChE Annual Meeting (2008).
20. "An Atomic-level Model for the Periplasmic Open State of Lactose Permease" Biophysical Society (2009).
21. "Improving the lipid force field of CHARMM: A quantum mechanical and experimental approach" ACS National Fall Meeting (2009).

#### Mentored Presentations

2008-Current

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. & 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. & J.B. Klauda "Structural Changes and Quantification of Ligand Affinity in Lactose Permease of *Escherichia coli*." ACS National Fall Meeting (2009).

#### Publications

2000-Current

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<sub>2</sub> and N<sub>2</sub> Adsorption in Nanoporous Carbon (C<sub>168</sub> 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<sub>2</sub>(O<sub>2</sub>)-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<sub>168</sub> 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<sub>70</sub> 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<sub>2</sub> Adsorption on the Outer Surface of and within a C<sub>60</sub> 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, <sup>31</sup>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. Pendse, P.Y., B.R. Brooks & J.B. Klauda. Cytoplasmic and Periplasmic Conformational Changes of Lactose Permease. *Biophys. J.* **In Prep.** (2009).