UNIVERSITY OF CALIFORNIA, BERKELEY

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Professor Teresa Head-Gordon	**274 Stanley Hall**
Department of Chemistry	**Berkeley, California 94720**
Department of Bioengineering	**(510) 666-2744**
Department of Chemical and Biomolecular Engineering	**thg@berkeley.edu**

Research Narrative

My research program encompasses the development of general theoretical and computational methodologies applied to chemistry and biophysics in the areas of water and aqueous hydration, proteins and macromolecular assemblies, non-disease and disease protein aggregation, materials and catalysis. I have also been involved in local and national service, education, and training, which extends to promoting and developing the blueprint for computational science and engineering for the future.

Education and Training

Case Western Reserve University, Cleveland, OH	B.S.	1979-1983	Chemistry
Carnegie Mellon University, Pittsburgh, PA	Ph.D.	1984-1989	Theo. Chem.

AT& T Bell Laboratories, Murray Hill, New Jersey, Postdoctoral Member Technical Staff, 1990-1992.

Professional Experience

Faculty Director, Professional Master's in Molecular Sciences and Software Engineering, 2018-
Co-Director, MolSSI: Molecular Sciences Software Institute, NSF National Center, 2016-
Co-Director, CalSolv: Solvation at UC Berkeley, 2016-
Chancellor's Professor, Dept. of Chemistry, UC Berkeley, 7/12-
Member of the Pitzer Center for Theoretical Chemistry, 7/12-
Faculty Staff Scientist, Chemical Sciences Division, Lawrence Berkeley National Laboratory 7/12-
Professor, Dept. of Chemical and Biomolecular Engineering, UC Berkeley, 7/11-
Professor, Dept. of Bioengineering, UC Berkeley, 7/07-
Assoc. Professor, Dept. of Bioengineering, UC Berkeley, 7/04-6/07
Member of the Center for Computational Biology, 1/03-present
Asst. Professor, Dept. of Bioengineering, UC Berkeley, 1/01-6/04
Member of Bioengineering, Biophysics, and AS&T Graduate Groups, UC Berkeley, 1/01-
Department Head of Computational Structure Group, Physical Biosciences LBNL, 10/01-10/02
Faculty affiliate of QB3 Institute, 10/01-
Faculty Staff Scientist, Physical Biosciences Division, Lawrence Berkeley National Laboratory, 1/01-
Senior Staff Scientist, Physical Biosciences Division, Lawrence Berkeley National Laboratory, 8/00-12/31/00.
Staff Scientist, Physical Biosciences Division, Lawrence Berkeley National Laboratory, 8/92-8/00.

Professional Activities
Intramural

Academic Senate, Committee on Academic Planning and Resource Allocation (CAPRA), 2019-2021
Berkeley Collegium: Narrowing the gap between teaching and research, 2018-2019
Systemwide UCOC Committee on Committees, 2018-2019
LBNL Chemical Sciences Division Staff Committee, 2017- present
Academic Senate, Committee on Committees, 2016-2018
BioE Vice Chair, Master Programs, Bioengineering Department, 2016-2018
Steering Committee, Bioengineering Department, 2016-2018
Chem, Undergraduate senior advising, Fall 2013, Fall/Spring 2016
Chem, Advanced Graduate Student advising, Theory 2012-2015
BioE Vice Chair, Graduate Affairs, Bioengineering Department, 2012- 2014
BioE Co-Chair, Graduate Committee, 2010-2012
BioE Executive Committee, Bioengineering Department, 2007-2010
BioE Vice Chair, Faculty Welfare, Bioengineering Department, 2008-2010

BioE Undergraduate advising, 2007-present
BioE Vice Chair, Graduate Affairs, Bioengineering Department, 2006-2008
COE Member, Engineering Ethics & Social Responsibility, 2014-2016
COE Member, Broadening Participation Committee, 2012-2013
COE/BioE Adjudicator for College and Junior Transfers to BioE, 2003-2007
COE Member, E7 Committee, 2009-2012
COE Member of the Biology in the College of Engineering Taskforce, 2007-2008
COE Committee on Computational Engineering Science, 2001-2008
UCB/UCSF Exec. Comm. (ex-officio), Joint Graduate Group Bioengineering, 2007-2011
UCB/UCSF Admissions Comm., Joint Graduate Group Bioengineering 2006-2012, 2014
UCB/UCSF Head Graduate Advisor, Joint Graduate Group in Bioengineering, 2006-2007
UCB ad hoc committees (confidential).
UCB/BioE Facilitator for NRC Assessment of Berkeley's Research Doctoral Programs, 2006-2007
UCB Executive Committee, Computational Biology Initiative, University of California, Berkeley, 2003-2008

Extramural

BES Representative of the SciDAC-4 Coordination Committee, DOE, 2017-2021.
Member, NIH Macromolecular Structure and Function D Study Section, July 1, 2017 - June 30, 2023
Advisory Board, NSF Center for Chemical Innovation; Center for Aerosol Impacts on Climate and the Environment (CAICE), UC San Diego, California
Panel, NSF Computational Chemistry/Science Gateway Workshop, May 9 - 11, 2017, Jackson State University, Jackson Mississippi
Organizer (with Jeff Neaton and Steve Louie); NSF Materials Workshop, February 2-3, 2017, Berkeley, California.
Reviewer, Pacific Northwest National Laboratory Molecular Theory and Modeling. April 13-15, 2016, Richland, WA.
Panel, MolSSI Interoperability workshop, Virginia Tech, June 5-7, 2017
Director for Academic, Industry and Government Lab Outreach, Molecular Sciences Software Institute, 2016-2021
Reviewer, DOE Office of Science Graduate Student Research (SCGSR) Program's 2016 Solicitation 2
Organizer, Advanced Potential Energy Surfaces, Telluride Science Research Center, June 13-18, 2015, Telluride, CO
ACS PHYS Division Councilor, 1/2014-12/2016
NIH Special Emphasis study section, June 23, 2014.
Appointment Committee for Professor in Physical Chemistry, Ruhr Universitat Bochum, June 5-6, 2013
NSF Review Panel, CCI, February 11-13, 2013.
NSF Review Panel, SSI-SSE, November 7-8, 2011.
NSF/EPSRC Workshop. Invited Panel Member, Oxford UK, June 13-15, 2011.
ACS National Award Panel, 2011-2013
NSF Review Panel, Graduate Research Fellowships, February 10-13, 2011.
NSF Review Panel, Protein Databank Site Visit, November 1-2, 2010.
DOD, Extreme Scale Applications Study (ESAS), September 2010-April 2011.
NIH/NIGMS Modeling and Analysis of Biological Systems study section, 2007-2012.
NSF Vision for R&D in Simulation-Based Engineering and Science in the Next Decade, April 22-23, 2009.
U.S. DOE Large Scale Computing and Storage Requirements for BER, May 8, 2009.
National Academies of Science. Member of panel on "Study on potential impact of advances in high-end computing in science and engineering", 2006-2008.
Program reviewer for Basic Energy Science/DOE, Molecular Theory project at PNNL, March 18-20, 2007
Co-Chair of Workshop on Cyberinfrastructure for NSF Chemistry, 7/04-10/04.
Lead Writer for Biophysical section of DOE/SCALES, July, 2003
Member of Subcommittee on 21st Century Biology NSF Biological Sciences (Directorate) Advisory Committee (BIOAC), July, 2003.
Lead Writer for Biophysical section of DOE/Genomes to Life Goal 4 Roadmap, March, 2002
Panelist for NSF Physical and Theoretical Chemistry Division CAREER awards, 2002
Panelist for NSF Mathematical and Physical Sciences Directorate ADVANCE Fellows, 2001
National Selection Committee for DOE Computational Science Graduate Fellowship Program, 2001.

Co-led a nation-wide community effort with Dr. John Wooley (associate vice chancellor for research at UC San Diego) in the editing and writing of a white paper on computational biology (see http://cbcg.lbl.gov/ssi-csb). This effort highlighted

the computational needs of the computational biology community and placed the community at the forefront of various initiative that includes the agencies of DOE, NSF, DOD, NASA, NOAA, and NIH.

Advisory and Editorial Boards

External Elector, Board of Electors for Professorship in Chemistry (1968), University of Cambridge
Scientific Advisory Board. DFG German Cluster of Excellence, RESOLV, 2018-
Editorial Advisory Board Member, Molecular Physics, 2018-2020
Editorial Advisory Board Member, Journal of Chemical Physics, 2017-2020
Telluride Science Research Council, General Member Advisor, 2016-
NSF BioXFEL Science and Technology Center, External Advisory Board, 2014
Editorial Advisory Board Member, Theoretical Chemistry Accounts, 2011-2012
Editorial Advisory Board Member, Journal of Physical Chemistry, 2009-2011
Editorial Advisory Board Member, Journal of Computational Chemistry, 2003-
Editor, Biophysical Journal, 2003-2006.
Editorial Board Member for the SIAM book series on Computational Science and Engineering, 2004-2008

Honors and Awards

Allergan Distinguished Lecturer, CSU Long Beach, April 8, 2020
39th Esther and Bingham J. Humphrey Memorial Lecturer, University of Vermont, Oct. 5, 2019
Fellow, American Chemical Society, 2018
Fellow, ReSolv German Center of Excellence, Bochum, 2018
Fellow, American Institute of Medical and Biomedical Engineers, 2016
Chancellors Professor, UC Berkeley 2012-2020
Plenary Lecture. From Computational Biophysics to Systems Biology 2017 (CBSB2017). University of Cincinnati in Cincinnati, OH, USA on May 18-20, 2017.
Plenary Lecture. CCP5 Annual General Meeting, Harper Adams University, U.K. September 12-14, 2016
Plenary Lecture. Royal Society of Chemistry Mini-Symposium on Advanced Potential Energy Surfaces, University of Southampton, UK, April 8, 2016
Frontiers in Materials Science Lecture, Pacific Northwest National Lab, January 25, 2015
Keynote Speaker, BioE Honor Society, UC Berkeley April 19, 2014
Keynote Speaker. Freiburg Institute for Advanced Studies, Freiberg, Germany, Sept. 25-29, 2013.
MasterWorks Talk, Supercomputing 2009, Portland, Oregon Nov. 14-20, 2009.
Keynote Speaker. MM2009, Surfers Paradise, Queensland Australia, July 28, 2009.
Plenary Lecture. International Workshop on Molecular Structure and Dynamics of Interfacial Water, Shanghai, China, December 14-21, 2007.
Keynote Speaker. Maria Goeppert-Mayer Symposium, San Diego, California, October 12, 2007.
Schlumberger Fellow. Sabbatical Fellow at Cambridge University, United Kingdom (2005-2006).
Schlumberger Lecture. Cambridge University, United Kingdom, February 15, 2006.
Clare Hall Faculty, Cambridge University, United Kingdom (2006-present)
IBM-SUR Award. A gift from IBM of a 40 processor IBM/SP (2001).

Graduate Students, Postdoctoral Fellows, Staff

H. Sienny Shang (M.S. in Biophysics, 1994; Associate Research Fellow, Academia Sinica Institute of Astronomy and Astrophysics); Jon Sorenson (NSF Fellowship, Ph.D. in Chemistry, 1995-2000; Software Group Lead, Invitae); Greg Hura (PhD in Biophysics, 1998-2004; Research Scientist, LBNL and Associate Adjunct Professor, University of California Santa Cruz); Liz Verschell (M.S. in Biophysics, Eugene Cota-Robles Fellowship, 2002-2008; Veterinary surgeon, Lincoln UK), Nicolas Fawzi (Ph.D. BioE, 2003-2007; Assistant Professor, Department of Molecular Pharmacology, Physiology & Biotechnology, Brown University); Matthew Lin (Ph.D. BioE, 2004-2009; Biomedical Engineer, Thomas Ried Lab, NIH); Brian Carnes (M. S. BioE, 2004-2007; Software Engineer, Google); Margaret Johnson (PhD. BioE, 2004-2008; Assistant Professor, Department of Biophysics, Johns Hopkins U.); Candace Gilet (M. S. Physics, 2005; Computational Scientist, University of Michigan); Enghui Yap (Ph.D. BioE, 2010; Sr. Data Scientist, OnDeck); Katherine Ball (Biophysics, 2008-2013; Asst. Prof. Skidmore College); Cheng Peng (CSC Research fellow, 2008-2010); Xin Geng (CSC Research fellow, 2011-2012); Asmit Bhowmick (CBE, 2011-2016, postdoc LBNL); Saurabh Belsare (BioE, 2012-2017, postdoc UCSF); Lisa Felberg (CBE, 2012-2017; Software Engineer, Square); Sukanya Sasmal (CBE, 2012-2017; postdoc UC Irvine); Alex Albaugh (CBE, 2012-2018; postdoc Northwestern); James Lincoff (CBE, 2014-2019; postdoc UCSF), Jerri Li (Chemistry, 2018-), Shuai Liu (Chemistry, 2018-2019; Machine Learning Engineer, Facebook), Lars Urban (German Masters visiting scholar, 2018-2019); Nancy Guan (Chemistry, 2019-)

Dr. Shijun Zhong (Postdoc, 1999-2000; Prof. Dalian University of Technology); Dr. Chao-Ping Hsu (Miller Postdoctoral Fellow, 1999-2001; Prof. of Chemistry, Academia Sinica, Taiwan); Dr. Voichita Dadarlat (Visiting Postdoc, 2000-2001; Research Scientist, Purdue University); Dr. Silvia Crivelli (Postdoc, 1997-2002; Staff Scientist, NERSC, LBNL); Dr. Louis Clark (Postdoc, 2002-2003; Scientist, Codexis); Dr. Scott Brown (Postdoc, 2001-2003; Director of Computational Chemistry, Sunovion Pharmaceuticals); Dr. Daniela Russo (Postdoc, 2001-2004; Staff Scientist, ILL, France); Dr. Pradipta Bandyopadhyay (Postdoc, 2003; Prof. of Biophysics, Jawaharlal Nehru University, India); Dr. Rajesh Murarka (Postdoc, 2004-2006; Prof. of Chemistry, IISER, Bhopal); Dr. Itay Lotan (Postdoc, 2004-2005; Quantitative Analyst in Israel); Dr. Cecile Maldier-Jugroot (Postdoc, 2004-2007; Prof. Chemistry/ChemE Royal Military College, Canada); Dr. Jory Ruscio (Postdoc, 2007-2009; Senior Software Engineer at Bleacher Report); Dr. Jonathan Kohn (Postdoc, 2006-2009; Group Leader at Bio-Rad Labs); Dr. Alex Sodt (Postdoc, 2007-2010; NIH principal investigator); Dr. Gary Clark (Postdoc, 2008-2010); Dr. Po Hu (Postdoc, 2009-2011; Actuarial Analyst at California Casualty Management Company); Dr. Jerome Nilmeier (Postdoc, 2009; Data scientist IBM); Dr. Paul Nerenberg (Postdoc, 2010-2011; Asst. Prof. of Biophysics, Cal State LA); Dr. Sudip Chakraborty (Postdoc, 2010-2011; Fast Track Scientist, Indian Institute of Science Bangalore); Dr. Marielle Soniat (Postdoc, 2015-2016), Dr. Omar Demerdash (Postdoc, 2013-2017; Staff Scientist, ORNL); Dr. Mert Gur (Postdoc, 2014; Asst. Professor, Istanbul Technical University), Dr. Luis Ruiz Pestana (2015-2019; Asst. Prof. U. Miami); Dr. Valerie Vaissier (2017-2019; Asst. Prof. Virginia Tech); Dr. Kochise Bennett (2017-2019; Chief Research Scientist, Valravn Capital); Dr. Akshaya Das (2018-); Dr. Sara Cheng (2018-); Dr. Itai Leven (2018-), Dr. Jagna Witek (2019-), Dr. Wan-Lu Li (2019-), Dr. Hongxia Hao (2019-), Dr. Farnaz Heidar Zadeh (2019-), Dr. Mojtaba Haghighatlari (2019-).

University Teaching

CHEMISTRY 1A: General Chemistry (Fall 2015, 2016, 2020)
CHEMISTRY 195/295: Machine Learning for the Chemical Sciences (Spring 2019)
BIOENGINEERING 103: Engineering Molecules 2 (Fall 2016, Fall 2018, Fall 2019)
CHEMISTRY130/MCB100: Biophysical Chemistry (Spring, 2013, 2014)
BIOENGINEERING 100: Ethics in Science and Engineering (Fall 2007, 2008, Spring 2010-2012, Fall 2012-)
BIOENGINEERING 143/243: Computational Methods In Biology (Spring, 2002-05, 2007-09, Fall 2009-2011)
BIOENGINEERING 131/231: Introduction To Computational Biology (Fall 2002-2005)
COMPUTER SCIENCE 267: Applications Of Parallel Computers (1 Lecture) (1999-2002, 2005)
COMPUTER SCIENCE 294: Challenges In Comp. Bio. (Lecture) Fall, 2000
ENGINEERING 39B: Introduction To Computational Biology (Spring, 2002)
BIOENGINEERING 24: Aspects of Bioengineering (Spring, 2003)

Publications

1. V. Vaissier Welborn, W.-L. Li, T. Head-Gordon (2020). Interplay of Encapsulated Water and a Supramolecular Capsule for Catalysis of Reductive Elimination Reaction from Gold. *Nature Comm.* 11, Article number: 415.
2. L. Ruiz Pestana, H. Hao, T. Head-Gordon (2020). Diels-Alder Reactions in Water are Determined by Microsolvation. *Nano Lett.* 20, 1, 606-611.
3. J. Li, K. C. Bennett, Y. Liu, M. V. Martin, T. Head-Gordon (2020). Accurate Prediction of Chemical Shifts for Aqueous Protein Structure for "Real World" Cases using Machine Learning. *Chem. Sci.* 11, 3180-3191.
4. E. C. Rossomme, C. N. Lininger, A. T. Bell, T. Head-Gordon, M. Head-Gordon (2020). Electronic Structure Calculations Permit Identification of the Driving Forces Behind Frequency Shifts in Transition Metal Mono-carbonyls. *Phys. Chem. Chem. Phys.* 22, 781-798.
5. J. Lincoff, M. Krzeminski, M. Haghighatlari, J. M.C. Teixeira, G.-N. W. Gomes, C. C. Gardinaru, J. Forman-Kay, T. Head-Gordon (2020). Extended Experimental Inferential Structure Determination Method for Evaluating the Structural Ensembles of Disordered Protein States. *Comm. Chem. accepted* (*ArXiv:1912.12582*)
6. M. Haghighatlari, J. Li, F. Heidar-Zadeh, Y. Liu, X. Guan, T. Head-Gordon (2020). Learning to Make Chemical Predictions: the Interplay of Feature Representation, Data, and Machine Learning Algorithms. *Chem, minor revisions (ArXiv: 2003.001575)_*
7. G.-N. Gomes, M. Krzeminski, E. W. Martin, T. Mittag, T. Head-Gordon, J. D. Forman-Kay, C. C. Gradinaru (2020). Integrating smFRET, SAXS and NMR Data to Infer Structural Ensembles of an Intrinsically-Disordered Protein. *Submitted ArXiv:1912.02735*
8. D. An, S. Y. Cheng, T. Head-Gordon, L. Lin, J. Lu (2020). Convergence of a Stochastic-Extended Lagrangian Molecular Dynamics Method for Polarizable Forcefield Simulation. *Submitted (arXiv:1904.12082)*
9. F. Novelli, L. Ruiz Pestana, K.C. Bennett, E. Adams, F. Sebastiani, C. Hoberg, N. Stavrias, G. Schwaab, T. Head-Gordon, M. Havenith (2020). Strong Anisotropy in Liquid Water Upon Librational Excitation Using Terahertz Laser Fields. *Submitted (ArXiv:1809.04261).*

10.   F. Sebastiani, T. A. Bender, S. Pezzotti, W.-L. Li, G. Schwaab, R. G. Bergman, K. N. Raymond, F. D. Toste, T. Head-Gordon, M. Havenith (2020). Encapsulated Water in a Supramolecular $Ga_4L_6^{-12}$ Cage is Neither Ice- nor Bulk Water-like. *J. Am. Chem. Soc. submitted*

11.   V. Vaissier Welborn, T. Head-Gordon (2019). Fluctuations of electric fields in the active site of the enzyme Ketosteroid Isomerase. *J. Am. Chem. Soc. Comm.* 141 (32) 12487-12492.

12.   V. Vaissier Welborn, T. Head-Gordon (2019). Computational design of synthetic enzymes. *Chem. Rev.* 119 (11), 6613-6630.

13.   A. Albaugh, M. Tuckerman, and T. Head-Gordon (2019). Combining iteration-free polarization with large time step stochastic-isokinetic integration. *J. Chem. Theory Comput.* 15 (4) 2195–2205

14.   J. Lincoff, S. Sasmal, T. Head-Gordon (2019). The combined force field-sampling problem in simulations of disordered amyloid-β peptides. *J. Chem. Phys.* 150, 104108.

15.   J. Dziedzic, T. Head-Gordon, M. Head-Gordon, C.-K. Skylaris (2019). Mutually polarizable QM/MM model with in situ optimized localized basis functions. *J. Chem. Phys.* 150, 074103.

16.   T. Head-Gordon, F. Paesani (2019). Water is not a dynamic polydisperse branched polymer. *Proc. Natl. Acad. Sci. (Letter to the Editor)* 116 (27) 13169-13170.

17.   S. Liu, J. Li, K. C. Bennett, B. Ganoe, T. Stauch, M. Head-Gordon, D. Ushizima, A. Hexemer, T. Head-Gordon (2019). A Multi-resolution 3D-DenseNet for chemical shift prediction in NMR crystallography. *J. Phys. Chem. Lett.* 10, 4558-4565

18.   I. Leven, T. Head-Gordon (2019). Inertial Extended-Lagrangian scheme for solving charge equilibration force fields. *Phys. Chem. Chem. Phys.* 21, 18652-18659.

19.   A. K. Das, L. Urban, I. Leven, M. Loipersberger, A. Aldossary, M. Head-Gordon, T. Head-Gordon (2019). Development of an advanced force field for water using variational energy decomposition analysis. *J. Chem. Theory Comput.* 15 (9), 5001-5013

20.   Y. Qiu, P. S. Nerenberg, T. Head-Gordon, L.-P. Wang (2019). Systematic optimization of water models using liquid/vapor surface tension data. *J. Phys. Chem. B* 123 (32) 7061-7073.

21.   I. Leven, T. Head-Gordon (2019). C-GeM: Coarse-Grained Electron Model for Predicting the Electrostatic Potential in Molecules. *J. Phys. Chem. Lett.* 10, 6820-6826

22.   M. Loipersberger, J. Lee, Y. Mao, A. Das, K. Ikeda, J. Thirman, T. Head-Gordon, M. Head-Gordon (2019). Energy Decomposition Analysis for Interactions of Radicals: Theory and Implementation at the MP2 Level with Application to Hydration of Halogenated Benzene Cations and Complexes between $CO2-•$ and Pyridine and Imidazole. *J. Phys. Chem. A* 123, 44, 9621-9633.

23.   V. Vaissier Welborn, L. Ruiz Pestana, T. Head-Gordon (2018). Computational optimization of electric fields for better catalysis design. *Nature Catalysis* 1, 649–655.

24.   V. Vaissier, S. C. Sharma, K. Schaettle, T. Zhang, T. Head-Gordon (2018). Computational optimization of electric fields for improving catalysis of a designed Kemp Eliminase. *ACS Catalysis* 8, 219-227.

25.   L. Ruiz Pestana, L. E. Felberg, T. Head-Gordon (2018). Coexistence of multilayered phases of nanoconfined water: the importance of flexible confining surfaces. *ACS Nano* 2 (1), 448–454.

26.   P. S. Nerenberg and T. Head-Gordon (2018). New developments in force fields for biomolecular simulations. *Curr. Opin. Struct. Bio. 49, 129-138*.

27.   V. Vaissier Welborn, T. Head-Gordon (2018). Electrostatics generated by a supramolecular capsule stabilizes the transition state for carbon-carbon reductive elimination from a gold(III) complex. *J. Phys. Chem. Lett. 9(14), 3814-3818.*

28.   L. Ruiz Pestana, O. Marsalek, T. E. Markland, T. Head-Gordon (2018). The quest for accurate liquid water properties from first principles. *J. Phys. Chem. Lett. 9 (17), 5009-5016.*

29.   O. N. Demerdash, L.-P. Wang, T. Head-Gordon (2018). Advanced models for water simulations. *WIREs Computational Molecular Science 8 (1), e1355.*

30.   E. Jurrus, D. Engel, K. Star, K. Monson, J. Brandi, L. E. Felberg, D.H. Brookes, L. Wilson, J. Chen, K. Liles, M. Chun, P. Li, T. Dolinsky, R. Konecny, D. Koes, J. E. Nielsen, T. Head-Gordon, W. Geng, R. Krasny, M. Gunner, G.-W. Wei, M. J. Holst, J. A. McCammon, N. A. Baker (2018). Improvements to the APBS biomolecular solvation software suite. *Protein Sci 27 (1), 112-128.*

31.   L. Ruiz Pestana, N. Minnetian, L. Nielsen Lammers, T. Head-Gordon, (2018). Dynamical inversion of the energy landscape promotes non-equilibrium self-assembly of binary mixtures. *RSC Chemical Science, 9, 1640 - 1646.*

32.   S. Belsare, V. Pattni, M. Heyden, and T. Head-Gordon (2018). Solvent entropy contributions to catalytic activity in designed and optimized Kemp Eliminases. *J. Phys. Chem. B (Ken Dill Festschrift), 122 (21), 5300-5307.*

33.   K. Schaettle, L. R. Pestana, T. Head-Gordon, L. Nielsen Lammers (2018). A structural coarse-grained model for clays using simple iterative Boltzmann inversion, *J. Chem. Phys.* 148, 222809.

34. A. Albaugh, A. M. N. Niklasson, T. Head-Gordon (2018). Higher-order Extended Lagrangian Born-Oppenheimer Molecular Dynamics for Classical Polarizable Models. *J. Chem. Theory Comput. 14 (2), 499–511.*

35. A. Krylov, T. L. Windus, T. Barnes, E. Marin-Rimoldi, J. Nash, B. Pritchard, D. G. A. Smith, D. Altarawy, P. Saxe, C. Clementi, T. D. Crawford, R. Harrison, S. Jha, V. S. Pande, T. Head-Gordon (2018). Computational chemistry software and its advancement as illustrated through three grand challenge cases for molecular science. *J. Chem. Phys. Perspective* 149, 180901.

36. A. K. Das, O. N. Demerdash, T. Head-Gordon (2018). Improvements to the AMOEBA Force Field by Introducing Anisotropic Atomic Polarizability of the Water Molecule. *J. Chem. Theory Comput.* 14 (12), 6722–6733.

37. A. Albaugh and T. Head-Gordon (2017). A new method for treating Drude polarization in classical molecular simulation. *J. Chem. Theory Comput.* 13(11):5207-5216.

38. A. Bhowmick, S. Sharma, T. Head-Gordon (2017). The importance of the scaffold for *de novo* enzymes: A Case Study with Kemp Eliminases. *J. Am. Chem. Soc.* 139(16):5793-5800.

39. L. Ruiz Pestana, K. Kolluri, T. Head-Gordon, and L. Nielsen Lammers (2017). Direct exchange mechanism for interlayer ions in non-swelling clays. *Environ. Sci. & Tech.* 51 (1), 393–400

40. N. Mardirossian, L. Ruiz Pestana, J. C. Womack, C.-K. Skylaris, T. Head-Gordon, M. Head-Gordon (2017). On the use of the rVV10 nonlocal correlation functional in the B97M-V density functional. *J. Phys. Chem. Lett.* 8, 35–40.

41. A. Esser*, S. Belsare*, D. Marx, and T. Head-Gordon (2017). Mode specific THz spectra of solvated amino acids using the AMOEBA polarizable force field. *Phys. Chem. Chem. Phys.* 19, 5579-5590.

42. A. Albaugh, A. Niklasson, and T. Head-Gordon (2017). Accurate classical polarization solution with no self-consistent field iterations. *J. Phys. Chem. Lett.* 8, 1714–1723

43. V. Vitale, J. Dziedzic, A. Albaugh, A. Niklasson, T. Head-Gordon, C.-K. Skylaris (2017). Performance of extended Lagrangian schemes for molecular dynamics simulations with classical polarizable force fields and density functional theory. *J. Chem. Phys.* 146, 124115

44. A. C. Carr, L. E. Felberg, V. A. Piunova, J. E. Rice, T. Head-Gordon, W. C. Swope (2017). The effect of hydrophobic core topology and composition on the structure and kinetics of star polymers, a molecular dynamics study. *J. Chem. Theory Comput.* 121 (13), 2902–2918.

45. L. E. Felberg, D. H. Brookes, E. Jurrus, N. Baker, and T. Head-Gordon (2017). PB-AM: An open-source, fully analytical linear Poisson-Boltzmann solver. *J. Comp. Chem. (Brooks Festschrift)* 38 (15), 1275-1282

46. L. Ruiz Pestana, N. Mardirossian, M. Head-Gordon, T. Head-Gordon (2017). Ab initio simulations of liquid water using high quality meta-GGA functionals. *Chemical Science* 8, 3554 – 3565.

47. L.-P. Wang, K. A. McKiernan, J. Gomes, K. A. Beauchamp, T. Head-Gordon, J. E. Rice, W. C. Swope, T. J. Martínez, V. S. Pande (2017). Building a more predictive protein force field: a systematic and reproducible route to AMBER-FB15. *J. Phys. Chem. B* 121 (16), 4023–4039.

48. Y. Mao, Y. Shao, J. Dziedzic, C.-K. Skylaris, T. Head-Gordon, M. Head-Gordon (2017). Performance of the AMOEBA water model in the vicinity of QM solutes: a diagnosis using energy decomposition analysis. *J. Chem. Theory Comput.* 13 (5), 1963–1979.

49. S. Sasmal, J. Lincoff, and T. Head-Gordon (2017). Effect of a paramagnetic spin label on the intrinsically disordered peptide ensemble of amyloid-β. *Biophys. J.* 113 (5), 1002-1011.

50. O. N. Demerdash, Y. Mao, T. Liu, M. Head-Gordon, T. Head-Gordon (2017). Assessing many-body contributions to intermolecular interactions of the AMOEBA force field using energy decomposition analysis of electronic structure calculations. *J. Chem. Phys.* 147, 161721.

51. D. H. Brookes and T. Head-Gordon (2016). Experimental inferential structure determination of ensembles for intrinsically disordered proteins. *J. Am. Chem. Soc.* 138 (13), 4530–4538.

52. A. Bhowmick, S. Sharma, T. Head-Gordon (2016). The role of side chain entropy and mutual information for improving the de novo design of Kemp Eliminases KE07 and KE70. *Phys. Chem. Chem. Phys.* 18, 19386-19396

53. O. N. Demerdash and T. Head-Gordon (2016). Electrostatic embedding schemes for the many-body approximation of classical polarizable models. *J. Chem. Theory Comput.* 12 (8), 3884–3893

54. Y. Mao, P. R. Horn, N. Mardirossian, C.-K. Skylaris, T. Head-Gordon, M. Head-Gordon (2016). Approaching the basis set limit for DFT calculations using an environment-adapted minimal basis with perturbation theory: Formulation, proof of concept, and a pilot implementation. *J. Chem. Phys.* 145, 044109.

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<u>Invited Presentations (since 1999)</u>

1.   *Coarse Graining Electrons: Fast and Accurate Representations of Electrostatic Interactions*. 2020 Allergen Lecturer. CSU Long Beach, April 8, 2020.

2.   *Chemical Reactivity in Complex Environments: New Methods and Models.* Symposium on Molecular Capsules: from Design to Application, CATL division, ACS National Meeting & Exposition, Philadelphia, PA, March 22 - 26, 2020.

3.   *Chemical Reactivity in Complex Environments: New Methods and Models.* Department of Chemistry Colloquium, University of Michigan March 12, 2020.

4. *Coarse Graining Electrons: Fast and Accurate Representations of Electrostatic Interactions*. Department of Chemistry Colloquium, University of Maryland, College Park March 9, 2020.

5. *APS Symposium Organizer with M. Bonn.* American Physical Society, Division of Chemical Physics Focus Symposium "Water Dynamics in Different Environments: Experiment and Theory", Denver, Colorado March 2-6, 2020.

6. *Fast and Accurate Representations of Electrostatic Interactions*. Beyond point charges: novel electrostatic developments in force fields. CECAM Workshop, Lausanne, Switzerland, December 16 – 18, 2019.

7. *Coarse Graining Electrons: Fast and Accurate Representations of Electrostatic Interactions*. Department of Chemistry Colloquium, Florida State University, December 6, 2019.

8. *Chemical Reactivity in Complex Environments*. 15th Condensed Phase and Interfacial Molecular Science. Washington DC, November 4-6, 2019.

9. *Many-Body Force Fields for Water: Reaching Spectroscopic Accuracy.* WaterEurope: Multiscale simulations and coarse-grained models for water and aqueous systems. CECAM Workshop, Lausanne, Switzerland, October 21 – 23, 2019

10. *Coarse Graining Electrons: Fast and Accurate Representations of Electrostatic Interactions* (Keynote Lecture). Department of Chemistry, University of Vermont, Esther and Bingham J. Humphrey Memorial Symposium, October 4–5, 2019.

11. *Anisotropic Atomic Polarizability, Charge Transfer, and Charge Equilibration Models Solved with Reduced SCF and SCF-Less Methods.* Quantum Systems in Chemistry, Physics, and Biology, Workshop XXIV, Park City, Utah, September 22–27, 2019

12. *Chemical Reactivity in Complex Environments (Keynote Lecture)*. Current Trends in Theoretical Chemistry VIII. Kraków, Poland, September 1–5, 2019.

13. *Coarse-Grained Models for Liquid-Liquid Phase Separation of Intrinsically Disordered Proteins*. Symposium on Advances in Multiscale Modeling, COMP division, ACS Fall 2019 National Meeting & Exposition in San Diego, CA, August 25–29, 2019.

14. *Anisotropic Atomic Polarizability, Charge Transfer, and Charge Equilibration Models Solved with Reduced SCF and SCF-Less Methods.* TINKER-CHARMM Workshop, Paris, France July 18–22, 2019

15. *How to Make an Enzyme: Computational Optimization of Electric Fields for Better Catalysis Design*. 10th congress of the International Society of Theoretical Chemical Physics (ISTCP) in Computational Biophysics. Tromsø, Norway, July 11–17, 2019.

16. *How to Make an Enzyme: Computational Optimization of Electric Fields for Better Catalysis Design*. Free Energy Calculations: Entering the Fourth Decade of Adventure in Chemistry and Biophysics. Santa Fe, New Mexico, June 16–21, 2019.

17. *Chemical Reactivity in Complex Environments*. Northern West Coast Theoretical Meeting, UC Berkeley, Berkeley, California, May 19, 2019.

18. *Computational optimization of electric fields for better catalysis design.* Symposium on Elucidating the Roles of Electric Fields in Catalysis, CATL division, ACS National Meeting & Exposition, Orlando, Florida March 31–April 4, 2019.

19. *Combined force-field sampling problem in simulations of disordered amyloid-β peptides*. Symposium on Sampling Conformations & Pathways in Biomolecular Systems: Recent Developments & Applications, COMP division, ACS National Meeting & Exposition, Orlando, Florida March 31–April 4, 2019.

20. *Advanced force fields with anisotropic atomic polarizability and charge transfer and solved with SCF-less methods.* Symposium on Electron-Molecule & Molecule-Molecule Interactions. COMP division, ACS National Meeting & Exposition, Orlando, Florida March 31–April 4, 2019.

21. *The Role of Interfaces for Chemical Transformations and Transport under Confinement.* Aqueous solutions, solvated interfaces, and ionic polarization (DCOMP, DCP), American Physical Society, Boston Massachusetts, March 4–8, 2019.

22. *The Role of Interfaces for Water and Binary Systems under Confinement.* Conference on Ab-Initio Modelling of Molecular Processes Under Confinement. Madrid, Spain, December 3–5, 2018.

23. *The Role of Interfaces for Water and Binary Systems under Confinement.* Theoretical Chemistry Colloquium, Oxford University, Oxford, U. K. October 15, 2018

24. *The Role of Interfaces for Water and Binary Systems Under Confinement.* Division of Inorganic Chemistry, Women in Nanotechnology. 256th ACS National Meeting, Boston, MA, August 19–23, 2018.

25. *New Methods and Models for Condensed Phase Simulations.* Division of Chemical Education, Frontiers in Computational Chemistry: Bridging the Gap Between Theory & Experiment. Symposium in honor of Jeff Madura. 256th ACS National Meeting, Boston, MA, August 19–23, 2018.

26. *Reducing and Eliminating Self-Consistent Field Calculations in Classical and Ab Initio Simulations.* Solving or Circumventing Eigenvalue Problems in Electronic Structure Theory. MolSSI Workshop and ELSI Conference, Richmond, Virginia, August 15–17, 2018.

27. *New Methods and Models for Condensed Phase Simulations.* 2018 Gordon Conference on Computational Chemistry. Mount Snow, West Dover, Vermont, July 22–27, 2018.

28. *New Methods and Models for Condensed Phase Simulations.* Many-Body Interactions: From Quantum Mechanics to Force Fields. TSRC, Telluride, Colorado, July 9–13, 2018.

29. *New Methods and Models for Condensed Phase Simulations.* TINKER Workshop. Austin, Texas June 2–4, 2018.

30. *New Methods and Models for Condensed Phase Simulations.* VIII Modeling and Design of Molecular Materials, Polanica Zdrój, Poland June 24–28, 2018.

31. *New Methods and Models for Condensed Phase Simulations.* Assessing Complex Free Energy Surfaces from Molecular Simulations from Electronic Structure to Mesoscopic Processes. 101st Canadian Chemistry Conference and Exhibition, Canadian Society for Chemistry, Edmonton May 27–31, 2018

32. *Computational Methods and Models for Generating and Evaluating Protein Ensembles.* Computational Modelling of Biomolecular Systems: From Structure to Function. 101st Canadian Chemistry Conference and Exhibition, Canadian Society for Chemistry, Edmonton May 27–31, 2018.

33. *How to Win Scientific Friends and Influence Scientific Frenemies: Team Science.* 2018 Computational and Theoretical Chemistry Research PI Meeting. Basic Energy Sciences, DOE, Gaithersburg, MD. May 22–24, 2018.

34. *Computational Methods and Models for Generating and Evaluating Protein Ensembles.* Department of Molecular Pharmacology, Physiology, and Biotechnology, Brown University, March 15, 2018

35. *New Methods and Models for Condensed Phase Simulations.* ICERM workshop Fast Algorithms for Generating Static and Dynamically Changing Point Configurations. Brown University, March 14, 2018

36. *Methods and Models for Condensed Phase Simulations of Water.* 58th Sanibel Symposium, celebrating Bob Parr and his legacy Feb. 18–23, 2018.

37. *New Methods and Models for Condensed Phase Simulations.* Chemistry Colloquium, Iowa State University, January 12, 2018.

38. *New Methods for Generating and Evaluating Conformational Ensembles.* Gordon Research Conference: Protein Dynamics, Galveston, Texas, January 7–12, 2018.

39. *The Role of Interfaces for Water and Binary Systems under Confinement.* RESOLV Colloquium, Ruhr University, Bochum, Germany, October 25, 2017.

40. *The Role of Interfaces for Water and Binary Systems under Confinement.* 13th Condensed Phase and Interfacial Molecular Science. Washington DC, October 18, 2017.

41. *New Methods and Models for Condensed Phase Simulations.* WATOC 2017, Munich, Germany, August 27–September 1, 2017.

42. *New Methods for Generating and Evaluating Conformational Ensembles.* Biophysical Society: Conformational Ensembles from Experimental Data and Computer Simulations, Berlin, Germany, August 25–29, 2017

43. *Statistical Fluctuations, Dynamics, Scaffolds, Electric Fields, and De Novo Enzyme Catalysis.* American Chemical Society, Catalysis division. Washington DC, August 22, 2017

44. *Statistical Fluctuations, Dynamics, Scaffolds, Electric Fields, and De Novo Enzyme Catalysis.* Telluride Science Research Center Workshop on Protein Dynamics. Telluride, CO July 31 - August 4, 2017.

45. *Computational Methods and Models for Condensed Phase Simulation.* American Conference on Theoretical Chemistry (ACTC), Boston Massachusetts, July 16 - 21, 2017.

46. *Computational Methods and Models for Intrinsically Disordered Peptides.* Gordon Research Conference: Computational Aspects of Biomolecular NMR; Sunday River, Maine June 11-16, 2017.

47. *Molecular Sciences Software Institute and Computational Chemistry;* American Chemical Society, California Section; Chevron auditorium, Richmond, CA May 31, 2017.

48. *Computational Methods and Models for Intrinsically Disordered Peptides.* CBSB2017: From Computational Biophysics to Systems Biology. University of Cincinnati, May 18-20, 2017.

49. *Molecular Sciences Software Institute and Molecular Simulation.* Computational Chemistry/Science Gateway Workshop, Jackson State University, Mississippi, May 9-11, 2017

50. *Statistical Fluctuations, Dynamics, Scaffolds, Electric Fields, and De Novo Enzyme Catalysis.* Merck Chemistry Seminars; Rahway, New Jersey, April 28, 2017.

51. *Methods and models for condensed phase simulation of water;* ACS COMP: Computational Studies of Water; San Francisco, Ca. April 2-6, 2017

52. *The Role of Statistical Fluctuations and Electrostatics in the Improvements of De Novo Enzyme Catalysis*; ACS PHYS: Long Range Correlated Motions in Proteins, San Francisco, Ca. April 2-6, 2017

53. *Computational Methods and Models for Intrinsically Disordered Peptides.* 58th Experimental NMR Conference (ENC): Pacific Grove, California, March 26-31, 2017.

54. *Polarizable Force Fields for Condensed Phase Simulation.* Tinker Software Developers Conference, Washington University in St. Louis; March 16-18, 2017

55. *Two Illustrative Cases for Cyberinfrastructure: Advanced Force Fields and Intrinsically Disordered Proteins.* Workshop for Cyberinfrastructure/MolSSI. Rice University Houston, Tx. October 8-10, 2016.

56. *Polarizable Force Fields for Condensed Phase Simulation (Plenary Lecture)* CCP5 Annual General Meeting, Harper Adams University, U.K. September 12-14, 2016

57. *Polarizable Force Fields for Condensed Phase Simulation* Annual EMLG-JMLG Meeting, Chania, Crete, Greece, September 11 – 16, 2016.

58. *Polarizable Force Fields for Condensed Phase Simulation* ACS COMP: Modeling Water and Solvation in Biochemistry: Developments and Applications. Philadelphia, PA August 21-25, 2016.

59. *Computational Methods and Models for Intrinsically Disordered Peptides,* ACS PHYS: Intrinsically Disordered Proteins: Structure, Function, and Interactions. Philadelphia, PA August 21-25, 2016.

60. *Polarizable Force Fields for Condensed Phase Simulation* TSRC: Many-Body Interactions: From Quantum Mechanics to Force Fields. Telluride, Colorado, July 12-16, 2016.

61. *Polarization Approximations for Atomistic and Coarse-Grained Models.* TSRC: Ions in Solution and Molecular Biology: Theory, Modeling, and Experiment. Telluride, Colorado. July 12-16, 2016.

62. *Statistical Fluctuations, Dynamics and De Novo Enzyme Catalysis.* GdCh - Kolloquium: Ruhr University, Bochum Germany, June 30, 2016

63. *Statistical Fluctuations, Dynamics and De Novo Enzyme Catalysis.* CECAM: Enzyme Engineering: Bright Strategies from Theory and Experiments, Lausanne, June 27-29, 2016

64. *Statistical Fluctuations, Dynamics and De Novo Enzyme Catalysis.* Plenary Speaker, Royal Society of Chemistry Mini-Symposium on Advanced Potential Energy Surfaces, University of Southampton, UK, April 8, 2016

65. *Advanced Potential Energy Surfaces for Condensed Phase Simulation* CECAM: Beyond point charges: novel electrostatic developments in force fields. Lausanne, April 3-7, 2016.

66. *Polarizable Force Fields for Condensed Phase Simulation* ACS PHYS. San Diego, California, March 13-17, 2016.

67. *Computational Methods and Models for Intrinsically Disordered Peptides,* ACS COMP. San Diego, California, March 13-17, 2016.

68. *Statistical Fluctuations, Dynamics and De Novo Enzyme Catalysis.* Chemical and Biomolecular Engineering seminar, University of Illinois, Urbana. March 10, 2016

69. *Advanced Potential Energy Surfaces for Condensed Phase Simulation* Symposium on Synergistic Relationships between Computational Chemistry and Experiment, Pacifichem, December 15-20, 2015.

70. *Advanced Potential Energy Surfaces for Water Simulations.* Symposium on Liquids and Glassy Soft Materials: Theoretical and Neutron Scattering Studies, Materials Research Society, November 29 - December 4, 2015, Boston, Massachusetts.

71. *Atomistic and Coarse-Grained Models and Methods for Electrostatics.* 11th Condensed Phase and Interfacial Molecular Science. Washington DC, November 3, 2015.

72. *All Atom and Coarse-Grained Models and Methods for Electrostatics.* Mathematical Biosciences Institute Workshop 2: Multiple Faces of Biomolecular Electrostatics. Columbus, Ohio, October 12-16, 2015.

73. *Development and Deployment of Chemical Software for Advanced Potential Energy Surfaces.* Telluride Workshop. THG, J. Ponder, J. Essex, co-organizers, June 14-20, 2015.

74. *Statistical Fluctuations, Dynamics and De Novo Enzyme Catalysis.* Albany 2015: The 19th Conversation, University of Albany, New York, June 9-13, 2015.

75. *Advanced Potential Energy Surfaces for Solvation.* German Bunsen-Society for Physical Chemistry, Bunsentagung 2015, Ruhr-Universität Bochum, Germany, May 14-16, 2015

76. *Statistical Fluctuations, Dynamics and De Novo Enzyme Catalysis.* Physical Chemistry Seminar, University of Oregon, May 4, 2015.

77. *Determining the Structural Ensemble of Intrinsically Disordered Disease Peptides combining Theory and Experiment: Applications to Alzheimer's Disease Biology.* Lorentz Center Workshop on Amyloid Aggregation: Single Molecule Approaches to a Many Molecule Problem, Leiden University, Netherlands April 13 - 17, 2015

78. *Determining the Structural Ensemble of Intrinsically Disordered Disease Peptides combining Theory and Experiment: Applications to Alzheimer's Disease Biology.* ACS PHYS. Denver, Colorado, March 22, 2015.

79. *Advanced Potential Energy Surfaces for Water Simulations.* ACS COMP. Denver, Colorado, March 25, 2015.

80. *Advanced Potential Energy Surfaces for Condensed Phase Simulation.* Frontiers in Materials Science Lecture Series. Pacific Northwest National Laboratories. Jan. 26, 2015.

81.   *The Future of Molecular Simulation.* NSF Conceptualization Workshop. Houston, Texas Jan. 22-24, 2015.

82.   *New Polarizable Models for Water.* Workshop on Fundamental Problems in the Physics and Chemistry of Water. Houston, Texas Jan. 16, 2015.

83.   *Statistical Fluctuations, Dynamics and De Novo Enzyme Catalysis.* CCP-BioSim, Leeds, UK Jan. 7-9, 2015.

84.   *Determining the Structural Ensemble of Intrinsically Disordered Disease Peptides combining Theory and Experiment: Applications to Alzheimer's Disease Biology.* University of Illinois, Urbana-Champagne. Theoretical and Computational Biophysics Seminar series. Nov. 10, 2014.

85.   *Advanced Potential Energy Surfaces for Condensed Phase Simulation.* WATOC 2014. Santiago, Chile Oct. 5-10, 2014.

86.   *Statistical Fluctuations, Dynamics and De Novo Enzyme Catalysis.* DFT-Day: New Approaches in Theoretical Chemistry, Santiago, Chile Oct. 4, 2014.

87.   *The Future of Molecular Simulation.* NSF Conceptualization Workshop. Berkeley, CA Sept. 18-20, 2014.

88.   *Methods and Models and Software for Molecular Simulation.* The Future of Computational Chemistry. PHYS, ACS in San Francisco, CA August 10-14, 2014.

89.   *Conformational Sampling Methods and Applications to Protein Kinases.* Modeling of Protein Kinases and Phosphorylation. COMP, ACS in San Francisco, CA August 10-14, 2014.

90.   *Polarization Approximations for Atomistic and Coarse-Grained Models*. International Conference on Chemical Bonding, Kauai, Hawaii, on July 24-28, 2014.

91.   *Polarization Approximations for Atomistic and Coarse-Grained Models.* TSRC: Ions in Solution and Molecular Biology: Theory, Modeling, and Experiment. Telluride, Colorado. July 7-11, 2014.

92.   *Problem-driven Coarse Grained Models.* Coarse-graining as a Frontier of Statistical Mechanics, Santa Fe, New Mexico, June 15-19, 2014.

93.   *Session Chair: Misfolding and Aggregation.* Gordon Research Conference on Biopolymers. Salve Regina, Rhode Island. June 1-6, 2014.

94.   *Engineering, Ethics, and the Future of Energy.* Lecture to BioE Honor Society Competition for Regional High Schools. UC Berkeley, April 19, 2014

95.   *Statistical fluctuations, Dynamics and De Novo Enzyme Catalysis.* Hauptman Woodward Medical Research Institute, Buffalo, New York, March 26, 2014

96.   *Panelist: Software Institutes in Building Communities of Scientific Software Practice.* Software Sustainability / SSI-SSE PI Workshop, Westin, Arlington, VA. February 24, 2014.

97.   *Atomistic and Coarse-Grained Models for Biomolecular Simulations.* Biophysical Society, San Francisco February 16, 2014

98.   *All Atom and Coarse-Grained Studies of the Alzheimer's Amyloid-β Peptide.* Biophysics Department Seminar. Johns Hopkins University, December 2, 2013.

99.   *All Atom and Coarse-Grained Studies of the Alzheimer's Amyloid-β Peptide.* Computational Biology Seminar series, Duke University, October 28, 2013

100.   *The 2013 Nobel Prize in Chemistry.* General audience talk. School of Management, University of San Francisco, October 21, 2013.

101.   *Atomistic and Coarse-Grained Models of Water and Solutes*. Keynote speaker. Black Forest Focus on Protein Dynamics: From Water Hydration to Crowding Effects. Freiburg Institute for Advanced Studies. Freiberg, Germany, September 25-29, 2013

102.   *Atomistic and Coarse-Grained Models of Water*. ACS Symposium Theory and Experiment on Water and Hydration. Indianapolis, Indiana September 8-12, 2013.

103.   *Determining the Structural Ensemble of Amyloid-β Peptides in Aqueous and Membrane Environments.* Laboratory of Chemical Physics, National Institutes of Health. Washington, D.C. July 26, 2013.

104.   *Session Chair,* GRC on Biological molecules in the Gas Phase and in Solution. Holderness School, New Hampshire July 21-26, 2013.

105.   *Engineering, Ethics, and the Future of Energy.* Lecture to National Leadership Student Council. Berkeley Art Museum, July 8, 2013.

106.   *Computing Experimental Observables from Molecular Simulation: Insights and Predictions.* Niels Bohr International Academy. Copenhagen, Denmark June 26-30, 2013.

107.   *Solvation Influence on Enzyme Catalysis and Intrinsically Disordered Peptides*. RESOLV International Symposium on Solvation. Ruhr Universitat, Bochum Germany June 3-7, 2013.

108.   *Computing Experimental Observables from Molecular Simulation: Insights and Predictions.* Department of Chemistry, UC Riverside May 15, 2013.

109. *All Atom and Coarse-Grained Studies of the Alzheimer's Amyloid-β Peptide.* Department of Chemistry, University of Maryland April 26, 2013

110. *Dynamical Measurements of Native and De Novo Enzyme Catalysis.* Workshop at Durham Institute for Advanced Studies. Durham, UK April 17-20, 2013.

111. *Dynamical Measurements of Native and De Novo Enzyme Catalysis.* Conference on Protein Dynamics and Function. Durham University, UK April 15-17. 2013

112. *Statistical fluctuations, Dynamics and De Novo Enzyme Catalysis.* IBM Almaden. San Jose, Ca April 4, 2013.

113. *Session Chair,* 2013 Berkeley Mini Statistical Mechanics Meeting. January 11-13, 2013.

114. *Dynamical Measurements of Native And De Novo Enzyme Catalysis.* PHYS, American Chemical Society in Philadelphia, PA August 19-23, 2012.

115. *Dependence of the Biomolecular Rate of Protein-Protein Association under Crowding Conditions.* COMP, American Chemical Society in Philadelphia, PA August 19-23, 2012.

116. *New Force Fields for Molecular Processes at Liquid Interfaces.* COMP, American Chemical Society in Philadelphia, PA August 19-23, 2012.

117. *Coarse-Grained Studies of the Alzheimer's Amyloid-β Peptide.* COMP, American Chemical Society in Philadelphia, PA August 19-23, 2012.

118. *Intrinsically Disordered Proteins: When Water Really Matters.* Gordon Research Conference on Computational Chemistry. Mt. Snow, Vermont. July 22-27, 2012.

119. *Energy Landscapes of Native and De Novo Enzyme Catalysis.* ESF-LFUI Conference on Energy Landscapes. Obergurgl, Austria. July 16-21, 2012.

120. *Fixed Charge and Polarizable Force Fields: Part 1.* TSRC Many-Body Interactions: From Quantum Mechanics to Force Fields. Telluride, Colorado. July 2-6, 2012.

121. *Fixed Charge and Polarizable Force Fields: Part 2.* TSRC Interfacial Molecular and Electronic Structure and Dynamics. Telluride, Colorado. July 2-6, 2012.

122. *Incorporating Dynamics into Design of De Novo Enzyme Catalysis.* Gordon Research Conference on Biopolymers. Salve Regina, Rhode Island. June 3-8, 2012.

123. *From Monomer Structure to Fibril Polymorphism: Computational and Experimental Studies of the Alzheimer's Aβ Peptide.* Department of Computational Biology, University of Pittsburgh, Pennsylvania, March 25, 2012.

124. *Dynamical Measurements of Native and De Novo Enzyme Catalysis.* Chemical Biology, Vanderbilt University, Nashville Tennessee. February 15, 2012.

125. *Computing Experimental Observables from Molecular Simulation: Insights and Predictions.* Department of Chemistry, UC Berkeley January 24, 2012.

126. *Coarse-Graining and Multiscale Models for Biological Systems.* US-UK ACV Network, Nottingham University UK, Nov. 4-7, 2011.

127. *From Monomer Structure to Fibril Polymorphism: Computational and Experimental Studies of the Alzheimer's Aβ Peptide.* Department of Biomedical Engineering, University of Texas A&M, College Station, Texas, October 10, 2011.

128. *Computing Experimental Observables from Molecular Simulation: Insights and Predictions.* PHYS, American Chemical Society in Denver, Colorado August 28-Sept. 1, 2011.

129. *Explorations of Water and Hydration by Experiment and Theory.* Gordon Research Conference on Biological Molecules in the Gas Phase. Andover, New Hampshire July 31- Aug. 31, 2011.

130. *Bioethics of Emerging Technologies for the Physician.* American Medical Student Association, UC Berkeley, March 31, 2011.

131. *Coarse-Graining and Multiscale Models for Biological Systems.* Modeling Electrostatics in Molecular Biology Conference. Clemson University, South Carolina April 4 -6, 2011.

132. *Incorporating Measurements of Dynamics in Computational De Novo Enzyme Design.* Joint BioEnergy Institute, Emeryville, Ca. March 4, 2011.

133. *Interplay of Experiment and Theory for Biological and Chemical Systems.* Department of Chemistry, Northwestern University, Evanston, Illinois, February 16, 2011.

134. *The Structure of Ambient Water*. Computational Materials Science and Chemistry Network. Princeton University, New Jersey, Dec. 6-8, 2010.

135. *Coarse-Graining and Multiscale Models for Biological and Chemical Systems.* Workshop on Novel Simulation Approaches to Soft Matter Systems. Max Planck Institute for the Physics of Complex Systems, Dresden, Germany, September 20 -24, 2010.

136. *Coarse-Graining and Multiscale Models for Biological and Chemical Systems.* Symposium on Multiscale Modeling and Simulations. PHYS, American Chemical Society in Boston, Massachusetts August 21-26, 2010.

137.   *Interplay of Experiment and Theory for Biological and Chemical Systems.* Yale University, Connecticut, August 19-20, 2010.

138.   *Overview of Water in Biology* (session chair). Gordon Research Conference on Water & Aqueous Solutions, Holderness School, New Hampshire, August 8-13, 2010.

139.   *Thermodynamic and Dynamical Anomalies of Water.* Dynasoft 2010: Dynamics in Soft Condensed Matter, Cargese, Corsica, July 31-August 8, 2010.

140.   *Energy Landscapes and Water Anomalies.* Energy Landscapes Workshop, Chemnitz, Germany, June 21-July 5, 2010.

141.   *Biological Interfaces: Theoretical and Experimental Investigations* Recent Advances at the Bio/Abio Interface, Christchurch, New Zealand, June 22-24, 2010.

142.   *Explorations of Water by Experiment and Theory.* Telluride workshop on Many-Body Interactions, Telluride, Colorado, June 12-18, 2010.

143.   *Hydration Water Dynamics Near Biological Interfaces.* Invited speaker for symposium on biological water. American Physical Society, Portland, Oregon, March 16, 2010.

144.   *Coarse-Graining Approaches for Biological Systems.* Workshop on Multiscale Modeling and Simulations of Hard and Soft Materials at JNCASR, Bangalore, India, December 7 - 20, 2009.

145.   *Challenges and Opportunities in Biomolecular Simulation.* MasterWorks Talk, Supercomputing 2009, Portland, Oregon Nov. 14-20, 2009.

146.   *From Monomer Structure to Polymorphism: Computational and Experimental Studies of the Alzheimer's Aβ Peptide.* Dept. of Chemical & Biomolecular Engineering, U. Akron, October 13, 2009.

147.   *Coarse-Graining Approaches for Chemical and Biological Systems.* Department of Chemical Engineering, Tulane University, September 25, 2009.

148.   *From Monomer Structure to Polymorphism: Computational and Experimental Studies of the Alzheimer's Aβ Peptide.* PHYS, American Chemical Society in Washington DC August 16-20, 2009.

149.   *Dynamics and Protein Enzyme Design.* Workshop on Function and Dynamics of Biomolecules. Keveli Institute of Theoretical Physics, Beijing, China, July 29-August 7, 2009.

150.   *Coarse-Graining Approaches for Biological Systems.* MM2009, Keynote Lecturer, Gold Coast (Surfers Paradise), Queensland, Australia, July 26-29, 2009.

151.   *Hydration Water Dynamics Near Biological Interfaces.* Proteins and Water Workshop, Tempe, Arizona, May 10-13, 2009.

152.   *Challenges and Opportunities in Biomolecular Simulation.* Large Scale Production Computing Requirements for Biological and Environmental Research. Washington DC, May 7-8, 2009.

153.   *Challenges and Opportunities in Biomolecular Simulation.* National Academies of Science workshop: Vision for R&D in Simulation-Based Engineering and Science in the Next Decade. Washington DC, April 22-23, 2009.

154.   *From Monomer Structure to Polymorphism: Computational and Experimental Studies of the Alzheimer's Aβ Peptide.* American Society for Biochemistry and Molecular Biology, New Orleans, Louisiana, April 18- 22, 2009.

155.   *From Monomer Structure to Polymorphism: Computational and Experimental Studies of the Alzheimer's Aβ Peptide.* Center for Computational Biology (CCB) Colloquium, Washington University, St. Louis, Mo. April 13, 2009.

156.   *Polarizable Models: Hydration Water Dynamics Near Biological Interfaces.* PHYS, American Chemical Society in Salt Lake City, Utah March 22-26, 2009.

157.   *Challenges and Opportunities in Enzyme Design.* Synthetic Biology Retreat. Berkeley, CA March 14, 2009.

158.   *From Monomer Structure to Polymorphism: Computational and Experimental Studies of the Alzheimer's Aβ Peptide.* Department of Chemistry, University of Cincinnati, November 21, 2008.

159.   *Coarse-Graining Approaches for Biological Systems.* Institute for Mathematics and its Applications. Development and Analysis of Multiscale Methods, University of Minnesota, November 3-7, 2008

160.   *From Monomer Structure to Polymorphism: Computational and Experimental Studies of the Alzheimer's Aβ Peptide.* Department of Chemistry, Utah University, October 27, 2008.

161.   *A Molecular View of Bulk and Interfacial Water from Theory and Experiment.* Department of Chemistry, New York University, October 17, 2008.

162.   *A Molecular View of Bulk and Interfacial Water from Theory and Experiment.* Eighth Conference of the World Association of Theoretically Oriented Chemists (WATOC). Sydney, Australia, September 16-21, 2008.

163.   *A Molecular View of Bulk and Interfacial Water from Theory and Experiment.* Symposium on Water mediated interactions: PHYS, American Chemical Society in Philadelphia, Pa. August 17-21, 2008.

164. *Coarse-Grained Molecular Models of Protein Complexation.* SIAM Conference on the Life Sciences, Mini-symposium on Mathematical Challenges in Multiscale Biosystems Modeling, Montreal, Quebec, Canada. August 4- 7, 2008.

165. *A Molecular View of Bulk and Interfacial Water from Theory and Experiment.* International Workshop on Aqueous Solutions and Their Interfaces, Crete, Greece, June 22-27, 2008

166. *Investigations Using NMR And Simulation Using Polarizable Force Fields On Ab Peptide Structure.* Workshop on the Development of Force Fields using Ab Initio Electronic Structure Calculations. Telluride Science Research Center, Colorado, July 6-11, 2008.

167. *Contrasting Disease and Non-Disease Protein Aggregation.* Symposium on Multiscale Modeling in Biophysics: PHYS, American Chemical Society in New Orleans, Louisiana, April 6-10, 2008.

168. *Enhanced sampling methods for characterizing Ab peptide structure.* Symposium on replica exhange: COMP, American Chemical Society in New Orleans, Louisiana, April 6-10, 2008.

169. *From Monomer Structure to Polymorphism: Computational and Experimental Studies of the Alzheimer's Aβ Peptide.* Department of Chemistry, Ohio State University, February 5, 2008.

170. *A Molecular View of Bulk and Interfacial Water from Theory and Experiment.* Plenary Speaker, International Workshop on Molecular Structure and Dynamics of Interfacial Water, Shanghai, China, December 14-21, 2007.

171. *A Molecular View of Liquid Water and Aqueous Hydration from Theory and Experiment.* Department of Chemistry, University of New Orleans, Nov. 16, 2007.

172. *Contrasting Disease and Non-Disease Protein Aggregation.* Department of Chemistry, Case Western Reserve University, Oct. 18, 2007.

173. *A Molecular View of Bulk and Interfacial Water from Theory and Experiment.* Keynote Speaker, Maria Goeppert-Mayer Symposium, Regional ACS meeting San Diego, California, October 12, 2007.

174. *A Molecular View of Liquid Water and Aqueous Hydration from Theory and Experiment.* Department of Chemistry, Kent State University, Fall, 2007.

175. *A Molecular View of Liquid Water and Aqueous Hydration from Theory and Experiment.* Department of Polymer Chemistry, Akron University, Fall, 2007.

176. *The Relationship between Bulk Water and Protein Dynamical Transitions.* Symposium on Hydration: From clusters to aqueous solution: PHYS, American Chemical Society in Boston, MA, August 19-23, 2007.

177. *Contrasting Disease and Non-Disease Protein Aggregation.* Mini-symposium on Computational Biomechanics: From Biomolecules to Organisms. 9th US National Congress on Computational Mechanics, San Francisco July 23-26, 2007.

178. *From Monomer Structure to Polymorphism: Computational and Experimental Studies of the Alzheimer's Aβ Peptide.* Presentation to ITRI Institute in Taiwan, UC Berkeley, June 11, 2007.

179. *From Monomer Structure to Polymorphism: Computational and Experimental Studies of the Alzheimer's Aβ Peptide..* Department of Chemistry, UC Berkeley, April 3, 2007.

180. *A Molecular View of Liquid Water and Aqueous Hydration from Theory and Experiment..* Department of Chemistry, U. C. Santa Barbara, December 4, 2006.

181. *Determining the Critical Nucleus and Mechanism of Fibril Elongation of the Alzheimer's Aβ1-40 Peptide.* Laboratory of Chemical Physics, National Institutes of Health. Washington, D.C. October 26, 2006.

182. *A Molecular View of Liquid Water and Aqueous Hydration from Theory and Experiment.* Condensed Phase and Interfacial Molecular Science, Airlie Conference Center, Virginia, October 22-25, 2006.

183. *Understanding Hydrophobic Solvation using Not-Water Models.* 62nd Southwest Regional Meeting of the American Chemical Society in Houston, TX, October 19-22.

184. *A Molecular View of Liquid Water from Theory and Experiment.* Chemical Biophysics Mini-symposia. University of Pennsylvania, October 12, 2006.

185. *A Molecular View of Liquid Water from Theory and Experiment.* Harvey Mudd College and Pomona College, California, October 10, 2006.

186. *Cyber-enabled Chemistry.* Symposia organizer for the American Chemical Society, September 10-15, 2006.

187. *A Molecular View of Liquid Water from Theory and Experiment.* ISIS seminar at Rutherford Appleton Laboratory, Oxford, UK July 18, 2006.

188. *Protein Folding and Aggregation* Isolated Biomolecules and Biomolecular Interactions: Theory and Experiment. Trest Castle, Czech Republic, May 9-14, 2006.

189. *Protein Folding and Aggregation*, CECAM Workshop on Protein Aggregation. Lyon, France, May 22-25, 2006.

190. *A Molecular View of Liquid Water from Theory and Experiment.* Institut fuer Physikalische und Theoretische Chemie Johann Wolfgang Goethe Universitaet, Frankfurt, Germany April 10, 2006.

191. *A Molecular View of Liquid Water from Theory and Experiment.* Physical Chemistry seminar. Nottingham University, UK, March 15, 2006.
192. *A Molecular View of Liquid Water from Theory and Experiment.* Schlumberger Lecture. Cambridge University, UK, February 15, 2006.
193. *A Molecular View of Bulk Liquid and Hydration Water.* Physical Chemistry seminar. Lugano, Switzerland, February 13, 2006.
194. *A Molecular View of Bulk Liquid and Hydration Water.* Physical Chemistry seminar. Oxford University, UK, January 30, 2006.
195. *Protein Folding and Aggregation.* Biophysics Seminar Series, Cambridge University, UK, January 20, 2006.
196. *Contrasting Disease and Non-Disease Protein Aggregation.* Gordon Research Conference on Protein Folding Dynamics, Ventura, California, January 8-13, 2006.
197. *A Molecular View of Bulk and Hydration Water.* Theoretical Chemistry Seminar, Cambridge University, October 12, 2005.
198. *Comparing Aggregation Mechanism and Morphologies between Disease and Non-Disease Proteins* Protein Society 19th Symposium, Boston, Massachusetts. July 30-August 3, 2005.
199. *Protein Folding and Aggregation.* Laboratory of Biophysics and Laboratory of Chemical Physics, National Institutes of Health. Washington, D.C. May 26, 2005.
200. *A Molecular View of Hydration Water Dynamics.* NIST Center for Neutron Research (NCNR), Washington, D.C. May 23, 2005.
201. *Cyberinfrastructure for Computational Biology and Chemistry.* CITRIS Corporate Day, NASA Ames/Santa Cruz, California April 18, 2005.
202. *Anomalous hydration dynamics as a function of temperature near a model hydrophobic peptide.* Symposium in Honor of Michael Klein. American Chemical Society, San Diego, California March 16-23, 2005.
203. *Protein Folding and Aggregation.* Center for Biomolecular Science and Engineering. University of California, Santa Cruz. February 8, 2005.
204. *Protein Folding and Aggregation.* Seventh Conference of the World Association of Theoretically Oriented Chemists (WATOC). Cape Town, South Africa, January 16-21, 2005.
205. *Co-organizer of NSF Workshop on Cyber-enabled Chemistry.* Washington D.C. NSF Oct. 3-5, 2004.
206. *Anomalous Hydration Dynamics As A Function Of Temperature Near A Model Hydrophobic Peptide.* Gordon Research Conference on Water and Aqueous Solutions. Holderness School, Plymouth, NH, Aug. 1-6, 2004
207. *Session leader on Aqueous Solutions.* Gordon Research Conference on Computational Chemistry. Holderness School, Plymouth, NH, July 4-9, 2004
208. *Hydration Dynamics Near a Model Protein Surface:Protein Function and Protein-Protein Assembly.* Gordon Research Conference on Interfacial Water in Cell Biology. Mt. Holyoke College, S. Hadley, MA, June 6-11, 2004.
209. *Protein Folding and Aggregation.* Chemistry department, Rice University, April 27, 2004.
210. *Role of Hydration Forces in Protein Folding, Structure, and Function.* Chemistry department, U. Houston, April 28, 2004.
211. *The Role of Hydration Forces in Protein Folding, Structure, and Function.* Chemical Physics seminar series, Caltech, March 9, 2004.
212. *Protein Folding and Aggregation.* Life Sciences Division, Lawrence Berkeley Laboratory, January 20, 2004.
213. *Protein Minimalist Models for Annotating Whole Genomes.* Center for Biological Modeling, Michigan State University, November 6, 2003
214. *Role of Hydration Forces in Protein Folding and Structure Prediction.* PENCE (Protein Engineering Network of Centres of Excellence) Seminar Series, University of Toronto, November 7, 2003.
215. *Computational Biology: Towards Understanding Disease Processes such as Alzheimer's & Parkinson's.* Celebrating Engineering Excellence, COE Alumni presentation, UC Berkeley, September 13, 2003.
216. *Stanley Building Groundbreaking Panel.* University of California, Berkeley, May 30, 2003.
217. *Cool Walking: A New Markov Chain Monte Carlo Sampling Method.* Symposium on Integrating Diverse Computational Approaches to Complex Problem Solving. ACS, New Orleans, Louisiana, March 23-27, 2003.
218. *Physiochemical Minimalist Models and Protein Design.* Colloquium in Protein Structure, Function and Dynamics, University of Puerto Rico's Protein Research Center, February 5-8, 2003.
219. *Protein Minimalist Models for Annotating Whole Genomes.* President's Meeting of the International Society of Quantum Biology and Pharmacology, Snowbird, Utah, December 13-14, 2002.
220. *Synchrotron Experiments and Theory: Pure Water as a Function of Temperature.* Symposium on Classical and Quantum Statistical Mechanics Studies of Solvation. ACS, Boston, Massachusetts, August 18-22, 2002.

221. *Protein Structure Prediction and Solvation Potentials of Mean Force.* Symposium on Water in Novel Environments and Biological Systems. ACS, Boston, Massachusetts, August 18-22, 2002.

222. *Simulation, Neutron, and X-ray Scattering Experiments for Pure Liquid Water.* Symposium on Applications of Neutron Scattering in Structural Biology and Biophysics. ACS, Boston, Massachusetts, August 18-22, 2002.

223. *Nominator for Berkeley as the Site of WATOC (World Association for Theoretically-Oriented Chemists) 2008.* Presentation given in Lugano, Switzerland, August 3, 2002.

224. *The Role of Hydration Forces in Protein Folding and Structure Prediction.* Department of Chemistry, Monash University, Melbourne, Victoria Australia June 26, 2002.

225. *Chemical Bonding Effects in Electron Crystallography.* Annual Meeting of the American Crystallographic Association, San Antonio, Texas, May 25-30, 2002.

226. *A Global Optimization Approach to Protein Structure Prediction.* 42nd Sanibel Symposium, St. Augustine, Florida, February 23-March 1, 2002.

227. *Protein Structure Prediction and Solvation Potentials of Mean Force*, Workshop on Self-Organizing Biomolecules: The Evolving Picture, Santa Fe, New Mexico, January 13-18, 2002.

228. *Facing the Challenges in Structural and Functional Genomics,* IBM T. J. Watson Research Center, Blue Gene team, Yorktown, New York, February 22, 2001.

229. *Experiment and Simulation in Protein Folding.* IBM Workshop for the Blue Gene Project. Break out session leader. San Diego, March 30-31, 2001.

230. *Facing the Challenges in Structural and Functional Genomics*, ACS, San Diego, April 1-5, 2001.

231. *Computational Complexity in Molecular and Genomic-Scale Biology*, National Research Council Committee on Frontiers at the Interface of Computing and Biology, Boston, Massachusetts, May 9, 2001.

232. *Synchrotron Experiments and Theoretical Analysis of Pure Water*, NATO Advanced Research Workshop: New kinds of phase transitions: transformations in disordered substances. Volga river, Russia, May 24-28, 2001.

233. *Matching Simulation and Experiment: Minimalist Models for Annotating Whole Genomes*. Gordon Research Conference on Biological Molecules in the Gas Phase. New London, Connecticut June 10-15, 2001.

234. *Synchrotron Experiments and Theory: Pure Water as a Function of Temperature.* Gordon Research Conference on the Chemistry and Physics of Liquids. Holderness, New Hampshire August 6-10, 2001.

235. *Computational Complexity in Molecular and Genomic-Scale Biology,* Department of Bioengineering, UC Berkeley, August 14, 2001.

236. *Workshop on Polarizability for Biomolecular Simulation (Co-organzier)*, Snowbird, Utah, Dec. 12-14, 2001.

237. *Session Chair of Coupling Simulation Theory and Experiment.* LJIS '2000: Quantitative Challenges In The Post-Genomic Sequence Era: A Workshop And Symposium, January 11-15, 2000.

238. *Facing the Challenges in Structural and Functional Genomics,* Biosciences Division, Argonne National Laboratory, January 24, 2000.

239. *Facing the Challenges in Structural and Functional Genomics,* Institute for Biomolecular Dynamics, University of Chicago, January 26, 2000.

240. *Facing the Challenges in Structural and Functional Genomics,* Department of Chemistry, University of North Carolina, Chapel Hill, January 31, 2000.

241. *Facing the Challenges in Structural and Functional Genomics,* Department of Chemistry, Indiana University, Bloomington, February 3, 2000.

242. *Aqueous Hydration Forces for Extremophiles.* Session of The Role of Water for Life Under Precarious Circumstances, AAAS meeting. Washington D. C., February 17-21, 2000.

243. *Computational Biology, Protein Structure Prediction, and Folding.* Symposium on the 21st Century: How Far Can Computation Go with the Hardest Problems, American Chemical Society, San Francisco, March 26-30, 2000.

244. *Matching Simulation And Experiment: A New Simplified Model For Simulating Protein Folding.* By invitation to RECOMB '2000. Japan, April 11-15, 2000.

245. *Facing the Challenges in Structural and Functional Genomics,* NASA-Ames, Moffit Field, CA. July 5, 2000.

246. *Facing the Challenges in Structural and Functional Genomics,* Department of Chemistry, UC Berkeley, September 12, 2000.

247. *Solvation Potentials of Mean Force for Protein Structure Prediction.* 4th Community Wide Experiment on the Critical Assessment of Techniques for Protein Structure Prediction (CASP4), Pacific Grove, CA, Dec. 7, 2000.

248. *Computational Challenges in Structural and Functional Genomics.* NERSC Scientific Computing Group, LBNL, April 15, 1999.

249. *Computational Challenges in Structural and Functional Genomics.* DOE Computational Sciences seminar series. Washington D. C. April 21, 1999.

250.   *Determining the Role of Aqueous Hydration Forces in Protein Folding.* National Institutes of Health, Washington D.C. April 22, 1999.

251.   *Lectures on Structural Genomics, Protein Folding and Prediction, and Hydration Forces*, Advanced School on Proteins, National Tsinghua University, Hsinchu, Taiwan, June 7-11, 1999.

252.   *Electronic and Classical Reaction Field Models for Aqueous Solvation*, Workshop on Treatment of Electrostatic Interactions in Computer Simulations of Condensed Media, Santa Fe, New Mexico, June 23-25, 1999.

253.   *Global Optimization Approaches to Protein Structure Prediction: α-Helical Proteins.* Polish-American Workshop on Theoretical Chemistry and Molecular Modeling, Wroclaw, Poland, July 1-6, 1999.

254.   *Determining the Role of Aqueous Hydration Forces in Protein Folding.* Americal Chemical Society, New Orleans, Louisiana, August 22-26, 1999.

255.   *Matching Simulation and Experiment: A New Simplified Model For Simulating Protein Folding.* Dept. of Physics, UC Davis. October 28, 1999.

256.   *Overview of Computational Biology,* Workshop on Computational Biology. Supercomputing '99, Portland, Oregon, November 11-17, 1999.