JAMES T. KINDT

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PROFESSIONAL AND EDUCATIONAL BACKGROUND

9/2013 – present	**Professor, Department of Chemistry, Emory University**
9/2007 – 8/2013	**Associate professor**
9/2001- 8/2007	**Assistant professor**
Honors:	Camille Dreyfus Teacher-Scholar Award, 2006.
	Alfred P. Sloan Research Fellowship, 2005.
	Camille and Henry Dreyfus New Faculty Award, 2001.
9/1999 – 7/2001	**Post-doctoral fellow**
	Department of Chemistry and Biochemistry, UCLA
	Advisor: Professor William M. Gelbart
9/1994 – 8/1999	**Graduate student;** Ph.D. awarded December 1999
	Department of Chemistry, Yale University, New Haven, CT
	Advisor: Professor John C. Tully (9/1996-8/1999)
	Professor Charles A. Schmuttenmaer (1/1995-8/1996)
Honors:	Richard Wolfgang Prize for Academic Accomplishment, Yale Chemistry Department, 1999-2000
	NSF Graduate Fellowship (Fall 1994 - Spring 1997)
	Sterling Prize, Yale Graduate School (Fall 1994 - Spring 1995)
9/1990 – 5/1994	**Haverford College,** Haverford, PA
	B.A., *summa cum laude,* with High Honors in chemistry
	Barry M. Goldwater Scholarship (Fall 1992 – Spring 1994)

TEACHING

Fall 2013	*Chem 331, Physical Chemistry I*
Spring 2012, 2013	*Chem 332, Physical Chemistry II*
Spring 2010, 2011,2015	*Chem 142, General Chemistry II*
Fall 2005-07,2003,2002	*Chem 300, Physical Chemistry for the Life Sciences*
Spring 2007, Fall 2004	*Chem 435s/Chem 470s Molecular Simulation in Chemistry and Biology* (new course)
Spring 2003-05, 2008, 2014; Fall 2009, 2011,2015	*Chem 536, Statistical Mechanics and Simulation Methods*
Fall 2001, 2008, 2010, 2012, 2014	*Chem 533, Kinetics and Thermodynamics*
Summer 2014	*Chem 468* (co-taught seminar course in Siena program)

Current research supervision of 4 graduate students and 1 undergraduate student.

CURRENT RESEARCH SUPPORT

American Chemical Society – Petroleum Research Fund (8/2014-8/2016) $110,000 “Molecular simulation studies of clathrate hydrate phase nucleation”

National Science Foundation (CHE-1213904) (7/2012 - 6/2016) $402,998 “Simulation studies of permeability and melting behavior in gel-phase lipid bilayers.” (no-cost extension)

XSEDE computer network allocation (XS-MCB110144) (1/2015-12/2015) 256,000 CPU-hours, “Simulations of lipid bilayers: permeability, melting dynamics, and peptide folding.”

PENDING RESEARCH SUPPORT

National Science Foundation, Division of Chemistry, CTMC (7/2016-6/2019) $454,969, "New simulation approaches to thermodynamics and kinetics of aggregation in solution"

National Science Foundation, Division of Materials Research, CMMT (9/2016-8/2019) $263,696, "Packing of particles at surfaces and interfaces: new simulation approaches"

PAST RESEARCH SUPPORT

National Science Foundation (CHE-0911285) (7/2009 – 1/2013) $387,724 “Molecular simulations of mixed-lipid bilayers.”

XSEDE computer network allocation (XS-MCB110144) (9/2011-10/2012) 301,120 CPU-hours. “Simulation of edges and domain boundaries in lipid bilayers.”

Teragrid computer network start-up allocation (TG-MCB100166) (9/2010-9/2011), 200,000 CPU-hours. “Molecular simulations of mixed-lipid bilayers”

Camille Dreyfus Teacher-Scholar Award (6/2006 – 6/2011) $75,000.

National Science Foundation (CHE-0616383) (7/2006 – 6/2009) $395,661. “Simulation and theory of molecular and mesoscale structure in mixed bilayers and bicelles”

National Science Foundation (CHE-0316076) "Monte Carlo simulation of self-assembled polymers, domains, and disks", (7/2003-6/2006) $249,600.

Alfred P. Sloan Research Fellowship (9/2005-8/2007) $45,000.

ACS-PRF type G, "Monte Carlo simulations of lipid bicelles and monolayer domains." (9/2002-8/2004) $35,000.

Emory University Research Committee "Mechanics of DNA translocation in nucleosomes: Sliding with a twist?" (6/2002-5/2003) $30,000

Camille and Henry Dreyfus New Faculty Award (9/2001-8/2003) $40,000.

CURRENT GROUP MEMBERS

Lewen Yang, 5th year Ph.D. student
Lara Patel, 4th year Ph.D. student
Keon Reid, 3rd year Ph.D. student
Ziwei Guo, 2nd year Ph.D. student
Erdong Lu, Emory College Senior, Honors student

FORMER GROUP MEMBERS

Dr. Ana West, 2013 Ph.D. Postdoc, University of Minnesota.
Dr. Fuchang Yin, 2011 Ph.D. Software engineer, Athena Software.
Dr. Patrick Coppock, 2010 Ph.D. Assistant Professor, Georgia Gwinnett College
Dr. Xinjiang Lü, Ph.D. 2007 Ph.D. Software engineer, Vitrue
Dr. Yong (Frank) Jiang, Ph.D 2007. AIG Corporation
Dr. Hao Wang (postdoc), Boyalife Biotechnology
Dr. Jason de Joannis (postdoc), Senior Consultant, Accelrys, Inc.
(on-site consultant to Wyeth Pharmaceuticals)
Dr. Yann Bouret (postdoc), Chargé de recherche CNRS, Univ. de Nice Sophia-Antipolis
Dr. Shi-jin Zhao (postdoc), assistant professor, Shanghai University, Dept. Mater. Sci.
Dr. Birgit Albrecht, (visiting graduate student from Oxford University)
assistant professor at Loyola University, Baltimore
Albertha Sabree (summer SURE fellow, Agnes Scott College)
Makoto Mori, EC '11, Emory School of Medicine
Jasmine Peterson (summer SURE fellow), Valdosta State University '10
Kanwei Li, EC '08, Software Engineer
Jennifer Colucci, EC '08, Ph.D. program in Biochemistry at Emory
Erik Hoffman, EC '08
Kunal Khanna, EC '07, M.S. in Chemistry at McGill University
LaKedra Pam (honors thesis student, EC '06), Vanderbilt medical school
Jeffrey Gaulding (honors thesis student, EC '06), Ph.D. student at Georgia Tech
Larissa Spell Fenn (summer SURE fellow, Mercer University) Ph.D. student at Vanderbilt University
Ted T. Chang, (undergraduate research student, EC '04) University of Virginia medical school
Danielle McShan (summer SURE fellow, Talladega College) M.S. student at Jackson State U.

COLLABORATORS:

Professors Brian Dyer, Fredric Menger, Tim Lian, Khalid Salaita	(Emory University)
Professor Max Berkowitz	(University of North Carolina)
Professor Hailing Zhang	(Mercer University)
Professor Ka Yee Lee	(University of Chicago)
Professor Hiroaki Saito	(Kanazawa University, Japan)
Professor Absalom Zamorano	(IPN, Mexico City)

RECENT RESEARCH PRESENTATIONS

Invited talks:

"Phase behavior of equilibrium polymers and networks by Monte Carlo simulation", ACS Colloid and Surface Science Conference, Atlanta, June 18, 2003.

"Monte Carlo methods for equilibrium polymers and other self-assembled systems", Center for Simulational Physics weekly seminar, University of Georgia, Athens, July 1, 2003.

"Understanding lipid bilayer membranes through computer simulation." University of the South, Chemistry department seminar, Sewanee, TN, October 23, 2003.

"Molecular and mesoscale modeling of membranes." Marshall University, Chemistry departmental seminar, Huntington, WV, November 7, 2003

"Molecular and mesoscale modeling of membranes." University of North Carolina, Pembroke, Chemistry and Physics departmental seminar, Pembroke, NC., January 30, 2004.

"Molecular and mesoscale modeling of membranes," Emerson Center Lectureship Award Symposium, Emory University, May 1, 2004.

"Reversible Polymerization and Gelation: Insights from Monte Carlo Simulations using Simple Models." Division of Chemical Sciences seminar, University of Science and Technology of China, Hefei, China, February 28, 2005.

"Molecular and mesoscale modeling of (mixed) membranes," Department of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, October 22, 2005.

"Molecular simulation approaches to lipid mixtures," Institut Européen de Chimie et Biologie, Bordeaux, France, November 21, 2005.

"Molecular simulation of mixed-lipid bilayers," Séminaire du département de chimie, Ecole Normale Supérieure, Paris, November 23, 2005.

"Molecular and mesoscale modeling of membranes," Physical Chemistry Seminar, Yale University, New Haven, CT, February 14, 2006

"Molecular and mesoscale modeling of membranes," Department of Chemistry and Biochemistry, University of Mississippi, March 2, 2006

"Molecular and mesoscale modeling of mixed membranes," Physical Chemistry Seminar, University of North Carolina, Chapel Hill, March 22, 2006

"Modeling Mixed Lipid Membranes," Physical Chemistry Seminar, University of Washington, April 12, 2006.

"Molecular and mesoscale modeling of mixed membranes," Physical Chemistry seminar, University of Notre Dame, April 20, 2006.

"Computational explorations of lipid membranes, disks, ribbons, and vesicles," Physical Chemistry seminar, Emory University, October 16, 2006.

"Simulations of mixed-lipid bilayers," Physical Chemistry seminar, University of Southern California, November 20, 2006.

"Simulating mixed bilayers," Physical Chemistry seminar, University of California, Los Angeles, November 20, 2006.

"Simulations of mixed-lipid bilayers," Physical Chemistry seminar, University of California, Irvine, November 21, 2006.

"Molecular Dynamics and Thermodynamics of Mixed-Lipid Bilayers," Joint Symposium of Chemical Kinetics and Renewable Energy: From Gas Phase to Condensed Phase,

in honor of Professor M.C. Lin", National Chiao Tung University, Hsinchu, Taiwan, June 7, 2007

"Simple equilibrium model for tripodal particle aggregation," Foundations of Nanoscience 2008: Self-assembled Architectures and Devices, Snowbird, Utah, April 25, 2008.

"Investigating material properties of lipid bilayers through molecular simulation," 1st South-East Workshop on Soft Materials, Georgia Institute of Technology, May 9, 2008.

"Molecular Simulation of Mixed-Lipid Bilayers," Computational Chemistry seminar, Beijing University of Chemical Technology, February 20, 2009.

"Molecular Simulation of Mixed-Lipid Bilayers," Physical Chemistry seminar, Beijing Normal University, February 21, 2009.

"Atomistic Simulation of Phase Separation in Lipid Bilayers," Telluride Science Research Center workshop, Biological Membranes and Membrane Proteins: Challenges for Theory and Experiment, July 30, 2009.

"Atomistic simulation of mixed-lipid bilayers: Mixed methods for mixed membranes," Atlanta Area Chemical Physics series, Georgia Tech, April 4, 2011.

"Simulations of mixing and demixing behavior in multicomponent lipid bilayers," Biological Membranes and Membrane Proteins meeting, Snowmass Village, June 29 2011.

"Molecular simulation approaches to lipid composition variations in membranes", Georgia State University Department of Chemistry, April 27, 2012.

"Atomistic, Coarse-grained, and Statistical Thermodynamic Modeling of "Bicelle" Lipid Mixtures", 95th Canadian Chemistry Conference and Exhibition in Calgary, May 26-30, 2012.

"Molecular simulation studies of lipid bilayer phase behavior", Telluride Science Research Center workshop, Mechanistic Studies in Membrane Biophysics: Experiments and Theory, March 2013.

"Molecular simulation studies of edges in bilayers and bicelles", APS March Meeting, March 2013.

"Bilayer gel-fluid transition: studies of dynamics and anomalous permeability", Snowmass Biophysics Workshop: Biological Membranes and Membrane Proteins, July 23, 2013.

"Modeling Bilayers Near Phase Transitions", New Mexico Institute of Mining and Technology, Chemistry Departmental Seminar, September 6, 2013.

"Modeling Lipid Bilayer Behavior in the Gel Phase and Across the Melting Transition", Carnegie Mellon University, Department of Physics, Biophysics Seminar, October 22, 2013.

" 'Bicelle' Lipid Mixtures: Atomistic, Coarse-grained, and Thermodynamic Modeling", Southeastern Regional Meeting of the American Chemical Society, Atlanta, November 15, 2013.

"Modeling Lipid Bilayer Behavior in the Gel Phase", Atlanta Area Molecular and Cellular Biophysics Symposium, Emory University, December 10, 2014.

"Thermodynamics of Cluster Formation from Simple Simulations" CRC-EC Joint International Symposium on Chemical Theory for Complex Systems, Emory University, January 10, 2014.

"Computer Simulations of Lipid Bilayers", Chemical Sciences Seminar, Università degli Studi di Siena, Italy, June 19, 2014

"How molecules get into and through lipid bilayers: explorations by molecular simulation" Department of Natural and Forensic Sciences, Albany State University, Georgia, October 13, 2015

"Computational studies of phase transitions in lipid bilayers: How fast do they melt, and what makes them leaky when they freeze?" Georgia Gwinnett College, School of Science and Technology, November 19, 2015

"How molecules get into and through lipid bilayers: explorations by molecular simulation" Winston-Salem State University, North Carolina, MARC U*STAR program seminar, November 24, 2015

Contributed talks:

"Monte Carlo simulations of self-assembled polymers and networks." 226th A.C.S. National Meeting, New York, September 11, 2003

"Monte Carlo studies of the membrane disk-vesicle transition." Southeast Regional Meeting of the A.C.S., Atlanta, November 18, 2003.

"Monte Carlo simulation of lipid bicelle phase behavior." Annual A.P.S. March Meeting, Montreal, March 22, 2004.

"A multiscale simulation approach to lipid bilayer vesicle formation." Annual A.P.S. March Meeting, Montreal, March 25, 2004.

"Phase behavior of self-assembled chains: Insights from Monte Carlo simulation and statistical theory." Southeast Theoretical Chemists' Association Meeting, Knoxville, July 18, 2005.

"Molecular simulation studies of tail-length effects in mixed-lipid bilayers." Annual A.P.S. March Meeting, Baltimore, March 15, 2006.

"Mixed methods for mixed membranes: Tail mutation moves for rapid equilibration in mixed-lipid bilayer simulations." 231st A.C.S. National Meeting, Atlanta, March 27, 2006.

"Atomistic simulation of local composition variations in mixed-lipid bilayers." 232nd A.C.S. National Meeting, San Francisco, September 11, 2006.

"Cholesterol-induced demixing of saturated and unsaturated phosphatidylcholine lipids: Insights from atomistic simulation." A.C.S. National Meeting, Salt Lake City, March 26, 2009.

"Atomistic simulations of DPPC/DOPC/cholesterol mixtures: Making contact with the experimental phase diagram using mixed MD/MC methods." A.C.S. National Meeting, Anaheim, March 28, 2011.

"Cooperativity in cholesterol-induced demixing of saturated and unsaturated lipids." APS March Meeting, Boston, March 2, 2012.

"Solvent Repacking Monte Carlo: Application to Phase Behavior of Hard-Disk Mixtures." APS March Meeting, San Antonio, March 2, 2015.

SERVICE ACTIVITIES

University service: Co-chair, Emory – Laney Graduate School STEM Research and Career Symposium (2014, 2015, 2016); Chair of Leadership Committee, Emerson Center for Scientific Computation (Fall 2009-Fall 2013). Laney Graduate School Assistant Dean Search Committee

(Spring 2012). Emory Scholars Selection Committee (2011-2012). FAME group faculty advisor (2007-2008). Emory College Educational Policy Committee (2004-2006). Emerson Lectureship Committee (2006-2009). Computational and Life Sciences Initiative Education Committee and Faculty Search Committee (2007-2008). Emory College SIRE grant selection committee (Fall 2008). Graduate School Honor Code Hearing Committees (Summer 2008; Spring 2012); Office of Research Compliance IRIC Committee (Spring 2014).

Departmental service: Search Committee Chair (Fall 2014-Spring 2015); Chair of Outreach Committee (Fall 2014-Spring 2015); Chair of joint Chemistry-Winship Cancer Institute Search Committee (Fall 2013-Spring 2014). Director of Graduate Studies for Chemistry (Fall 2009-Summer 2011); Co-director of Graduate Studies (Fall 2008-Spring 2009); Member of graduate, (2001-2012), undergraduate (2004-present), budget (2010-2012), outreach (Fall 2012-Spring2013), and curriculum redevelopment (Fall 2014-present) committees. Chair of departmental Computer Committee (2005-2010). Chair of Departmental Search Advisory Committee (2006-2008). Emory College Honors program coordinator for Chemistry Department (2005-2009). BS/MS program coordinator for Chemistry Department (2005-2014.)

Service beyond Emory:

NM-INBRE Faculty Research Mentoring Program (2013-present). Provide mentoring support to an assistant professor at New Mexico Tech.

Panelist for TeraGrid/XSEDE Resource Allocations Committee, Fall 2010- Summer 2013. (quarterly meetings to review proposals for computer time at 6 national supercomputer facilities)

Peer review for journals and granting agencies: *J. Chem. Phys.*, *J. Phys. Chem. B*, *Langmuir*, *Macromolecules*, *J. Am. Chem. Soc., Biophys. J*; *Biochemistry; ChemPhysChem; Biopolymers; J. Comp. Chem.; Soft Matter; Acta Biomaterialia; PLoS Comp. Biol.; Int. J. Quantum Chem.; J. Mol. Liq.*, *J. Chem. Ed.; Materials*; *Adv. Colloid and Interfac. Sci.*; NSF, ACS-Petroleum Research Fund, and Research Corporation.

Panelist/virtual panelist for NSF grant review: 2008, 2014

Co-organizer of Atlanta Area Chemical Physics symposium, a monthly seminar held jointly with Georgia Institute of Technology (2003-2008).

Chair, 35th annual Southeast Theoretical Chemists' Association meeting, at Emory University, May 19-20, 2006. Website: http://www.chemistry.emory.edu/faculty/kindt/SETCA2006.htm

OUTREACH: Videos of molecular simulations produced with explanatory narration for a general audience: http://www.youtube.com/user/TheKindtGroup/

PUBLICATIONS: (* indicates undergraduate co-author)

50) L. Bolling-Patel and J. T. Kindt. "Coarse-grained molecular simulations of the melting kinetics of small unilamellar vesicles." *Soft Matter*, under revision (10/2015).

49) L. Yang and J. T. Kindt. "Line tension assists membrane permeation at the transition temperature in mixed-phase lipid bilayers." Submitted to *Phys. Chem. Chem. Phys.* (10/2015).

48) J. T. Kindt, "Grand canonical Monte Carlo using solvent repacking: Application to phase behavior of hard disk mixtures." *J. Chem. Phys.* **143**, 124109 (2015). dx.doi.org/10.1063/1.4931731

47) K. Uppulury, P. S. Coppock and J. T. Kindt, "Molecular simulation of the DPPE lipid bilayer gel phase: Coupling between molecular packing order and tail tilt angle." *J. Phys. Chem. B* **119**, 8725-8733 (2015). dx.doi.org/10.1021/acs.jpcb.5b05720

46) L. Yang and J. T. Kindt, "Simulation study of the permeability of a model lipid membrane at the fluid-solid phase transition." *Langmuir,* **31**, 2187-2195 (2015). dx.doi.org/10.1021/la504269t

45) A. West and J. T. Kindt, "On the relationship between plateau modulus and shear relaxation time in transient networks." *Macromol. Theory Simul.*, **24**, 208-217 (2015). dx.doi.org/10.1002/mats.201400093

44) W. Zheng, Y. Liu, A. West, E. E. Schuler, K. Yehl, R. B. Dyer, J. T. Kindt, and K. Salaita. "Quantum dots encapsulated within phospholipid membranes: phase-dependent structure, photostability, and site-selective functionalization." *J. Am. Chem. Soc.* **136**, 1992-1999 (2014). http://pubs.acs.org/doi/abs/10.1021/ja411339f

43) A. West, K. Ma*, J. L. Chung*, and J. T. Kindt. "Simulation studies of structure and edge tension of lipid bilayer edges: effects of tail structure and force-field." *J. Phys. Chem. A* **117**, 7114-7123 (2013). http://pubs.acs.org/doi/abs/10.1021/jp400371k

42) J. T. Kindt, "Accounting for Finite-Number Effects on Cluster Size Distributions in Simulations of Equilibrium Aggregation." *Journal of Chemical Theory and Computation*. **9**, 147-152 (2013). http://pubs.acs.org/doi/abs/10.1021/ct300686u

41) S. Nagarajan, E. E. Schuler, K. Ma*, J. T. Kindt, and R. B. Dyer, "Dynamics of the gel to liquid-crystal phase transformation in lipid bilayer vesicles." *J. Phys. Chem B.* **116**, 13749-13756 (2012). http://dx.doi.org/10.1021/jp309832u

40) D. C. Turner, F. Yin, J. T. Kindt, and H. Zhang. "Understanding pharmacokinetic food effects using molecular dynamics simulation coupled with physiologically based pharmacokinetic modeling." *Biopharmaceutics and Drug Disposition*, **33**, 510-521 (2012). http://onlinelibrary.wiley.com/doi/10.1002/bdd.1818/full

39) F. Yin and J. T. Kindt, "Hydrophobic mismatch and lipid sorting near OmpA in mixed bilayers: Atomistic and coarse-grained model simulations." *Biophys. J.* **102**, 2279-2287 (2012).

38) A. West and J.T. Kindt, "Effects of defects on shear stress relaxation in self-assembled protein networks." *Soft Matter* **8**, 2895 - 2906 (2012).

37) K.L.H. Lam, H. Wang, T. A. Siaw, M. R. Chapman, A. J. Waring, J. T. Kindt, and K.Y.C. Lee, "Mechanism of membrane disruption by antimicrobial peptides." *Biochimica et Biophysica Acta* **1818**, 194-204 (2012).

36) J. T. Kindt, "Atomistic simulation of mixed-lipid bilayers: Mixed methods for mixed membranes." *Molecular Simulation* **37**, 516-524 (2011).

35) M. L. Berkowitz and J. T. Kindt, "Molecular Detailed Simulations of Lipid Bilayers." In *Reviews of Computational Chemistry, Volume 27*, ed. K. Lipkowitz. (J. Wiley & Sons, 2011).

34) J. de Joannis, P. S. Coppock, F. Yin, M. Mori*, A. Zamorano, and J. T. Kindt. "Atomistic Simulation of Cholesterol Effects on Miscibility of Saturated and Unsaturated Phospholipids: Implications for Liquid-Ordered/Liquid-Disordered Phase Coexistence." *J. Am. Chem. Soc.* **133**, 3625-3634 (2011).

33) P. S. Coppock and J. T. Kindt, "Determination of phase transition temperatures for atomistic models of lipids from temperature-dependent stripe domain growth kinetics." *J. Phys. Chem. B,* **114**, 11468-73 (2010).

32) F. Yin and J. T. Kindt, "Atomistic simulation of hydrophobic matching effects on lipid composition near a helical peptide embedded in mixed-lipid bilayers", *J. Phys. Chem. B* **114,** 8076-8080 (2010).

31) Y. Jiang, H. Wang, J. T. Kindt, "Atomistic simulations of 'bicelle' mixtures." *Biophys. J.*, **98**, 2895-2903 (2010).

30) D. C. Turner, F. Yin, J. T. Kindt, H. Zhang, "Molecular dynamics simulations of glycocholate-oleic acid mixed micelle assembly." *Langmuir* **26**, 4687-4692 (2010).

29) P. S. Coppock, J. T. Kindt, "Atomistic simulations of mixed-lipid bilayers in the gel and fluid phases." *Langmuir* **25**, 352-359 (2009).

28) H. Wang, J. de Joannis, Y. Jiang, *J. C. Gaulding, B. Albrecht, F. Yin, *K. Khanna, and J. T. Kindt, "Bilayer edge and curvature effects on partitioning of lipids by tail length: Atomistic simulations." *Biophys. J.* **95**, 2647-2657 (2008).

27) *L. S. Pam, *L. L. Spell, and J. T. Kindt, "Simulation and theory of flexible equilibrium polymers under poor solvent conditions." *J. Chem. Phys.*, **126**, 134906 (1-10) (2007).

26) F. M. Menger, Hailing Zhang, J. de Joannis, and J. T. Kindt, "Solubilization of Paclitaxel (Taxol) by Peptoad Self-Assemblies." *Langmuir*, **23**, 2308-2310 (2007).

25) Y. Jiang and J. T. Kindt, “Simulations of edge behavior in a mixed-lipid bilayer: Fluctuation analysis.” *Journal of Chemical Physics* **126**, 045105-1 – 045105-9 (2007).

24) J. de Joannis, Y. Jiang, F. Yin, and J. T. Kindt, “Equilibrium distributions of DPPC and DLPC in a mixed lipid bilayer: Atomistic semi-grand canonical ensemble simulations.” *Journal of Physical Chemistry B*. **110**, 25875-25882 (2006).

23) X. Lü and J. T. Kindt, “Theoretical analysis of polydispersity in the nematic phase of self-assembled semiflexible chains.” *Journal of Chemical Physics* **125**, 054909-1 – 054909-3 (2006).

22) *K. Khanna, *T. T. Chang, and J. T. Kindt “Complementarity and clustering in a simple model mixed bilayer.” *Journal of Chemical Physics* **124**, 036102-1 – 036102-3 (2006).

21) J. de Joannis, F. Y. Jiang, and J. T. Kindt, “Coarse-grained model simulations of mixed lipid systems: Composition and line tension of a stabilized bilayer edge.” *Langmuir* **22**, 998-1005 (2006).

20) J. T. Kindt, “Simulation and theory of self-assembly and network formation in reversibly cross-linked equilibrium polymers.” *Journal of Chemical Physics*, **123**, 144901-1 – 144901-11 (2005).

19) S.-J. Zhao and J. T. Kindt, “Monte Carlo calculations of the free-energy landscape of vesicle formation and growth.” *Europhysics Letters,* **69**, 839-845 (2005).

18) F. Y. Jiang, Y. Bouret, and J. T. Kindt, “Molecular dynamics simulations of the lipid bilayer edge.” *Biophysical Journal* **87,** 182-192 (2004).

17) X. Lü and J. T. Kindt, “Monte Carlo simulation of the self-assembly and phase behavior of semiflexible equilibrium polymers.” *Journal of Chemical Physics* **120,** 10328-10338 (2004).

16) J. T. Kindt, “Grand canonical Monte Carlo simulation of equilibrium polymers and networks,” in *Mesoscale Phenomena in Fluid Systems*, ed. F. Case and P. Alexandridis, ACS Symposium Series 861, 298-312 (2003)

15) J. T. Kindt, "Simulation and theory of self-assembled networks: Ends, junctions, and loops." *Journal of Physical Chemistry B*, **106,** 8223-8232 (2002).

14) J. T. Kindt, "Pivot-coupled grand canonical Monte Carlo method for ring simulations." *Journal of Chemical Physics*, **116,** 6817-6825 (2002).

13) L. Sun, K. Petersen, Y. Alexeev, T. Windus, J. Kindt, and W. L. Hase, “Effect of the Ar-Ni(s) potential on the cross section for Ar + CH_4/Ni{111} collision-induced desorption.” *Journal of Chemical Physics*, **122**, 044704 (2005).

12) S. Tzlil, J. T. Kindt, W. M. Gelbart, and A. Ben-Shaul, "Forces and Pressures in DNA Packaging and Release from Viral Capsids." *Biophysical Journal*, **84,** 1616-1627 (2003).

11) J. Kindt, S. Tzlil, A. Ben-Shaul, and W. M. Gelbart. "DNA packaging and ejection forces in bacteriophage." *Proceedings of the National Academy of Sciences, USA* **98**, 13671 (2001).

10) J. T. Kindt and W. M. Gelbart, "Chain self-assembly and phase transitions in semiflexible polymer systems." *Journal of Chemical Physics*, **114,** 1432 (2001).

9) J. T. Kindt and J. C. Tully, "Dynamical corrugation: simulations of the sticking of CO on Cu (100)." *Surface Science*, **477,** 149 (2001).

8) J. T. Kindt and J. C. Tully, "Simulations of collision-induced absorption of hydrogen on Ni(111)." *Journal of Chemical Physics* **111,** 11060 (1999).

7) O. V. Prezhdo, J. T. Kindt, and J. C. Tully, "Perturbed ground state method for electron transfer." *Journal of Chemical Physics* **111,** 7818 (1999).

6) J. T. Kindt and C. A. Schmuttenmaer, "Theory for determination of the low-frequency time-dependent response function in liquids using time-resolved terahertz pulse spectroscopy." *Journal of Chemical Physics* **110,** 8589 (1999).

5) J. T. Kindt, J. C. Tully, M. Head-Gordon and M. A. Gomez, "Electron-hole pair contributions to scattering, sticking, and surface diffusion: CO on Cu(100)." *Journal of Chemical Physics* **109,** 3629 (1998).

4) J. T. Kindt and C. A. Schmuttenmaer, "Far-infrared absorption spectra of water, ammonia, and chloroform calculated from instantaneous normal mode theory." *Journal of Chemical Physics* **106,** 4389 (1997).

3) J. T. Kindt and C. A. Schmuttenmaer, "Far-infrared dielectric properties of polar liquids probed by femtosecond terahertz pulse spectroscopy." *Journal of Physical Chemistry* **100,** 10373 (1996).

2) R. C. Scarrow, B. A. Brennan, J. G. Cummings, H. Y. Jin, D. H. J. Duong, J. T. Kindt, M. J. Nelson, "X-ray spectroscopy of nitrile hydratase at pH 7 and 9." *Biochemistry* **35,** 10078 (1996).

1) J. T. Kindt, A. Woods, B. M. Martin, R. J. Cotter, and Y. Osawa, "Covalent alteration of the prosthetic heme of human hemoglobin by $BrCCl_3$: Cross-linking of heme to cysteine residue 93." *Journal of Biological Chemistry* **267,** 8739, (1992).