PABLO GASTON DEBENEDETTI

Dean for Research

Class of 1950 Professor in Engineering and Applied Science Professor of Chemical and Biological Engineering Princeton University

Born: March 30, 1953

Place of birth: Buenos Aires, Argentina

Citizenship: U.S.

EDUCATION

Ingeniero Químico (B.S., Chemical Engineering), Buenos Aires University (Argentina), 1978 M.S., Chemical Engineering, Massachusetts Institute of Technology, 1981 Ph.D., Chemical Engineering, Massachusetts Institute of Technology, 1985

PROFESSIONAL EMPLOYMENT

| 1977-78 1978-80 | Process Engineer, Exibro, Buenos Aires, Argentina Process Development Engineer, O.de Nora, Impianti Elettrochimici, Milan, Italy |
|----------------------|---|
| 1981-84 | Teaching and Research Assistant, Massachusetts Institute of Technology |
| | |
| FACULTY APPOINTMENTS | |
| 1985-90 | Assistant Professor of Chemical Engineering, Princeton University |
| 1990-94 | Associate Professor of Chemical Engineering, Princeton University |
| 1991-92 | Visiting Professor, Dept. of Chemical Eng., University of California, Berkeley |
| 1994- | Professor of Chemical Engineering, Princeton University |

ADMINISTRATIVE APPOINTMENTS

Class of 1950 Professor in Engineering and Applied Science

| 1990-91 | Director of Graduate Studies, Chem. Eng. Dept., Princeton University |
|-------------|--|
| 1992-94 | Director of Graduate Studies, Chem. Eng. Dept., Princeton University |
| 1996-04 | Chair of Chemical Engineering Department, Princeton University |
| 2006-08 | Director of Graduate Studies, Chem. Eng. Dept., Princeton University |
| 2008 | Acting Chair, Chemical Engineering Department, Princeton University |
| 2008-2013 | Vice Dean, School of Engineering and Applied Science, Princeton University |
| 2012 (Fall) | Acting Dean, School of Engineering and Applied Science, Princeton University |
| 2013- | Dean for Research, Princeton University |

PROFESSIONAL ACTIVITIES

Editorial Boards

1998-

Journal of Supercritical Fluids, 1988-2004 Journal of Chemical and Engineering Data, 1996-1998 Chemical Engineering Education, 2000-2009 Industrial and Engineering Chemistry Research, 2001-2004 The Journal of Chemical Physics, 2006-2009 AIChE Journal, Associate Editor for Perspectives, 2006-2010 AIChE Journal, Consulting Editor for Thermodynamics, 2012-Proceedings of the National Academy of Sciences, 2013-

Advisory Councils, Boards

Department of Chemical Engineering Graduate Program Academic Review, University of Cincinnati, 1996 NRC Panel for Chemical Science and Technology, Board of Assessment of NIST Programs, 1997-2000

Department of Chemical Engineering, Massachusetts Institute of Technology, Visiting Comm., 1997-2005

Department of Chemical & Biomolecular Engineering, Cornell University, Advisory Council, 1999-2005

Department of Chemical Engineering Academic Review, Vanderbilt University, 2000

School of Chemical Engineering Academic Review, Georgia Institute of Technology, 2001

Department of Chemical Engineering, City College of CUNY, Advisory Council, 2004-

Council for Chemical Research, Governing Board, 2004-2006

Center for Talented Youth, Johns Hopkins University; Cogito Project Advisory Board, 2005-

Department of Chemical Engineering, Pennsylvania State University, Advisory Council, 2006-2010

Board on Chemical Sciences and Technology, The National Academies, 2006-2012

Board on Chemical Sciences and Technology, The National Academies, co-Chair, 2011-2013

Department of Chemical Engineering, Columbia University, 2010-2016

Department of Sponsored Research, Massachusetts Institute of Technology, Visiting Committee, 2014-

Department of Chemical and Biochemical Engineering, Rutgers University, Advisory Council, 2017-

External Review Committee, Dept. of Chemical and Biomolecular Eng., U. of Pennsylvania, 2017

External Review Committee, The Journal of Chemical Physics, 2017

Award Committees

Alpha Chi Sigma Award subcommittee, American Institute of Chemical Engineers, 1994

Evaluator of Engineering Fellowship Applications, Guggenheim Foundation, 1996-2004

Colburn Award subcommittee, American Institute of Chemical Engineers, 2001

Chemical Engineering Peer Committee, National Academy of Engineering, 2002-2005

Awards Committee, American Institute of Chemical Engineers, 2001-2006

Blue-Ribbon Awards Committee, American Institute of Chemical Engineers, 2007-2008

World Cultural Council, Albert Einstein Prize Committee, 2010-2015

Bernard M. Gordon Prize Committee, National Academy of Engineering, 2011-2015

Blavatnik Award for Young Scientists, New York Academy of Sciences, 2011-

National Academy of Sciences, Class Membership Committee Member-at-Large (Section 31), 2017-2019

Organization of Technical Conferences

Chair, Area 1a, Thermodynamics and Transport Properties, American Institute of Chemical Engineers, 1996-1998

Organizing Committee, NATO Advanced Study Institute on Supercritical Fluids, Kemer, Turkey, July 12-24, 1998

Organizing Committee, 5th International Symposium on Supercritical Fluids (ISSF 2000), Atlanta, GA, April 9-11, 2000

Organizing Committee, 6^a Liblice Conference on the Statistical Mechanics of Liquids, Czech Republic, June 9-14, 2002

Co-Chair, Gordon Research Conference on Water and Aqueous Solutions, August 4-9, 2002

U.S. Frontiers of Engineering, National Academy of Engineering, Organizing Committee, Irvine, CA, September 19-21, 2002

U.S. Frontiers of Engineering, National Academy of Engineering, Chair, Organizing Committee, 2003-05 Co-Chair, CECAM Workshop on Metastability and Landscapes in Complex Systems, Lyon, France, May 22-24, 2003

Co-Chair, Symposium on "The Future of Chemical Engineering Research", Austin, TX, November 8, 2004

Organizing Committee, Council for Chemical Research Workshop on "Process Analytical Technology", Center for Advanced Research in Biotechnology, Rockville, MD, December 13, 2005

Co-organizer, Symposium on "Packing Problems, Classical Ground States, and Glasses," Princeton Center for Theoretical Physics, Princeton University, April 12-13, 2007

Chair, Council for Chemical Research Workshop on "Modeling Challenges in Process Development: Approaches in the Chemical and Pharmaceutical Industries," University of Maryland Biotechnology Institute, Rockville, MD, June 7-8, 2007

Organizing Committee, Faraday Discussion 146, "Wetting Dynamics of Hydrophobic and Structured Surfaces", Jefferson Hotel, Richmond, VA, April 12-14, 2010.

Co-organizer, Workshop on "Towards Unifying Concepts in the Physics of Aperiodic Systems", Princeton Center for Theoretical Science, Princeton University, October 14-15, 2011.

Co-organizer, International School of Physics Enrico Fermi on "Water: Fundamentals as the Basis for Understanding the Environment and Promoting Technology." Varenna, Italy, July 7-13, 2013.

Co-organizer, Workshop on "Origin of Biological Homochirality", Princeton Center for Theoretical Science, Princeton University, April 24-25, 2014.

Co-organizer, Workshop on "Ice Nucleation", Princeton Center for Theoretical Science, Princeton University, April 23-24, 2015.

University Service

Churchill Fellowships Selection Committee, 1986-87, 1987-88

Graduate School Fellowship Subcommittee, 1990-91

Public Lectures Committee, 1989-90, 1990-91

Graduate School Policy Subcommittee, 1993-94

President's Strategic Planning Committee (Graduate School), 1993-94

Student Life and Discipline Subcommittee, 1992-93

Faculty Committee on the Graduate School, 1990-91, 1992-93, 1993-94, 2006-2008

Priorities Committee, 1993-94, 1994-95

School of Engineering Wu Fellowship Committee, 1995-96

Intellectual Property Committee, 1997-98

Faculty Advisory Committee on Appointments and Advancements, 1998-99

School of Engineering and Applied Science, Space Committee, 2003-04

School of Engineering and Applied Science, Diversity Task Force, 2005-2008

Committee on Undergraduate Admission and Financial Aid, 2006-2009

Graduate School Policy Subcommittee, 2006-2008

Princeton Sustainability Committee, 2008-

Executive Committee, Princeton Inst. for Computational Science and Engineering (PICSciE), 2008-2013

University Research Board, 2009-2012

Executive Committee, Andlinger Center for Energy and the Environment, 2008-2013

Council on International Teaching and Research, Executive Committee, 2012-2013

Committee on Appointments and Advancements for Professional Researchers and Professional Specialists (C7) (Chair), 2013-

Conflict of Interest in Research Committee (Chair), 2013-

Executive Compliance Committee, 2013-

Executive Risk Management Committee, 2013-

University Research Board (Chair), 2013-

Strategic Planning Committee on Sponsored Research (Co-Chair), 2014-

Search Committee, Vice President for Princeton Plasma Physics Laboratory (Chair), 2015

Search Committee, Dean of the School of Engineering and Applied Science (Chair), 2015

Search Committee, Director of the Princeton Plasma Physics Laboratory, 2016-2017

Search Committee, Vice President for Innovation, 2018

HONORS AND AWARDS

- 1978 European Economic Community Fellow
- 1987 NSF Presidential Young Investigator Award
- 1989 Camille and Henry Dreyfus Teacher-Scholar Award
- 1991 John Simon Guggenheim Memorial Foundation Fellowship
- 1996 Best New Professional/Scholarly Book in Chemistry: *Metastable Liquids. Concepts and Principles*, Association of American Publishers
- 1997 Professional Progress Award, American Institute of Chemical Engineers
- 2000 National Academy of Engineering
- 2001 J.M. Prausnitz Award in Applied Chemical Thermodynamics
- 2008 Joel Henry Hildebrand Award in the Theoretical and Experimental Chemistry of Liquids, American Chemical Society
- 2008 William H. Walker Award for Excellence in Contributions to Chemical Engineering Literature, American Institute of Chemical Engineers
- 2008 Named one of "100 Chemical Engineers of the Modern Era", American Institute of Chemical Engineers
- 2008 American Academy of Arts and Sciences
- 2011 Fellow, American Association for the Advancement of Science
- 2012 National Academy of Sciences
- 2013 Fellow, American Institute of Chemical Engineers
- 2014 Honorary Professor, Beijing University of Chemical Technology
- 2014 Benjamin Garver Lamme Award, American Society for Engineering Education
- 2015 Fellow, American Physical Society
- 2017 Guggenheim Medal, Institution of Chemical Engineers

Teaching

- 2004 Excellence in Teaching Award, Engineering Council, Princeton University
- 2005 Excellence in Teaching Award, Engineering Council, Princeton University
- 2006 Excellence in Teaching Award, Engineering Council, Princeton University
- 2007 Excellence in Teaching Award, Engineering Council, Princeton University (Fall & Spring)
- 2008 Distinguished Teacher Award, School of Engineering and Applied Science, Princeton University
- 2008 President's Award for Distinguished Teaching, Princeton University
- 2013 Excellence in Teaching Award, Engineering Council, Princeton University (Lifetime Achievement)
- 2016 Phi Beta Kappa Teaching Award, Princeton University

Honorary Lectures

- 1992 Robert W. Vaughan Memorial Lecture, Chem. Eng. Dept., California Institute of Technology
- 1997 Stanley Katz Memorial Lecture, Department of Chemical Engineering., City College of the City University of New York
- 1997 Kurt Wohl Memorial Lecture, Chemical Engineering Department, University of Delaware
- 1998 Ashton Cary Lecture, School of Chemical Engineering, Georgia Institute of Technology
- 2003 Dean's Distinguished Colloquia Series, College of Engineering and Applied Sciences, State University of New York, Stony Brook
- 2003 Rutgers Collaboratus XIII Distinguished Lecture, Department of Chemical and Biochemical Engineering, Rutgers University
- 2003 Berkeley Lectures in Chemical Engineering, Department of Chemical Engineering, University of California, Berkeley
- 2003 Area 1a Keynote Lecture, American Institute of Chemical Engineers
- 2005 Walker Lecture in Physical Chemistry, Departments of Chemistry and Chemical Engineering, Pennsylvania State University

- 2005 Donald L. Katz Lectureship, Department of Chemical Engineering, University of Michigan
- 2006 Patten Distinguished Lecturer, Dept. of Chemical and Biological Eng., U. of Colorado, Boulder
- 2007 Reilly Lectureship in Chemical and Biomolecular Engineering, Department of Chemical and Biomolecular Engineering, University of Notre Dame
- 2007 Michael M. Abbott Lecture, Department of Chemical and Biological Engineering, Rensselaer Polytechnic Institute
- 2007 Joe Smith Distinguished Lecture, Department of Chemical Engineering and Materials Science, University of California at Davis
- 2008 Kelly Lecturer, School of Chemical Engineering, Purdue University
- 2008 Hunter Henry Jr. Lecture, School of Chemical Engineering, Mississippi State University
- 2009 D.B. Robinson Distinguished Speaker, Schlumberger Lecture, Department of Chemical and Materials Engineering, University of Alberta
- 2011 Eli Ruckenstein Lecture, Department of Chemical and Biological Engineering, University at Buffalo, State University of New York
- 2012 William G. Lowrie Lectures, Department of Chemical and Biomolecular Engineering, The Ohio State University
- 2012 Fredrickson Lectures, Department of Chemical Engineering and Materials Science, University of Minnesota
- 2013 Julian C. Smith Lectures, Department of Chemical and Biomolecular Engineering, Cornell University
- 2013 Keynote Lecture, 13^a International Conference on Properties and Phase Equilibria for Products and Process Design, Iguazú Falls, Argentina
- 2013 Chair Lecture, Department of Chemistry, University of Nebraska
- 2013 Institute Lecture, American Institute of Chemical Engineers
- Warren L. McCabe Lecture, Dept. of Chemical and Biomolecular Engineering, North Carolina State University
- 2014 Honorary Professorship Lecture, Beijing University of Chemical Technology
- 2014 Bird, Stewart and Lightfoot Lecture, Department of Chemical and Biological Engineering, University of Wisconsin
- 2014 Molecular Physics Lecture, Liblice Conference on the Statistical Mechanics of Liquids, Sec, Czech Republic
- 2015 David M. Mason Lectures, Department of Chemical Engineering, Stanford University
- 2015 Molecular Physics Lecture, Thermodynamics 2015 Conference, Copenhagen, Denmark
- 2015 Barnett Dodge Distinguished Lecture, Department of Chemical and Environmental Engineering, Yale University
- 2015 W.E. Palke Memorial Lectures, Department of Chemistry and Biochemistry, University of California, Santa Barbara
- 2016 John A. Quinn Lecture, Department of Chemical and Biomolecular Engineering, University of Pennsylvania
- 2016 Distinguished Lindsay Speaker, Department of Chemical Engineering, Texas A&M University
- 2017 Guggenheim Medal Plenary Lecture, Thermodynamics 2017 Conference, Edinburgh, Scotland
- 2018 Distinguished Seminar Speaker Series, Dept. of Chemical and Environmental Eng., University of California, Riverside

RESEARCH INTERESTS

Thermodynamics and Statistical Mechanics of Liquids and Glasses Metastable Liquids
Water and Aqueous Solutions
Biopreservation
Nucleation
Protein Thermodynamics
Origin of Biological Homochirality

PROFESSIONAL SOCIETIES

American Association for the Advancement of Science American Chemical Society American Institute of Chemical Engineers American Physical Society American Society for Engineering Education

PABLO G. DEBENEDETTI

Bibliography

Book

Metastable Liquids. Concepts and Principles. Princeton University Press, 1996.

Edited Book

Supercritical Fluids. Fundamentals and Applications. E. Kiran, P.G. Debenedetti, and C.J. Peters, eds. NATO Science Series E: Applied Sciences. Vol. 366. Kluwer, **2000**.

Journal Articles

- 1. P.G. Debenedetti and C.G. Vayenas, Steady State Analysis of High Temperature Fuel Cells. Chem. Eng. Sci., 38, 1817, 1983.
- 2. P.G. Debenedetti, The Thermodynamic Fundamentals of Exergy. Chem. Eng. Ed., 18, 116, 1984.
- 3. C.G. Vayenas, P.G. Debenedetti, I. Yentekakis and L.L. Hegedus, Cross-Flow, Solid-State Electrochemical Reactors: a Steady-State Analysis. Ind. Eng. Chem. Fund., 24, 316, 1985.
- 4. P.G. Debenedetti, On the Relationship Between Principal Fluctuations and Stability Coefficients in Multicomponent Systems. **J. Chem. Phys.**, **84**, 1778, **1986**.
- 5. P.G. Debenedetti and M.C. D'Antonio, On the Nature of the Tensile Instability in Metastable Liquids and its Relationship to Density Anomalies. **J. Chem. Phys.**, **84**, 3339, **1986**.
- 6. P.G. Debenedetti, Generalized Massieu-Planck Functions: Geometric Representation, Extrema and Uniqueness Properties. **J. Chem. Phys.**, **85**, 2132, **1986**.
- 7. P.G. Debenedetti and S.K. Kumar, Infinite Dilution Fugacity Coefficients and the General Behavior of Dilute Binary Systems. **AIChEJ.**, **32**, 1253, **1986**.
- 8. P.G. Debenedetti and R.C. Reid, Diffusion and Mass Transfer in Supercritical Fluids. **AIChEJ.**, **32**, 2034, **1986**.
- 9. P.G. Debenedetti and M.C. D'Antonio, On the Entropy Changes and Fluctuations Occurring Near a Tensile Instability. **J. Chem. Phys.**, **85**, 4005, **1986**.
- 10. P.G. Debenedetti, Derivation of Operational Definitions for the Computer Calculation of Partial Molar Properties in Multicomponent Mixtures. **Chem. Phys. Lett.**, **132**, 325, **1986**.
- 11. M.C. D'Antonio and P.G. Debenedetti, Loss of Tensile Strength in Liquids Without Property Discontinuities: a Thermodynamic Analysis. **J. Chem. Phys.**, **86**, 2229, **1987**.

- 12. P.G. Debenedetti, Fluctuation-based Computer Calculation of Partial Molar Properties . I . Molecular Dynamics Simulation of Constant Volume Fluctuations. **J. Chem. Phys.**, **86**, 7126, **1987**.
- 13. P.G. Debenedetti, The Statistical Mechanical Theory of Concentration Fluctuations in Mixtures. J. Chem. Phys., 87, 1256, 1987.
- 14. P.G. Debenedetti, Clustering in Dilute, Binary Supercritical Mixtures: a Fluctuation Analysis. Chem. Eng. Sci., 42, 2203, 1987.
- P.G. Debenedetti, Fluctuation-based Computer Calculation of Partial Molar Properties. II. A Numerically Accurate Method for the Determination of Partial Molar Energies and Enthalpies. J. Chem. Phys., 88, 2681, 1988.
- 16. P.G. Debenedetti and M.C. D'Antonio, Stability and Tensile Strength of Liquids Exhibiting Density Maxima. AIChEJ., 34, 447, 1988.
- 17. P.G. Debenedetti and S.K. Kumar, The Molecular Basis of Temperature Effects in Supercritical Extraction. AIChEJ., 34, 645, 1988.
- 18. N.A. Collins, P.G. Debenedetti and S. Sundaresan, Disproportionation of Toluene over ZSM-5 under Near-Critical Conditions. **AIChEJ.**, **34**, 1211, **1988**.
- 19. P.G. Debenedetti, Thermodynamic Stability of Single-Phase Fluids and Fluid Mixtures Under the Influence of Gravity. **J. Chem. Phys.**, **89**, 6881, **1988**.
- 20. R.S. Mohamed, P.G. Debenedetti and R.K. Prud'homme, Effect of Process Conditions on Crystals Obtained from the Rapid Expansion of Supercritical Mixtures. **AIChEJ.**, **35**, 325, **1989**.
- 21. P.G. Debenedetti, Fluctuation Simulations and the Calculation of Mechanical Partial Molar Properties. **Molecular Simulation**, **2**, 33, **1989**.
- 22. P.G. Debenedetti and R.S. Mohamed, Attractive, Weakly Attractive, and Repulsive Near-Critical Systems. J. Chem. Phys., 90, 4528, 1989.
- 23. I.V. Yentekakis, P.G. Debenedetti and B. Costa, A Novel Fused Metal Anode Solid Electrolyte Fuel Cell for Direct Coal Gasification: A Steady State Model. Ind. Eng. Chem. Res., 28, 1414, 1989.
- 24. I.B. Petsche and P.G. Debenedetti, Solute-Solvent Interactions in Infinitely Dilute Supercritical Mixtures: A Molecular Dynamics Investigation. **J. Chem. Phys.**, **91**, 7075, **1989**.
- A.A. Chialvo, D.L. Heath and P.G. Debenedetti, A Molecular Dynamics Study of the Influence of Elongation and Quadrupole Moment Upon Some Thermodynamic and Transport Properties of Linear Heteronuclear Triatomic Fluids. J. Chem. Phys., 91, 7818, 1989.
- 26. P.G. Debenedetti, I.B. Petsche and R.S. Mohamed, Clustering in Supercritical Mixtures: Theory, Applications and Simulations. **Fluid Phase Equilibria**, **52**, 347, **1989**.
- 27. P.G. Debenedetti, Homogeneous Nucleation in Supercritical Fluids. AIChEJ., 36, 1289, 1990.

- 28. A.A. Chialvo and P.G. Debenedetti, On the Use of the Verlet Neighbor List in Molecular Dynamics. Computer Phys. Commun., 60, 215, 1990.
- 29. I.B. Petsche and P.G. Debenedetti, Influence of Solute-Solvent Asymmetry Upon the Behavior of Dilute Supercritical Mixtures. J. Phys. Chem., 95, 386, 1991.
- 30. A.A. Chialvo and P.G. Debenedetti, On the Performance of an Automated Verlet Neighbor List Algorithm for Large Systems on a Vector Processor. **Computer Phys. Commun.**, **64**, 15, **1991**.
- 31. A.A. Chialvo and P.G. Debenedetti, Use of the McQuarrie Equation for the Computation of Shear Viscosity via Equilibrium Molecular Dynamics. **Phys. Rev. A**, **43**, 4289, **1991**.
- 32. P.G. Debenedetti, V.S. Raghavan and S.S. Borick, Spinodal Curve of Some Supercooled Liquids. J. Phys. Chem., 95, 4540, 1991.
- 33. J.W. Tom and P.G. Debenedetti, Particle Formation with Supercritical Fluids A Review. **J. Aerosol Sci.**, 22, 555, 1991.
- 34. J.W. Tom and P.G. Debenedetti, Formation of Bioerodible Polymeric Microspheres and Microparticles by Rapid Expansion of Supercritical Solutions. **Biotech.Prog.**, 7, 403, 1991.
- 35. A.A. Chialvo and P.G. Debenedetti, Study of Solute-Solvent Interactions at Infinite Dilution via the Coupling Parameter Approach. **Molecular Simulation**, **7**, 265, **1991**.
- 36. A.A. Chialvo and P.G. Debenedetti, Molecular Dynamics Study of Solute-Solute Microstructure in Attractive and Repulsive Supercritical Mixtures. **Ind. Eng. Chem. Res.**, **31**, 1391, **1992**.
- 37. P.G. Debenedetti and A.A. Chialvo, Solute-Solute Correlations in Infinitely Dilute Supercritical Mixtures. J. Chem. Phys., 97, 504, 1992.
- 38. A.A. Chialvo and P.G. Debenedetti, An Automated Verlet Neighbor List Algorithm with a Multiple Time Step Approach for the Simulation of Large Systems. **Computer Phys. Commun.**, **70**, 467, **1992**.
- 39. S.-D. Yeo, G.-B. Lim, P.G. Debenedetti and H. Bernstein, Formation of Microparticulate Protein Powders Using a Supercritical Fluid Anti-Solvent. **Biotech. Bioeng.**, **41**, 341, **1993**.
- 40. P.G. Debenedetti, J.W. Tom, X. Kwauk and S.-D. Yeo, Rapid Expansion of Supercritical Solutions (RESS): Fundamentals and Applications. **Fluid Phase Equil.**, **82**, 311, **1993**.
- 41. P.G. Debenedetti, J.W. Tom, S.-D. Yeo and G.-B. Lim, Application of Supercritical Fluids for the Production of Sustained Delivery Devices. J. Contr. Rel., 24, 27, 1993.
- 42. S.S. Borick and P.G. Debenedetti, Equilibrium, Stability and Density Anomalies in a Lattice Model with Core-Softening and Directional Bonding. **J. Phys. Chem.**, **97**, 6292, **1993**.
- 43. X. Kwauk and P.G. Debenedetti, Mathematical Modelling of Aerosol Formation by Rapid Expansion of Supercritical Solutions in a Converging Nozzle. **J. Aerosol Sci.**, **34**, 445, **1993**.

- 44. J.W. Tom and P.G. Debenedetti, Integral Equation Study of Microstructure and Solvation in Model Attractive and Repulsive Supercritical Mixtures. **Ind. Eng. Chem. Res.**, **32**, 2118, **1993**.
- 45. S.-D. Yeo, P.G. Debenedetti, M. Radosz and H.-W. Schmidt, Supercritical Anti-Solvent (SAS) Process for Substituted Para-Linked Aromatic Polyamides: Phase Equilibrium and Morphology Study. **Macromolecules**, **26**, 6207 **1993**.
- 46. R.J. Speedy and P.G. Debenedetti, The Entropy of a Network Crystal, Fluid and Glass. **Molec. Phys.**, **81**, 237, **1994**.
- 47. J.W. Tom, P.G. Debenedetti and R. Jérome, Precipitation of Poly(L-lactic acid) and Composite Poly(L-lactic acid) Pyrene Particles by Rapid Expansion of Supercritical Fluids. **J. Supercrit.** Fluids, **7**, 9, **1994**.
- 48. A. Chakravarthi, P.G. Debenedetti, S. Sastry and S.-D. Yeo, Thermal Expansion an Stability Limits of Generalized van der Waals Fluids. **J. Phys. Chem.**, **98**, 6876, **1994**.
- 49. D.S. Corti and P.G. Debenedetti, A Computational Study of Metastability in Vapor-Liquid Equilibrium. Chem. Eng. Sci., 49, 2717, 1994.
- 50. S.-D. Yeo, P.G. Debenedetti, S.Y. Patro and T.M. Przybycien, Secondary Structure Characterization of Microparticulate Insulin Powders. **J. Pharm. Sci.**, **83**, 1651, **1994**.
- 51. S.-D. Yeo, P.G. Debenedetti, M. Radosz, R. Giesa and H.-W. Schmidt, Supercritical Anti-Solvent (SAS) Process for a Series of Substituted Para-Linked Aromatic Polyamides. **Macromolecules**, **28**, 1316, **1995**.
- 52. S.S. Borick, P.G. Debenedetti and S. Sastry, A Lattice Model of Network-Forming Fluids with Orientation-Dependent Bonding: Equilibrium, Stability, and Implications for the Phase Behavior of Supercooled Water. J. Phys. Chem., 99, 3781, 1995.
- 53. D.S. Corti and P.G. Debenedetti, Metastability and Constraints: a Study of the Superheated Lennard-Jones Liquid in the Void-Constrained Ensemble. Ind. & Eng. Chem. Res., 34, 3573, 1995.
- 54. R.J. Speedy and P.G. Debenedetti, Persistence Time for Bonds in a Tetravalent Network Fluid. **Molec. Phys.**, **86**, 1375, **1995**.
- 55. J.K. Taylor, P.G. Debenedetti, W.W. Graessley and S.K. Kumar, Compressibility Effects in the Analysis and Interpretation of Neutron Scattering Data from Polymer Blends. **Macromolecules**, **29**, 764, **1996**.
- M. Connolly, P.G. Debenedetti and H.-H. Tung, Freeze Crystallization of Imipenem. J. Pharm. Sci., 85, 174, 1996.
- 57. P.G. Debenedetti, M.M. Atakan and R.J. Speedy, Comment on 'Entropy Catastrophe and Configurational Entropies in Supercooled and Superheated Regimes', by K. Kishore and H.K. Shobha. **J. Chem. Phys.**, **104**, 5349, **1996**.

- 58. M.A. Winters, B.L. Knutson, P.G. Debenedetti, H.G. Sparks, T.M. Przybycien, C.L. Stevenson and S.J. Prestrelski, Precipitation of Proteins in Supercritical Carbon Dioxide. **J. Pharm. Sci.**, **85**, 586, **1996**.
- 59. S. Sastry, P.G. Debenedetti, F. Sciortino and H.E. Stanley, Singularity-Free Interpretation of the Thermodynamics of Supercooled Water. **Phys. Rev. E**, **53**, 6144, **1996**.
- 60. R.J. Speedy, P.G. Debenedetti, R.S. Smith, C. Huang and B.D. Kay, The Evaporation Rate, Free Energy, and Entropy of Amorphous Water at 150K. J. Chem. Phys., 105, 240, 1996.
- 61. M.A. Winters, P.G. Debenedetti, P.D. Condo, M. Radosz and H.-W. Schmidt, Effects of Compressed Carbon Dioxide on the Phase Equilibrium and Molecular Order of a Lyotropic Polyamide Solution. **Macromolecules**, **29**, 4904, **1996**.
- 62. C.J. Roberts and P.G. Debenedetti, Polyamorphism and Density Anomalies in Network-Forming Fluids: Zeroth- and First-Order Approximations. **J. Chem. Phys.**, **105**, 658, **1996**.
- 63. H. Inomata, S. Saito and P.G. Debenedetti, Molecular Dynamics Simulation of Infinitely Dilute Solutions of Benzene in Supercritical CO₂. **Fluid Phase Equil.**, **116**, 282, **1996**.
- 64. R.J. Speedy and P.G. Debenedetti, The Distribution of Tetravalent Network Glasses. **Molec. Phys.**, **88**, 1293, **1996**.
- 65. C.A. Eckert, B.L. Knutson and P.G. Debenedetti, Supercritical Fluids as Solvents for Chemical and Materials Processing. **Nature**, **383**, 313, **1996**.
- 66. C.J. Roberts, A.Z. Panagiotopoulos and P.G. Debenedetti, Liquid-Liquid Immiscibility in Pure Fluids: Polyamorphism in Simulations of a Network-Forming Fluid. **Phys. Rev. Lett.**, **77**, 4386, **1996**.
- 67. D.S. Corti, P.G. Debenedetti, S. Sastry and F.H. Stillinger, Constraints, Metastability, and Inherent Structures in Liquids. **Phys. Rev. E**, **55**, 5522, **1997**.
- 68. M.A. Winters, P.G. Debenedetti, J. Carey, H.G. Sparks, S.U. Sane and T.M. Przybycien, Long-Term and High-Temperature Storage of Supercritically-Processed Microparticulate Protein Powders. **Pharm. Res.**, 14, 1370, 1997.
- S. Sastry, D.S. Corti, P.G. Debenedetti and F.H. Stillinger, Statistical Geometry of Particle Packings: I. Algorithm for Exact Determination of Connectivity, Volume and Surface Areas of Void Space in Mono- and Polydisperse Sphere Packings. Phys. Rev. E, 56, 5524, 1997.
- 70. S. Sastry, P.G. Debenedetti and F.H. Stillinger, Statistical Geometry of Particle Packings: II. 'Weak Spots' in Liquids. **Phys. Rev. E**, **56**, 5533, **1997**.
- 71. J.K. Taylor-Maranas, P.G. Debenedetti, W.W. Graessley and S.K. Kumar, Compressibility Effects in Neutron Scattering by Polymer Blends. **Macromolecules**, **30**, 6943, **1997**.
- 72. P.G. Debenedetti and H. Reiss, Reversible Work of Formation of an Embryo of a New Phase Within a Uniform Macroscopic Mother Phase. **J. Chem. Phys., 108**, 5498, **1998**.

- 73. D.S. Corti and P.G. Debenedetti, Statistical Mechanics of Fluids Under Internal Constraints: Rigorous Results for the One-Dimensional Hard Rod Fluid. **Phys. Rev. E**, **57**, 4211, **1998**.
- 74. S. Sastry, P.G. Debenedetti and F.H. Stillinger, Signatures of Distinct Dynamical Regimes in the Energy Landscape of a Glass-Forming Liquid. **Nature**, **393**, 554 **1998**.
- 75. L.P. Rebelo, P.G. Debenedetti and S. Sastry, Singularity-Free Interpretation of the Thermodynamics of Supercooled Water. II: Thermal and Volumetric Behavior. **J.Chem.Phys.**, **109**, 626, **1998**.
- 76. C.J. Roberts, G.A. Karayiannakis and P.G. Debenedetti, Liquid-Liquid Immiscibility in Single-Component Network-Forming Fluids: Model Calculations, and Implications for Polyamorphism in Water. Ind. & Eng. Chem. Res., 37, 3012, 1998.
- 77. T.M. Truskett, S. Torquato, S. Sastry, P.G. Debenedetti, and F.H. Stillinger, A Structural Precursor to Freezing in the Hard-Disk and Hard-Sphere Systems. **Phys. Rev. E**, **58**, 3083, **1998**.
- 78. F.H. Stillinger, P.G. Debenedetti and S. Sastry, Resolving Vibrational and Structural Contributions to Isothermal Compressibility. **J.Chem.Phys.**, **109**, 3983, **1998**.
- 79. K.M. Layn, P.G. Debenedetti and R.K. Prud'homme, A Theoretical Study of Gemini Surfactant Phase Behavior. **J. Chem. Phys.**, **109**, 5651, **1998**.
- 80. S. Sastry, T.M. Truskett, P.G. Debenedetti, S. Torquato and F.H. Stillinger, Free Volume in the Hard-Sphere Liquid. **Molec. Phys.**, **95**, 289, **1998**.
- 81. J.K. Maranas, M. Mondello, G.S. Grest, S.K. Kumar, P.G. Debenedetti and W.W. Graessley, Liquid Structure, Thermodynamics, and Mixing Behavior of Saturated Hydrocarbon Polymers. 1. Cohesive Energy Density and Internal Pressure. **Macromolecules**, **31**, 6991, **1998**.
- 82. J.K. Maranas, S.K. Kumar, P.G. Debenedetti, W.W. Graessley, M. Mondello and G.S. Grest, Liquid Structure, Thermodynamics, and Mixing Behavior of Saturated Hydrocarbon Polymers. 2. Pair Distribution Functions and the Regularity of Mixing. **Macromolecules**, 31, 6998, 1998.
- 83. T.M. Truskett, S. Torquato and P.G. Debenedetti, Density Fluctuations in Many-Body Systems. **Phys. Rev. E**, **58**, 7369, **1998**.
- 84. M.A. Winters, D.Z. Frankel, P.G. Debenedetti, J. Carey, M. Devaney and T.M. Przybycien, Protein Purification with Vapor-Phase Carbon Dioxide. **Biotech. & Bioeng.**, **62**, 247, **1999**.
- 85. F.H. Stillinger and P.G. Debenedetti, Distinguishing Vibrational and Structural Equilibration Contributions to Thermal Expansion. **J. Phys. Chem. B**, **103**, 4052, **1999**.
- 86. T.M. Truskett and P.G. Debenedetti, The Statistical Geometry of Voids in Liquids. **Fluid Phase Equil.**, **158-160**, 549, **1999**.
- 87. T.M. Truskett, P.G. Debenedetti, S. Sastry and S. Torquato, A Single-Bond Approach to Orientation-Dependent Interactions and its Implications for Liquid Water. J. Chem. Phys., 111, 2647, 1999.

- 88. V.K. Shen and P.G. Debenedetti, A Computational Study of Homogeneous Liquid-Vapor Nucleation in the Lennard-Jones Fluid. **J. Chem. Phys.**, **111**, 3581, **1999**.
- 89. P.G. Debenedetti and H. Reiss, Reply to the Comment on: Reversible Work of Formation of an Embryo of a New Phase Within a Uniform Macroscopic Mother Phase [J.Chem.Phys. 108, 5498 (1998)]. J. Chem. Phys., 111, 3781, 1999.
- 90. C.J. Roberts and P.G. Debenedetti, Structure and Dynamics in Concentrated, Amorphous Carbohydrate-Water Systems by Molecular Dynamics Simulation. **J. Phys. Chem. B**, **103**, 7308, **1999**.
- 91. P.G. Debenedetti, F.H. Stillinger, T.M. Truskett and C.J. Roberts, The Equation of State of an Energy Landscape. **J. Phys. Chem. B**, **103**, 7390, **1999**.
- 92. J. Werling and P.G. Debenedetti, Numerical Modeling of Mass Transfer in the Supercritical Antisolvent Process. **J. Supercrit. Fluids**, **16**, 167, **1999**.
- 93. C.J. Roberts, P.G. Debenedetti and F.H. Stillinger, Equation of State of the Energy Landscape of SPC/E Water. **J. Phys. Chem. B**, **103**, 10258, **1999**.
- 94. S. Sastry, P.G. Debenedetti, F.H. Stillinger, T.B. Schrøder, J.C. Dyre and S.C. Glotzer, Potential Energy Landscape Signatures of Slow Dynamics in Glass Forming Liquids. **Physica A**, **270**, 310, **1999**.
- 95. M. Utz, P.G. Debenedetti and F.H. Stillinger, Atomistic Simulation of Aging and Rejuvenation in Glasses. **Phys. Rev. Lett.**, **84**, 1471, **2000**.
- 96. S. Torquato, T.M. Truskett and P.G. Debenedetti, Is Random Close Packing of Spheres Well Defined? **Phys. Rev. Lett.**, **84**, 2064, **2000**.
- 97. T.M. Truskett, S. Torquato and P.G. Debenedetti, Towards a Quantification of Disorder in Materials: Distinguishing Equilibrium and Glassy Sphere Packings. **Phys. Rev. E**, **62**, 993, **2000**.
- 98. A. Vishnyakov, P.G. Debenedetti and A.V. Neimark, Statistical Geometry of Cavities in a Confined Metastable Fluid. **Phys. Rev. E**, **62**, 538, **2000**.
- 99. J. Werling and P.G. Debenedetti, Numerical Modeling of Mass Transfer in the Supercritical Antisolvent Process: Miscible Conditions. **J. Supercrit. Fluids**, **18**, 11, **2000**.
- 100. D.K. Stillinger, F.H. Stillinger, S. Torquato, T.M. Truskett and P.G. Debenedetti, Triangle Distribution and Equation of State for Classical Rigid Disks. **J. Stat. Phys.**, **100**, 49, **2000**.
- 101. F.H. Stillinger, D.K. Stillinger, S. Torquato, T.M. Truskett and P.G. Debenedetti, Equation of State of the Rigid Disk Fluid from its Triangle Distribution. **J. Chem. Phys.**, **113**, 10186, **2000**.
- 102. J.R. Errington and P.G. Debenedetti, Relationship Between Structural Order and the Anomalies of Liquid Water. **Nature**, **409**, 318, **2001**.

- 103. T.M. Truskett, P.G. Debenedetti and S. Torquato, Thermodynamic Implications of Confinement for a Water-Like Fluid. **J. Chem. Phys.**, **114**, 2401, **2001**.
- 104. V.K. Shen and P.G. Debenedetti, Density-functional Study of Homogeneous Bubble Nucleation in the Stretched Lennard-Jones Fluid. **J. Chem. Phys.**, **114**, 4149, **2001**.
- 105. P.G. Debenedetti and F.H. Stillinger, Supercooled Liquids and the Glass Transition. **Nature**, **410**, 259, **2001**; with F.H. Stillinger.
- 106. M. Utz, P.G. Debenedetti and F.H. Stillinger, Isotropic Tensile Strength of Molecular Glasses. J. Chem. Phys., 114, 10049, 2001.
- 107. M.R. Feeney, C. Brown, A. Tsai, D. Neumann and P.G. Debenedetti, Incoherent Quasi-Elastic Neutron Scattering from Fructose-Water Solutions. J. Phys. Chem. B, 105, 7799, 2001.
- 108. F.H. Stillinger, P.G. Debenedetti and T.M. Truskett, The Kauzmann Paradox Revisited. J. Phys. Chem. B, 105, 11809, 2001.
- 109. H.S. Ashbaugh, T.M. Truskett and P.G. Debenedetti, A Simple Molecular Thermodynamic Theory of Hydrophobic Hydration. J. Chem. Phys., 116, 2907, 2002.
- 110. F.H. Stillinger and P.G. Debenedetti, Energy Landscape Diversity and Supercooled Liquid Properties. **J. Chem. Phys.**, **116**, 3353, **2002**.
- M. Weber, L.M. Russell and P.G. Debenedetti, Mathematical Modeling of Nucleation and Growth of Particles Formed by the Rapid Expansion of Supercritical Solutions under Subsonic Conditions. J. Supercrit. Fluids, 23, 65, 2002.
- 112. C.J. Roberts and P.G. Debenedetti, Engineering Pharmaceutical Stability with Amorphous Solids. AIChEJ., 48, 1140, 2002.
- 113. M.S. Shell, P.G. Debenedetti and A.Z. Panagiotopoulos, Molecular Structural Order and Anomalies in Liquid Silica. **Phys. Rev. E**, **66**, 011202, **2002**.
- 114. V.K. Shen, P.G. Debenedetti and F.H. Stillinger, Energy Landscape and Tensile Strength of n-Alkane Glasses. **J. Phys. Chem. B**, **106**, 10447, **2002**.
- 115. T.M. Truskett, P.G. Debenedetti and S. Torquato, Comment on "Observations on an Equation of State for Water Confined in Narrow Slit-Pores" [J. Chem. Phys. 116, 2565 (2002)] **J. Chem. Phys.**, **117**, 8162, **2002**.
- 116. J.R. Errington, P.G. Debenedetti and S. Torquato, Cooperative Origin of Low-Density Domains in Liquid Water. **Phys. Rev. Lett.**, **89**, 215503, **2002**.
- 117. M.S. Shell, P.G. Debenedetti and A.Z. Panagiotopoulos, Generalization of the Wang-Landau Method for Off-Lattice Simulations. **Phys. Rev. E**, **66**, 056703, **2002**.
- 118. V.K. Shen and P.G. Debenedetti, A Kinetic Theory of Homogeneous Bubble Nucleation. **J. Chem. Phys.**, **118**, 768, **2003**.

- 119. J.R. Errington, P.G. Debenedetti and S. Torquato, Quantification of Order in the Lennard-Jones System. J. Chem. Phys., 118, 2256, 2003.
- 120. M.S. Shell, P.G. Debenedetti. E. La Nave and F. Sciortino, Energy Landscapes, Ideal Glasses, and their Equation of State. J. Chem. Phys., 118, 8821, 2003.
- 121. P.G. Debenedetti and H.E. Stanley, Supercooled and Glassy Water. Physics Today, 56 (6), 40, 2003.
- 122. F. Chávez-Ríos, P.G. Debenedetti, J.J. Luo, R.N. Dave and R. Pfeffer, Estimation of Characteristic Time Scales in the Supercritical Antisolvent Process. Ind. & Eng. Chem. Res., 42, 3156, 2003.
- 123. M.R. Feeney, P.G. Debenedetti and F.H. Stillinger, A Statistical Mechanical Model for Inverse Melting. J. Chem. Phys., 119, 4582, 2003.
- 124. F.H. Stillinger and P.G. Debenedetti, Phase Transitions, Kauzmann Curves, and Inverse Melting. **Biophys. Chem.**, **105**, 211, **2003**.
- 125. E. La Nave, F. Sciortino, P. Tartaglia, M.S. Shell and P.G. Debenedetti, Test of Non-Equilibrium Thermodynamics in Glassy Systems: the Soft-Sphere Case. **Phys. Rev. E**, **68**, 032103, **2003**.
- 126. M.S. Shell, P.G. Debenedetti and A.Z. Panagiotopoulos, An Improved Monte Carlo Method for the Calculation of the Density of States. **J. Chem. Phys.**, **119**, 9406, **2003**.
- 127. H.S. Ashbaugh, T.M. Truskett and P.G. Debenedetti, Response to Comment on: A Simple Molecular Thermodynamic Theory of Hydrophobic Hydration [J.Chem.Phys. 116, 2907 (2002)]. J. Chem. Phys., 119, 10450, 2003.
- 128. P.G. Debenedetti, Supercooled and Glassy Water. J. Phys.: Condens. Matt., 15, R1669, 2003.
- 129. M.R. Feeney and P.G. Debenedetti, A Theoretical Study of the Interfacial Properties of Supercooled Water. Ind. & Eng. Chem. Res., 42, 6396, 2003.
- 130. P.G. Debenedetti, F.H. Stillinger and M.S. Shell, Model Energy Landscapes. J. Phys. Chem. B, 107, 14434, 2003.
- 131. M.S. Shell, P.G. Debenedetti and A.Z. Panagiotopoulos, Saddles in the Energy Landscape: Extensivity and Thermodynamic Formalism. **Phys. Rev. Lett.**, **92**, 035506, **2004**.
- 132. S.L. Lee, P.G. Debenedetti, J.R. Errington, B.A. Pethica and D.J. Moore, A Calorimetric and Spectroscopic Study of DNA at Low Hydration. J. Phys. Chem. B, 108, 3098, 2004.
- 133. M.S. Shell and P.G. Debenedetti, Thermodynamics and the Glass Transition in Model Energy Landscapes. **Phys. Rev. E**, **69**, 051102, **2004**.
- 134. M.S. Shell, P.G. Debenedetti and F.H. Stillinger, Inherent Structure View of Self-Diffusion in Liquids. J. Phys. Chem. B, 108, 6772, 2004.

- 135. L. Chen, P.G. Debenedetti, C.W. Gear and I.G. Kevrekidis, From Molecular Dynamics to Coarse Self-Similar Solutions: a Simple Example Using Equation-Free Computation. **J. Non-Newt. Fluid Mech., 120**, 215, **2004**.
- 136. P.G. Debenedetti, Reply to Comment on "Supercooled and Glassy Water". J. Phys.: Cond. Matt., 16, 6815, 2004.
- 137. T.F. O'Connor, P.G. Debenedetti and J.D. Carbeck, Simultaneous Determination of Structural and Thermodynamic Effects of Carbohydrate Solutes on the Thermal Stability of Ribonuclease A. J. Amer. Chem. Soc., 126, 11794, 2004.
- 138. Y. Zhang, P.G. Debenedetti, R.K. Prud'homme and B.A. Pethica, Differential Scanning Calorimetry (DSC) Studies of Clathrate Hydrate Formation. **J. Phys. Chem. B**, **108**, 16717, **2004**.
- 139. M.S. Shell, P.G. Debenedetti and A.Z. Panagiotopoulos, Flat Histogram Dynamics and Optimization in Density of States Simulation of Fluids. **J. Phys. Chem. B**, **108**, 19748 **2004**.
- 140. E. La Nave, F. Sciortino, P. Tartaglia, M.S. Shell and P.G. Debenedetti, Reply to Comment on "Test of Nonequilibrium Thermodynamics in Glassy Systems: the Soft-Sphere Case." **Phys. Rev. E**, **71**, 033102, **2005**.
- 141. R.M. Lynden-Bell and P.G. Debenedetti, Computational Investigation of Order, Structure and Dynamics in Modified Water Models. J. Phys. Chem. B, 109, 6527, 2005.
- 142. F.H. Stillinger and P.G. Debenedetti, An Alternative View of Self Diffusion and Shear Viscosity. J. Phys. Chem. B, 109, 6604, 2005.
- 143. S.L. Lee, P.G. Debenedetti and J.R. Errington, A Computational Study of Hydration, Solution Structure, and Dynamics in Dilute Carbohydrate Solutions. J. Chem. Phys., 122, 204511, 2005.
- 144. N. Giovambattista, P.G. Debenedetti, F. Sciortino and H.E. Stanley, Structural Order in Glassy Water. **Phys. Rev. E**, **71**, 061505, **2005**.
- 145. P.G. Debenedetti, Structure, Dynamics and Thermodynamics in Complex Systems: Theoretical Challenges and Opportunities. **AIChEJ.**, **51**, 2391, **2005**.
- 146. S. Chatterjee, H.S. Ashbaugh and P.G. Debenedetti, Effects of non-Polar Solutes on the Thermodynamic Response Functions of Aqueous Mixtures. J. Chem. Phys., 123, 164503, 2005.
- 147. M.S. Shell, P.G. Debenedetti and F.H. Stillinger, Novel Computational Probes of Diffusive Motion. **J. Phys. Chem. B**, **109**, 21329, **2005**.
- 148. M.S. Shell, P.G. Debenedetti and F.H. Stillinger, Dynamic Heterogeneity and Non-Gaussian Behavior in a Model Supercooled Liquid. **J. Phys.: Condens. Matter**, **17**, S4035, **2005**.
- 149. C. Chakravarthy, P.G. Debenedetti and F.H. Stillinger, Generating Inherent Structures of Liquids: Comparison of Local Minimization Algorithms. **J. Chem. Phys.**, **123**, 206101, **2005**.

- 150. M.S. Shell, P.G. Debenedetti and A.Z. Panagiotopoulos, Computational Characterization of the Sequence Landscape in Simple Protein Alphabets. **Proteins. Struct., Funct. & Bioinformatics**, **62**, 232, **2006**.
- 151. M.S. Shell, P.G. Debenedetti and A.Z. Panagiotopoulos, A Conformal Solution Theory for the Energy Landscape and Glass Transition of Mixtures, **Fluid Phase Equil.**, **241**, 147, **2006**.
- 152. N. Giovambattista, P.J. Rossky and P.G. Debenedetti, Effect of Pressure on the Phase Behavior and Structure of Water Confined Between Nanoscale Hydrophobic and Hydrophilic Plates. **Phys. Rev. E**, **73**, 041604, **2006**.
- 153. S. Chatterjee and P.G. Debenedetti, Fluid-Phase Behavior of Binary Mixtures in which One Component Can Have Two Critical Points. **J. Chem. Phys.**, **124**, 154503, **2006**.
- 154. Y. Zhang, P.G. Debenedetti, R.K. Prud'homme and B.A. Pethica, Accurate Prediction of Clathrate Hydrate Phase Equilibria below 300K from a Simple Model. **J. Petr. Sci. & Eng.**, **51**, 45, **2006**.
- 155. Z. Yan, S. Buldyrev, N. Giovambattista, P.G. Debenedetti, and H.E. Stanley, Family of Tunable Spherically-Symmetric Potentials that Span the Range from Hard Spheres to Water-like Behavior, **Phys. Rev. E**, **73**, 051204, **2006**.
- 156. S.L. Lee, A.E. Hafeman, P.G. Debenedetti, B.A. Pethica, and D.J. Moore, Solid-State Stabilization of α-Chymotrypsin and Catalase with Carbohydrates, **Ind. & Eng. Chem. Res.**, **45**, 5134, **2006**.
- 157. T.G. Lombardo, P.G. Debenedetti, and F.H. Stillinger, Computational Probes of Molecular Motion in the Lewis and Wahnström Model of ortho-Terphenyl, **J. Chem. Phys.**, **125**, 174507, **2006**.
- 158. F.H. Stillinger, P.G. Debenedetti and S. Chatterjee. Scaled Particle Theory for Hard Sphere Pairs. I. Mathematical Structure. **J. Chem. Phys.**, **125**, 204504, **2006**.
- 159. S. Chatterjee, P.G. Debenedetti and F.H. Stillinger. Scaled Particle Theory for Hard Sphere Pairs. II. Numerical Analysis. **J. Chem. Phys.**, **125**, 204505, **2006**.
- N. Giovambattista, P.G. Debenedetti and P.J. Rossky, Hydration Behavior under Confinement by Nanoscale Surfaces with Patterned Hydrophobicity and Hydrophilicity. J. Phys. Chem. C, 111, 1323, 2007.
- 161. T.F. O'Connor, P. G. Debenedetti and J.D. Carbeck, Stability of Proteins in the Presence of Carbohydrates; Experiments and Modeling Using Scaled Particle Theory. **Biophys. Chem.**, **127**, 51, **2007**.
- 162. C. Chakravarthy, P.G. Debenedetti and F.H. Stillinger, Lindemann Measures for the Solid-Liquid Phase Transition. **J. Chem. Phys.**, **126**, 204508, **2007**.
- 163. N. Giovambattista, P.G. Debenedetti and P.J. Rossky, Effect of Surface Polarity on Water Contact Angle and Interfacial Hydration Structure. **J. Phys. Chem. B**, **111**, 9581, **2007**.

- 164. Z. Yan, S.V. Buldyrev, P. Kumar, N. Giovambattista, P.G. Debenedetti and H.E. Stanley, Structure of the First and Second Neighbor Shells of Water: Quantitative Relation with Translational and Orientational Order. **Phys. Rev. E**, **76**, 051201, **2007**.
- 165. B.A. Patel, P.G. Debenedetti, F.H. Stillinger and P.J. Rossky, A Water-Explicit Lattice Model of Heat-, Cold-, and Pressure-Induced Protein Unfolding. **Biophys. J.**, **93**, 4116, **2007**.
- 166. S.V. Buldyrev, P. Kumar, P.G. Debenedetti, P.J. Rossky, and H.E. Stanley, Water-Like Solvation Thermodynamics in a Spherically-Symmetric Solvent Model with Two Characteristic Lengths. **Proc.** Nat. Acad. Sci. USA, 104, 20177, 2007.
- 167. B.A. Patel, P.G. Debenedetti and F.H. Stillinger, A Method for Efficient Computation of the Density of States in Water-Explicit Biopolymer Simulations on a Lattice. **J. Phys. Chem. A**, **111**, 12651, **2007**.
- 168. N. Giovambattista, P.G. Debenedetti, C.N. López and P.J. Rossky. Hydrophobicity of Protein Surfaces. Distinguishing Geometry from Chemistry. **Proc. Nat. Acad. Sci. USA**, **105**, 2274, **2008**.
- S. Chatterjee, P.G. Debenedetti, F.H. Stillinger and R.M. Lynden-Bell. A Computational Investigation of Thermodynamics, Structure, Dynamics and Solvation Behavior in Modified Water Models. J. Chem. Phys., 128, 124511, 2008.
- 170. B.A. Patel, P.G. Debenedetti, F.H. Stillinger and P.J. Rossky. Effect of Sequence on the Conformational Stability of a Model Heteropolymer in Explicit Water. **J. Chem. Phys.**, **128**, 175102, **2008**.
- 171. T.G. Lombardo, N. Giovambattista and P.G. Debenedetti. Structural and Mechanical Properties of Glassy Water in Nanoscale Confinement. **Faraday Discuss.**, **141**, 359, **2009**.
- 172. S. Romero-Vargas Castrillón, N. Giovambattista, I.A. Aksay and P.G. Debenedetti. Effect of Surface Polarity on the Structure and Dynamics of Water in Nano-scale Confinement. **J. Phys. Chem. B**, **113**, 1438, **2009**.
- 173. N. Giovambattista, P.J. Rossky and P.G. Debenedetti. Phase Transitions Induced by Nanoconfinement in Liquid Water. **Phys. Rev. Lett.**, **102**, 050603, **2009**.
- 174. T.G. Lombardo, F.H. Stillinger and P.G. Debenedetti. Thermodynamic Mechanism for Solution Phase Chiral Amplification via a Lattice Model. **Proc. Nat. Acad. Sci. USA**, **106**, 15131, **2009**.
- 175. A.L. Ferguson, P.G. Debenedetti and A.Z. Panagiotopoulos. Solubility and Molecular Conformations of n-Alkane Chains in Water. **J. Phys. Chem. B**, **113**, 6405, **2009**.
- 176. N. Giovambattista, P.G. Debenedetti and P.J. Rossky. Effect of Temperature on the Structure and Phase Behavior of Water Confined by Hydrophobic, Hydrophilic and Heterogeneous Surfaces. J. Phys. Chem. B, 3, 2942, 2009.
- 177. S. Romero-Vargas Castrillón, N. Giovambattista, I.A. Aksay and P.G. Debenedetti. Evolution from Surface-Influenced to Bulk-Like Dynamics in Nanoscopically Confined Water (Letter). **J. Phys.** Chem. B, 113, 7973, 2009.

- 178. T. Cho, N. Byrne, D.J. Moore, B.A. Pethica, C.A. Angell and P.G. Debenedetti. Structure-Energy Relations in Hen Egg-White Lysozyme Observed During Refolding from a Quenched Unfolded State. ChemComm., issue 29, 4441, 2009.
- 179. N. Giovambattista, P.G. Debenedetti and P.J. Rossky. Enhanced Surface Hydrophobicity by Coupling of Surface Polarity and Topography. **Proc. Nat. Acad. Sci. USA**, **106**, 15181, **2009**.
- 180. Y. Liu, A.Z. Panagiotopoulos and P.G. Debenedetti. Low Temperature Fluid-Phase Behavior of ST2 Water. **J. Chem. Phys.**, **131**, 104508, **2009**.
- 181. Y. Liu, A.Z. Panagiotopoulos and P.G. Debenedetti. Finite Size Scaling Study of the Vapor-Liquid Critical Properties of Confined Fluids: Crossover from 3 Dimensions to 2 Dimensions. **J. Chem. Phys.**, 132, 144107, 2010.
- 182. A. Ferguson, A.Z. Panagiotopoulos, P.G. Debenedetti and I.G. Kevrekidis. Systematic Determination of Order Parameters for Chain Dynamics Using Diffusion Maps. **Proc. Nat. Acad. Sci. USA**, **107**, 13597, **2010**.
- 183. A.L. Ferguson, S. Zhang, I. Dikiy, A.Z. Panagiotopoulos, P.G. Debenedetti and A.J. Link. An Experimental and Computational Investigation of Spontaneous Lasso Formation in Microcin J25. **Biophys. J.**, 99, 3056, 2010.
- 184. H.W. Hatch, F.H. Stillinger and P.G. Debenedetti. Chiral Symmetry Breaking in a Microscopic Model with Asymmetric Autocatalysis and Inhibition. **J. Chem. Phys.**, **133**, 224502, **2010**.
- 185. L. Xu, N. Giovambattista, S.V. Buldyrev, P.G. Debenedetti and H.E. Stanley. Water-like Glass Polyamorphism in a Monoatomic Isotropic Jagla Model. J. Chem. Phys., 134, 064507, 2011.
- 186. R.M. Lynden-Bell, N. Giovambattista, P.G. Debenedetti, T. Head-Gordon and P.J. Rossky. Hydrogen Bond Strength and Network Structure Effects on Hydration of Non-Polar Molecules. **Phys. Chem. Chem. Phys.**, **13**, 2748, **2011**.
- 187. S. Romero-Vargas Castrillón, N. Giovambattista, I. Aksay and P.G. Debenedetti. Structure and Energetics of Thin Film Water. **J. Phys. Chem. C**, **115**, 4624, **2011**.
- 188. Z. Shi, P.G. Debenedetti and F.H. Stillinger. Properties of Model Atomic Free-Standing Films. J. Chem. Phys., 134, 114524, 2011.
- 189. S. Sarupria and P.G. Debenedetti. Molecular Dynamics Study of Carbon Dioxide Hydrate Dissociation. J. Phys. Chem. A, 115, 6102, 2011.
- A.L. Ferguson, A.Z. Panagotopoulos, P.G. Debenedetti and Y.G. Kevrekidis. Integrating Diffusion Maps with Umbrella Sampling: Application to Alanine Dipeptide. J. Chem. Phys., 134, 135103, 2011.
- 191. C.A. Cerdeiriña, P.G. Debenedetti, P.J. Rossky and N. Giovambattista. Evaporation Length Scales of Confined Water and Some Common Organic Liquids. **J. Phys. Chem. Lett.**, **2**, 1000, **2011**.

- 192. Y. Liu, A.Z. Panagiotopoulos and P.G. Debenedetti. Monte Carlo Simulations of High-Pressure Phase Equilibria of CO₂-H₂O Mixtures. **J. Phys. Chem. B**, **115**, 6629, **2011**.
- 193. A.L. Ferguson, A.Z. Panagiotopoulos, I.G. Kevrekidis and P.G. Debenedetti. Nonlinear Dimensionality Reduction in Molecular Simulation: The Diffusion Map Approach. (Frontiers Article). Chem. Phys. Lett., 509, 1, 2011.
- 194. Z. Shi, P.G. Debenedetti, F.H. Stillinger and P. Ginart. Structure, Dynamics and Thermodynamics of a Family of Potentials with Tunable Softness. J. Chem. Phys., 135, 084513, 2011.
- 195. G. Stirnemann, S. Romero-Vargas Castrillón, J.T. Hynes, P.J. Rossky, P.G. Debenedetti and D. Laage. Non-Monotonic Dependence of Water Dynamics on Surface Hydrophilicity: Competing Effects of Hydration Structure and Hydrogen Bond Strength. Phys. Chem. Chem. Phys., 13, 19911, 2011
- 196. S. Matysiak, P.G. Debenedetti and P.J. Rossky. Dissecting the Energetics of Hydrophobic Hydration of Polypeptides. J. Phys. Chem. B, 115, 14859, 2011.
- 197. Z. Su, S.V. Buldyrev, P.G. Debenedetti, P.J. Rossky and H.E. Stanley. Modeling Simple Amphiphilic Solutes in a Jagla Solvent. J. Chem. Phys., 136, 044511, 2012.
- N. Giovambattista, P.J. Rossky and P.G. Debenedetti. Computational Studies of Pressure, Temperature and Surface Effects on the Structure and Thermodynamics of Confined Water. Annu. Rev. Phys. Chem., 63, 179, 2012.
- S. Sharma and P.G. Debenedetti. Evaporation Rate of Water in Hydrophobic Confinement. Proc. Nat'l. Acad. Sci. USA, 109, 4365, 2012.
- 200. K.B. Daly, J.B. Benziger, P.G. Debenedetti and A.Z. Panagiotopoulos. Massively Parallel Chemical Potential Calculation on Graphics Processing Units. **Computer Phys. Commun.**, **183**, 2054, **2012**.
- 201. S. Matysiak, P.G. Debenedetti and P.J. Rossky. The Role of Hydrophobic Hydration in Protein Stability: a 3D Water-Explicit Protein Model Exhibiting Cold and Heat Denaturation. **J. Phys. Chem. B**, 116, 8095, 2012.
- 202. H. Hatch and P.G. Debenedetti. Molecular Modeling of Mechanical Stresses on Proteins in Glassy Matrices: Formalism. **J. Chem. Phys.**, **137**, 035103, **2012**.
- S. Romero-Vargas Castrillón, S. Matysiak, F.H. Stillinger, P.J. Rossky and P.G. Debenedetti. Phase Behavior of a Lattice Hydrophobic Oligomer in Explicit Water. J. Phys. Chem. B, 116, 9540, 2012.
- 204. S. Romero-Vargas Castrillón, S. Matysiak, F.H. Stillinger, P.J. Rossky and P.G. Debenedetti. Thermal Stability of Hydrophobic Helical Oligomers: a Lattice Simulation Study in Explicit Water. J. Phys. Chem. B, 116, 9963, 2012.
- 205. A.L. Ferguson, N. Giovambattista, P.J. Rossky, A.Z. Panagiotopoulos and P.G. Debenedetti. A Computational Investigation of the Phase Behavior and Capillary Sublimation of Water Confined Between Nanoscale Hydrophobic Plates. J. Chem. Phys., 137, 144501, 2012.

- 206. J.C. Palmer and P.G. Debenedetti. Computer Simulation of Water Sorption on Flexible Protein Crystals. J. Phys. Chem. Lett., 3, 2713, 2012.
- 207. S. Sarupria and P.G. Debenedetti. Homogeneous Nucleation of Methane Hydrate in Microsecond Molecular Dynamics Simulations. J. Phys. Chem. Lett., 3, 2942, 2012.
- 208. S. Sharma and P.G. Debenedetti. Free Energy Barriers to Evaporation of Water in Hydrophobic Confinement. **J. Phys. Chem. B**, **116**, 13282, **2012**.
- 209. Y. Liu, J.C. Palmer, A.Z. Panagiotopoulos and P.G. Debenedetti. Liquid-Liquid Transition in ST2 Water. J. Chem. Phys., 137, 214505, 2012.
- 210. F. Ricci, F.H. Stillinger and P.G. Debenedetti. Creation and Persistence of Chiral Asymmetry in a Microscopically Reversible Molecular Model. J. Phys. Chem. B, 117, 602, 2013.
- 211. Z. Shi, P.G. Debenedetti and F.H. Stillinger. Relaxation Processes in Liquids: Variations on a Theme by Stokes and Einstein. **J. Chem. Phys.**, **138**, 12A526, **2013**.
- J. Dowdle, S.V. Buldyrev, H.E. Stanley, P.G. Debenedetti and P.J. Rossky. Temperature and Length Scale Dependence of Solvophobic Solvation in a Single-site Water-like Liquid. J. Chem. Phys., 138, 064506, 2013.
- Y. Liu, T. Lafitte, A.Z. Panagiotopoulos and P.G. Debenedetti. Simulations of Vapor-Liquid Phase Equilibrium and Interfacial Tension in the CO2-H2O-NaCl System. **AIChEJ**, **59**, 3514, **2013**.
- 214. F.H. Stillinger and P.G. Debenedetti. Glass Transition Thermodynamics and Kinetics. **Annu. Rev.** Cond. Matter Phys., 4, 263, 2013.
- S. Sharma, S.K. Kumar, S.V. Buldyrev, P.G. Debenedetti, P.J. Rossky and H.E. Stanley, A Coarse-Grained Protein Model in a Water-like Solvent. Sci. Reports, 3, Art. 1841, doi: 10.1038/srep01841, 2013.
- 216. J.C. Palmer, R. Car and P.G. Debenedetti, The Liquid-Liquid Transition in Supercooled ST2 Water: a Comparison Between Umbrella Sampling and Well-Tempered Metadynamics. **Faraday Discuss.**, **167**, 77, **2013**.
- 217. K.B. Daly, J.B. Benziger, P.G. Debenedetti and A.Z. Panagiotopoulos, Molecular Dynamics Simulations of Water Sorption in a Perfluorosulfonic Acid Membrane. **J. Phys. Chem. B**, **117**, 12649, **2013**.
- 218. F. Ricci, F.H. Stillinger and P.G. Debenedetti, A Computational Investigation of Attrition-Enhanced Chiral Symmetry Breaking in Conglomerate Crystals. J. Chem. Phys., 139, 174503, 2013.
- V. Holten, J.C. Palmer, P.H. Poole, P.G. Debenedetti and M. Anisimov, Two-State Thermodynamics of the ST2 Model for Supercooled Water. **J. Chem. Phys., 140,** 104502, **2014.**
- 220. H.W. Hatch, F.H. Stillinger and P.G. Debenedetti, Computational Study of the Stability of the Miniproteins Trp-Cage and GB1 Beta-Hairpin, and of the AK16 Peptide, Under Negative Pressure. **J. Phys. Chem. B**, 118, 7761, 2014.

- 221. J.C. Palmer, F. Martelli, Y. Liu, R. Car, A.Z. Panagiotopoulos and P.G. Debenedetti, Metastable Liquid-Liquid Transition in a Molecular Model of Water. **Nature**, **510**, 385, **2014**.
- 222. A. Haji-Akbari and P.G. Debenedetti, The Effect of Substrate on Thermodynamic and Kinetic Anisotropies in Atomic Thin Films. **J. Chem. Phys., 141,** 024506, **2014.**
- 223. K. Daly, J.B. Benziger, A.Z. Panagiotopoulos and P.G. Debenedetti, Molecular Dynamics Simulations of Water Permeation Across Nafion Membrane Interfaces. **J. Phys. Chem. B**, **118**, 8798, **2014**.
- L. Cai, B.A. Pethica, P.G. Debenedetti and S. Sundaresan, Formation Kinetics of Cyclopentane-Methane Binary Clathrate Hydrate. Chem. Eng. Sci., 119, 147, 2014.
- 225. J.R. Vella, F.H. Stillinger, A.Z. Panagiotopoulos and P.G. Debenedetti, A Comparison of the Predictive Capabilities of the Embedded-Atom Method and Modified Embedded-Atom Method Potentials for Lithium. **J. Phys. Chem. B,** in press, http://dx.doi.org/10.1021/jp5077752, **2014.**
- 226. Y.E. Altabet and P.G. Debenedetti, The Role of Material Flexibility on the Drying Transition of Water Between Hydrophobic Objects: a Thermodynamic Analysis. **J. Chem. Phys.**, **141**, 18C535, **2014**.
- 227. A. Haji-Akbari, R.S. DeFever, S. Sarupria and P.G. Debenedetti, Suppression of Sub-Surface Freezing in Free-Standing Thin Films of a Coarse-Grained Model of Water. **Phys. Chem. Chem. Phys, 16,** 25916, **2014.**
- 228. K. Daly, A.Z. Panagiotopoulos, P.G. Debenedetti and J.B. Benziger, Viscosity of Nafion Oligomers as a Function of Hydration and Counterion Type: a Molecular Dynamics Study. **J. Phys. Chem. B**, 118, 13981, 2014.
- 229. J.C. Palmer and P.G. Debenedetti, Recent Advances in Molecular Simulation: a Chemical Engineering Perspective. **AIChE J., 61**, 370, **2015.**
- 230. S. Kim, J.C. Palmer and P.G. Debenedetti, A Computational Study of the Effect of Matrix Structural Order on Water Sorption by Trp-Cage Miniproteins. **J. Phys. Chem. B**, **119**, 1847 **2015**.
- 231. S. Kim, C.J. Dsilva, I.G. Kevrekidis and P.G. Debenedetti, Systematic Characterization of Protein Folding Pathways Using Diffusion Maps: Application to Trp-Cage Miniprotein. **J. Chem. Phys.**, **142**, 085101, **2015**.
- 232. M. Chen, J.R. Vella, A.Z. Panagiotopoulos, P.G. Debenedetti, F.H. Stillinger and E.A. Carter, Liquid Li Structure and Dynamics: a Comparison Between OFDT and Second Nearest-Neighbor Embedded-Atom Method. AIChE J., 61, 2841, 2015.
- 233. R.C. Remsing, E. Xi, S. Vembanur, S. Sharma, P.G. Debenedetti, S. Garde and A.J. Patel, Pathways to Dewetting in Hydrophobic Confinement. **Proc. Nat'l. Acad. Sci. USA**, **112**, 8181, **2015**.
- 234. D.J. Bozym, B. Uralcan, D.T. Limmer, M.A. Pope, N.J. Szameta, P.G. Debenedetti and I.A. Aksay, Anomalous Capacitance Maximum of the Glassy Carbon-Ionic Liquid Interface through Dilution with Organic Solvents. J. Phys. Chem. Lett., 6, 2644, 2015.

- 235. A. Haji-Akbari and P.G. Debenedetti, Direct Calculation of Ice Homogeneous Nucleation Rate for a Molecular Model of Water. **Proc. Nat'l. Acad. Sci. USA**, **112**, 10582, **2015**.
- 236. A. Haji-Akbari and P.G. Debenedetti, Thermodynamic and Kinetic Anisotropies in Octane Thin Films. **J. Chem. Phys.**, **143**, 214501, **2015**.
- 237. L. Cai, B.A. Pethica, P.G. Debenedetti and S. Sundaresan, Formation of Cyclopentane-Methane Binary Hydrate in Brine Solutions. **Chem. Eng. Sci.**, **141**, 125, **2016**.
- 238. M.M. Gianetti, A. Haji-Akbari, M.P. Longinotti and P.G. Debenedetti, Computational Investigation of Structure, Dynamics and Nucleation Kinetics of a Family of Modified Stillinger-Weber Model Fluids in Bulk and Free-Standing Thin Films. **Phys. Chem. Chem. Phys.**, **18**, 4102, **2016**.
- 239. R.S. Singh, J.W. Biddle, P.G. Debenedetti and M. Anisimov, Two-State Thermodynamics and the Possibility of a Liquid-Liquid Transition in Supercooled TIP4P/2005 Water. **J. Chem. Phys.**, **144**, 144504, **2016**.
- 240. J.C. Palmer, F. Martelli, Y. Liu, R. Car, A.Z. Panagiotopoulos and P.G. Debenedetti, Reply to "Metastability and no Criticality," by D. Chandler. **Nature**, **531**, E2, doi:10.1038/nature16540, **2016**.
- 241. C. Cerdeiriña and P.G. Debenedetti, Water Anomalous Thermodynamics, Attraction, Repulsion, and Hydrophobic Hydration. **J. Chem. Phys.**, **144**, 164501, **2016**.
- 242. J.C. Palmer, R.S. Singh, R. Chen, F. Martelli and P.G. Debenedetti, Density and Bond-Orientational Relaxations in Supercooled Water. **Mol. Phys.**, **114**, 2580, **2016**.
- 243. S. Kim, D.R. Gupta and P.G. Debenedetti, Computational Investigation of Dynamical Transitions in Trp-cage Miniprotein Powders. **Sci. Rep.**, **6**, 25612, doi: 10.1038/srep25612, **2016**.
- 244. B. Uralcan, I.A. Aksay, P.G. Debenedetti and D.T. Limmer, Concentration Fluctuations and Capacitive Response in Dense Ionic Solutions. **J. Phys. Chem. Lett.**, 7, 2333, **2016**.
- 245. S. Kim, J.C. Palmer and P.G. Debenedetti, Computational Investigation of Cold Denaturation in the Trp-cage Miniprotein. **Proc. Nat'l. Acad. Sci. USA**, **113**, 8991, **2016**.
- 246. F. Latinwo, F.H. Stillinger and P.G. Debenedetti, Molecular Model for Chirality Phenomena. J. Chem. Phys., 145, 154503, 2016.
- 247. J.R. Espinosa, J. M. Young, H. Jiang, D. Gupta, C. Vega, E. Sanz, P.G. Debenedetti and A.Z. Panagiotopoulos, On the Calculation of Solubilities via Direct Coexistence Simulations: Investigation of NaCl Aqueous Solutions and Lennard-Jones Binary Mixtures. J. Chem. Phys., 145, 154111, 2016.
- 248. Y.E. Altabet, F.H. Stillinger and P.G. Debenedetti, A Cavitation Transition in the Energy Landscape of Simple Cohesive Liquids and Glasses. J. Chem. Phys., 145, 211905, 2016.
- 249. J.W. Biddle, R.S. Singh, E.M. Sparano, F. Ricci, M.A. González, C. Valeriani, J.L. Abascal, P.G. Debenedetti, M.A. Anisimov and F. Caupin, Two-Structure Thermodynamics for the TIP4P/2005

- Model of Water Covering Supercooled and Deeply Stretched Regions. **J. Chem. Phys.**, **146**, 034502, **2017**.
- 250. J.R. Vella, M. Chen, F.H. Stillinger, E.A. Carter, P.G. Debenedetti and A.Z. Panagiotopoulos, Structural and Dynamic Properties of Liquid Tin from a New Modified Embedded-Atom Method Force Field. **Phys. Rev. B**, **95**, 064202, **2017**.
- 251. S. Kim, E.M. Sparano, R.S. Singh and P.G. Debenedetti, Microscopic Origin of Hysteresis in Water Sorption on Protein Matrices. **J. Phys. Chem. Lett.**, **8**, 1185, **2017**.
- 252. Y.E. Altabet, A. Haji-Akbari and P.G. Debenedetti, Effect of Material Flexibility on the Thermodynamics and Kinetics of Hydrophobically Induced Evaporation of Water. **Proc. Nat'l. Acad. Sci. USA**, **114**, E2548, **2017**.
- 253. A. Haji-Akbari and P.G. Debenedetti, Computational Study of Surface Freezing in a Molecular Model of Water. **Proc. Nat'l. Acad. Sci. USA**, **114**, 3316, **2017**.
- 254. R.S. Singh, J.C. Palmer, P.D.A. Pudney, P.K.C. Paul, C. Johannessen, P.G. Debenedetti, J. Raut, K. Lee, M. Noro and D. Tiemsesen, Molecular Modeling and Structural Characterization of a High-Glycine-Tyrosine hair Keratin Associated Protein, Phys. Chem. Chem. Phys., 19, 8575, 2017.
- 255. F. Ricci and P.G. Debenedetti, A Free Energy Study of the Liquid-Liquid Phase Transition of the Jagla Two-Scale Potential. **J. Chem. Sci.**, **129**, 801, **2017**.
- 256. J.R. Vella, M. Chen, S. Fürstenberg, F.H. Stillinger, E.A. Carter, P.G. Debenedetti and A.Z. Panagiotopoulos, Characterization of the Liquid Li-Solid Mo (110) Interface from Classical Molecular Dynamics for Plasma-Facing Applications. Nucl. Fusion, 57, 116036, 2017.
- 257. S. Kim, R.S. Singh, P.K.C. Paul and Pablo G. Debenedetti, Effects of Disulfide Bridges and Backbone Connectivity on Water Sorption by Protein Matrices. **Sci. Rep., 7**: 7957, doi:10.1038/s41598-017-08561-2, **2017**.
- 258. A. Haji-Akbari and P.G. Debenedetti, Surface Freezing in Water: a Nexus of Experiments and Simulations. J. Chem. Phys., 147, 060901, 2017.
- 259. Y.E. Altabet, R.Singh, F.H. Stillinger and P.G. Debenedetti, Thermodynamic Anomalies in Stretched Water. **Langmuir**, 33, 11771, 2017.
- Y.E. Altabet and P.G. Debenedetti, Communication: Relationship Between Local Structure and the Stability of Water in Hydrophobic Confinement. **J. Chem. Phys., 147**, 241102, **2017**.
- H. Jiang, A. Haji-Akbari, P.G. Debenedetti and A.Z. Panagiotopoulos, Forward Flux Sampling Calculation of Homogeneous Nucleation Rates from Aqueous NaCl Solutions. J. Chem. Phys. 148, 044505, 2018.
- Y.E. Altabet, A.L. Fenley, F.H. Stillinger and P.G. Debenedetti, Cavitation Transition in the Energy Landscape: Distinct Tensile Yielding Behavior in Strongly and Weekly Attractive Systems. J. Chem. Phys., 148, 114501, 2018.

- 263. J.C. Palmer, A. Haji-Akbari, R. Singh, F. Martelli, R. Car, A.Z. Panagiotopoulos and P.G. Debenedetti, Comment on "The Putative Liquid-Liquid Transition is a Liquid-Solid Transition in Atomistic Models of Water" [Parts I and II: J. Chem. Phys. 135, 134503 (2011); J. Chem. Phys. 138, 214504 (2013)]. J. Chem. Phys., 148, 137101, 2018.
- 264. C. Cerdeiriña and P.G. Debenedetti, Water's Thermal Pressure Drives the Temperature Dependence of Hydrophobic Hydration. **J. Phys. Chem. B**, 122, 3620 2018.
- 265. B. Uralcan, S.B. Kim, C.E. Markwalter, R.K. Prud'homme and P.G. Debenedetti, A Computational Study of the Ionic Liquid-Induced Destabilization of the Miniprotein Trp-Cage. **J. Phys. Chem. B**, 122, 5707, 2018.
- 266. G.H. Zerze, M.N. Khan, F.H. Stillinger and P.G. Debenedetti, Computational Investigation of the Effect of Backbone Chiral Inversions on Polypeptide Structure. J. Phys. Chem. B, 122, 6357, 2018.

Chapters in Books

- 1. P.G. Debenedetti, C.G. Vayenas, I. Yentekakis and L.L. Hegedus, Mathematical Modeling of Cross-Flow Solid State Electrochemical Reactors. **ACS Symp. Ser. 237**, Ch.10, **1984**.
- 2. P.G. Debenedetti and R.C. Reid, Binary Diffusion in Supercritical Fluids. p. 225 in Proc. Tech. Symp. 3, Supercritical Fluid Technology, J.M.L. Penninger, M. Radosz, M.A. McHugh and V.J. Krukonis, eds., Elsevier Science Publishers, Amsterdam, 1985.
- 3. R.S. Mohamed, D.S. Halverson, P.G. Debenedetti and R.K. Prud'homme, Solids Formation Following the Expansion of Supercritical Mixtures. Supercritical Science and Technology, K.P.Johnston and J.M.L. Penninger, eds., ACS Symp. Ser. No. 406, ch.23, 1989.
- 4. L.L. Lee, P. G. Debenedetti and H.D. Cochran, Fluctuation Theory of Supercritical Solutions. In Supercritical Fluid Technology, Reviews in Modern Theory and Applications, J. F. Ely and T. J. Bruno, eds., CRC Press, ch. 4, 1991.
- B.L. Knutson, D.L. Tomasko, C.A. Eckert, P.G. Debenedetti and A.A. Chialvo, Local Density Augmentation in Supercritical Solutions: a Comparison Between Fluorescence Spectroscopy and Molecular Dynamics Results. In Supercritical Fluid Technology. Theoretical and Applied Approaches in Analytical Chemistry, F.Bright and M.E.P. McNally, eds. ACS Symp. Ser. No. 488, Ch. 5, 1992.
- 6. J.W. Tom, G.-B. Lim, P.G. Debenedetti and R.K. Prud'homme, Applications of Supercritical Fluids in Controlled Release of Drugs. In Supercritical Engineering Science: Fundamentals and Applications, E. Kiran and J.F. Brennecke, eds. **ACS Symp. Ser. No. 514**, Ch. 19, **1993**.
- 7. P.G. Debenedetti, Supercritical Fluids as Particle Formation Media. In Supercritical Fluids Fundamentals for Application, E. Kiran and J.M.H. Levelt Sengers, eds., **NATO ASI, Ser. E, 273**, 719, **1994**.
- 8. P.G. Debenedetti, Solute-Solute Interactions: Theory and Simulation. In Supercritical Fluids Fundamentals for Application, E. Kiran and J.M.H. Levelt Sengers, eds., **NATO ASI, Ser. E, 273**, 439, **1994**.

- 9. B.L. Knutson, Jean W. Tom and P.G. Debenedetti, Preparation of Microparticulates Using Supercritical Fluids. In Microparticulate Systems for the Delivery of Proteins and Vaccines, S. Cohen and H. Bernstein, eds. Marcel Dekker, Inc., New York. Ch. 3, **1996**.
- 10. P.G. Debenedetti, Phase Separation by Nucleation and Spinodal Decomposition: Fundamentals. In Supercritical Fluids Fundamentals and Applications, E. Kiran, P.G. Debenedetti, and C.J. Peters, eds., **NATO Science Series**, **Ser. E**, **366**, 123, **2000**.
- 11. P.G. Debenedetti, F.H. Stillinger, T.M. Truskett and C.P. Lewis, Theory of Supercooled Liquids and Glasses: Energy Landscape and Statistical Geometry Perspectives. In Molecular Modeling and Theory in Chemical Engineering, A. Chakraborty, ed., Adv. in Chem. Eng., 28, 21, 2001.
- 12. P.G. Debenedetti and R.M. Lynden-Bell, Properties of Liquids Made from Modified Water Models. In Water and Life. The Unique Properties of H2O, R.M. Lynden-Bell, S. Conway Morris, J.D. Barrow, J.L. Finney and C.L. Harper, Jr, eds., ch.6, **CRC Press**, **2010**.

Book Reviews

- 1. Supercritical Fluid Extraction. Principles and Practice, by M. McHugh and V. Krukonis, Butterworths, Boston, 1986. **AIChEJ.**, **33**, 1406, **1987**.
- 2. Molecular Dynamics Simulation. Elementary Methods, by J.M. Haile, Wiley, New York, 1992. **AIChEJ**, 39, 1097, 1993.
- 3. Statistical Mechanics of Phase Transitions, by J.M. Yeomans, Oxford University Press, 1992. J. Amer. Chem. Soc., 115, 12230, 1993.
- 4. Innovations in Supercritical Fluids: Science and Technology, edited by K.W. Hutchenson and N.R. Foster, ACS Symp. Ser. 608, American Chemical Society, Washington, DC, 1995. **AIChEJ., 42**, 2698, **1996**.
- 5. Chemical Thermodynamics: Basic Theory and Methods, 5th ed., by I.M. Klotz and M. Rosenberg, 1994. Chem. Eng. Educ., 30, 69, 1996.

Miscellaneous

- 1. One Substance, Two Liquids? Invited News and Views article, Nature, 392, 127, 1998.
- 2. D.A. Saville, W.B. Russel and P.G. Debenedetti, Bill Schowalter, Preface to Schowalter Festschrift Issue, Ind. & Eng. Chem. Res., 41, 6215, 2002.
- 3. P.G. Debenedetti, B.L. Knutson, K.P. Johnston and J.F. Brennecke, In Honor of Charles A. Eckert, Preface to Eckert Festschrift Issue, **Ind. & Eng. Chem. Res., 42**, 6263, **2003**.

- 4. P. G. Debenedetti and S. Torquato, Frank H. Stillinger, Theoretical Chemist: a Tribute, Preface to Stillinger Festschrift Issue, **J. Phys. Chem. B**, **108**, 19569, **2004**.
- 5. When a Phase is Born. Invited News and Views article, **Nature**, **441**, 168, **2006**.
- 6. P.G. Debenedetti, T.K. Vanderlick, A.J. Myers and J.A. Quinn, In Honor of Eduardo Glandt, Preface to Glandt Festschrift, **Ind. & Eng. Chem. Res.**, **45**, 5419, **2006**.
- 7. P.G. Debenedetti, Bill Russel: a Tribute, Preface to Russel Festschrift Issue, **Ind. & Eng. Chem. Res.**, **45**, 6877, **2006**.
- 8. Invited Journal Club article, Nature, 446, 835, 2007.
- 9. P.G. Debenedetti and S. Sarupria, Hydrate Molecular Ballet. Invited Perspective article, **Science**, **326**, 1070, **2009**.
- 10. C. Vega, J.L.F. Abascal and P.G. Debenedetti, Physics and Chemistry of Water and Ice, Preface to co-guest-edited themed issue, **Phys. Chem. Chem. Phys.**, **13**, 19660, **2011**.
- 11. P.G. Debenedetti and S.C. Glotzer, Tribute to H. Eugene Stanley, Preface to co-guest-edited Festschrift, **J. Phys. Chem. B**, **115**, 13963, **2011**.
- 12. P.G. Debenedetti, Stretched to the Limit. Invited News and Views article, Nature Physics, 9, 7, 2013.

Patents

- 1. Formation of Protein Microparticles by Anti-Solvent Precipitation, Australian Patent 668367, August 20, 1996 [with G.-B. Lim and R.K. Prud'homme]
- 2. Formation of Protein Microparticles by Anti-Solvent Precipitation, European Patent EP 0542314 B1, October 29, 1998 [with G.-B. Lim and R.K. Prud'homme]
- 3. Preparation of Protein Microparticles by Supercritical Fluid Precipitation, US Patent 6,063,910, May 16, 2000 [with G.-B. Lim and R.K. Prud'homme]

PABLO G. DEBENEDETTI⁵

I. Named, Invited and Plenary Lectures

1988

"Cluster Formation in Near-Critical Systems: Classical and Non-Classical Modeling". International Symposium on Thermodynamics in Chemical Engineering and Industry, Beijing, China, June 2, 1988.

1989

"Clustering in Supercritical Mixtures: Theory, Applications, and Simulations". Fifth International Conference on Fluid Properties and Phase Equilibria for Chemical Process Design, Banff Center, Banff, Canada, May 2, 1989.

1992

"Particle Formation by Rapid Expansion of Supercritical Solutions". Engineering Foundation Meeting on Vapor-Phase Manufacture of Ceramics, Kona, Hawaii, January 13, 1992.

"Use of Supercritical Fluids for the Production of Controlled Release Devices". Gordon Research Conference on Polymers for Biosystems, Oxnard, California, February 28, 1992.

"Application of Supercritical Fluids for the Production of Sustained Delivery Devices". Second European Symposium on Controlled Drug Delivery, Noordwijk aan Zee, Holland, April 1, 1992.

"Structure and Dynamics of Supercooled Liquids: Spinodals, Glasses, and Some Open Questions on the Theory of Metastability." Robert W. Vaughan Memorial Lecture. Department of Chemical Engineering, California Institute of Technology, April 14, 1992.

1993

"Supercritical Fluids: Fundamentals and Applications". 6th International Congress on Engineering and Food, Chiba, Japan, May 26, 1993.

1994

"Towards an Understanding of Supercooled and Glassy Water." International Symposium on Molecular Thermodynamics and Molecular Simulation, Kyoto University, Kyoto, Japan, January 12, 1994.

"Phase Equilibrium, Thermal Expansion, and Stability Limits of a Model Network-Forming Fluid: Implications for the Phase Behavior of Supercooled Water". Gordon Research Conference on Water and Aqueous Solutions, Holderness School, Plymouth, New Hampshire, August 7, 1994.

"The Thermodynamics of Supercooled Water: a Critical Review". 12th International Conference on the Properties of Water and Steam, Orlando, Florida, September 13, 1994.

1995

"Thermodynamics of Supercooled and Glassy Water." Murphree Award Symposium honoring Charles A. Eckert, ACS Spring Meeting, Anaheim, California, April 3, 1995.

"Supercritical Fluids", a four-lecture course. Astra-Hässle, Mölndal, Sweden, May 22-23, 1995.

"Materials Processing with Supercritical Fluids". Invited tutorial. American Association for Aerosol Research, 14th annual meeting. Pittsburgh, Pennsylvania, October 9, 1995.

[§] This list includes only named, invited, plenary lectures (I) and seminars (II). Contributed talks and posters are not included.

1996

"Particle Formation from Supercritical Fluids." International Fine Particle Research Institute Annual Meeting, Nancy, France, June 11, 1996.

"The Glass Transition: Thermodynamic and Dynamic Viewpoints." 1996 Colorado Protein Stability Conference, Breckenridge, Colorado, July 13, 1996.

"Metastable Water." Gordon Research Conference on Physics and Physical Chemistry of Water and Aqueous Solutions, Holderness School, Plymouth, New Hampshire, August 5, 1996.

"Materials Processing with Supercritical Fluids." Third International Symposium on High Pressure Chemical Engineering, ETH (Swiss Federal Institute of Technology), Zürich, Switzerland, October 8, 1996.

1997

"Thermodynamics of Polyamorphic Phase Transitions in Network-Forming Fluids." International Symposium on Molecular Thermodynamics and Molecular Simulation, Hosei University, Tokyo, Japan, January 14, 1997.

"Holes, Packings and Networks" Towards a Rigorous Understanding of Liquids Under Extreme Conditions." Stanley Katz Memorial Lecture, Department of Chemical Engineering, City College of the City University of New York, May 12, 1997.

"Thermodynamics of Supercooled and Glassy Water." 13th Symposium on Thermophysical Properties, Boulder, CO, June 23, 1997.

"Models of Liquid Polyamorphism." Gordon Research Conference on the Chemistry and Physics of Liquids, Holderness School, Plymouth, New Hampshire, August 5, 1997.

"Towards a Fundamental Understanding of Liquids Under Extreme Conditions." Kurt Wohl Memorial Lecture, Department of Chemical Engineering, University of Delaware, September 19, 1997.

"Materials Processing with Supercritical Fluids." Engineering Foundation Conference on Separation Technology: Separations for Clean Production, Davos, Switzerland, October 28, 1997.

1998

"Thermodynamics of Supercooled and Glassy Water." March Annual Meeting of the American Physical Society, Symposium on The Chemistry and Physics of Water, Los Angeles, California, March 16, 1998.

"Statistical Geometry, Energy Landscapes, and the Glass Transition." Murphree Award Symposium Honoring Stanley I. Sandler, American Chemical Society Meeting, Dallas, Texas, April 1, 1998.

"Liquids at Extreme Conditions: Natural Occurrence, Engineering Applications, and Scientific Challenges." Ashton Cary Lecture, School of Chemical Engineering, Georgia Institute of Technology, Atlanta, Georgia, April 13, 1998.

"Thermodynamics of Supercooled and Glassy Water." Ashton Cary Lecture, School of Chemical Engineering, Georgia Institute of Technology, Atlanta, Georgia, April 14, 1998.

"Statistical Geometry and Energy Landscapes in Liquids and Glasses: Fundamentals and Applications." Eighth International Conference on Properties and Phase Equilibria for Product and Process Design. Noordwijkerhout, The Netherlands, April 30, 1998.

"Statistical Geometry and Energy Landscapes in Liquids and Glasses." 5th Liblice Conference on the Statistical Mechanics of Liquids, Zelezna Ruda, Czech Republic, June 9, 1998.

"Phase Separation by Nucleation and Growth, and by Spinodal Decomposition: Fundamentals." NATO Advanced Study Institute, Supercritical Fluids. Fundamentals and Applications, Kemer, Turkey, July 20, 1998.

"Towards an Improved Understanding of Supercooled Liquids and Glasses." Professional Progress Award Lecture, American Institute of Chemical Engineers, Miami Beach, Florida, November 17, 1998.

1999

"The Equation of State of an Energy Landscape." 81st Statistical Mechanics Conference, Rutgers University, New Brunswick, New Jersey, May 9, 1999.

"Statistical Geometry and Energy Landscapes in Liquids and Glasses." Symposium in Honor of Eli Ruckenstein, State University of New York, Buffalo, June 19, 1999.

"Thermodynamics of Supercooled and Glassy Water." ACS National Meeting, New Orleans, August 24, 1999.

"Thermodynamics of Supercooled and Glassy Water." International Bunsen Discussion Meeting on Metastable Water, Schloss Nordkirchen, Germany, September 23, 1999.

2000

"Materials Processing with Supercritical Fluids. Pharmaceutical Applications." 5^a International Symposium on Supercritical Fluids, Atlanta, Georgia, April 9, 2000.

"Recent Developments on the Statistical Geometry of Amorphous Packings." 2nd International TRI-Princeton Workshop on Characterization of Porous Materials: from Angstroms to Millimeters, Princeton, New Jersey, June 19, 2000.

"Recent Advances in the Theory of Metastable Fluids and Glasses." 14^a Symposium on Thermophysical Properties, Boulder, Colorado, June 28, 2000.

"Recent Developments in the Theory of Bulk and Confined Water." 3st Joint China/USA Chemical Engineering Conference – CUChE3 – Beijing, China, September 28, 2000.

2001

"Towards a Quantification of Disorder in Liquids and Solids." Cullimore Lecture, New Jersey Institute of Technology, Newark, New Jersey, January 24, 2001.

"Recent Developments in the Theory of Bulk and Confined Water." Symposium on "Probing Molecular Aqueous Environments in Chemistry and Biology," American Chemical Society National Meeting, San Diego, California, April 2, 2001.

"Preservation of Biomolecules in Carbohydrate-Water Glasses." Ipatieff Award Symposium Honoring Joan Brennecke, American Chemical Society National meeting, San Diego, California, April 4, 2001.

"Recent Developments in the Theory of Amorphous Aqueous Systems." The Amorphous State: a Critical Review. Churchill College, Cambridge University, May 16, 2001.

"Ubiquitous but Unusual, Odd but Ordered: Recent Developments in Aqueous Thermodynamics." John M. Prausnitz Award Lecture. 9^a International Conference on Properties and Phase Equilibria for Product and Process Design. Kurashiki, Japan, May 23, 2001.

"Recent Developments in the Theory of Bulk and Confined Water." Euresco Conference on Water at the New Millenium. Obernai, France, September 11, 2001.

"Recent Developments in the Theory of Bulk and Confined Water." Session in Honor of James Wei. Annual

meeting of the American Institute of Chemical Engineers, Reno, Nevada, November 6, 2001.

"Recent Developments in the Theory of Supercooled Liquids and Glasses." Session on Thermodynamics of Amorphous Solids and Metastable Liquids. Annual meeting of the American Institute of Chemical Engineers, Reno, Nevada, November 8, 2001.

2002

"Thermodynamics of Glasses: the Kauzmann Paradox Revisited, Energy Landscape Diversity, and Supercooled Liquid Properties." Second conference on Unifying Concepts in Glass Physics. Accademia dei Lincei, Rome, Italy, February 28, 2002.

"Thermodynamics and Energy Landscapes." American Physical Society Division of Polymer Physics short course on Glasses and the Glass Transition. APS meeting, Indianapolis, Indiana, March 16, 2002.

"Recent Progress in Aqueous Thermodynamics." First North American Lectures in Chemical Engineering. Mexican Petroleum Institute, Mexico City, Mexico, April 25, 2002.

"Towards an Improved Understanding of Glasses and Viscous Liquids." First North American Lectures in Chemical Engineering. Institute of Physics, Mexican National Autonomous University, Mexico City, Mexico, April 26, 2002.

"Supercooled Liquids and Glasses." A three-lecture course. Physics Department, University of Rome "La Sapienza", Rome, Italy, May 13, 15, 17, 2002.

"Supercooled and Glassy Water." A three-lecture course. Physics Department, University of Rome III, Rome, Italy, May 20, 22, 24, 2002.

"Recent Developments in the Theory of Supercooled Liquids and Glasses." 6 Liblice Conference on the Statistical Mechanics of Liquids, Spindleruv Mlyn, Czech Republic, June 10, 2002.

"Relationship Between Structural Order and Liquid-Phase Anomalies: Similarities and Differences Between Water and Silica." CECAM Workshop: Understanding the Similarities of SiO2, H2O and Other Systems with Local Tetrahedral Order, Lyon, France, July 24, 2002.

2003

"Metastability, Confinement and Hydrophobicity: Recent Progress in Aqueous Thermodynamics." Dean's Distinguished Colloquia Series, College of Engineering and Applied Sciences, State University of New York at Stony Brook, February 26, 2003.

"Metastability, Confinement and Hydrophobicity: Recent Progress in Aqueous Thermodynamics." Thirteenth Annual Merck Distinguished Lecture Series. Department of Chemical and Biochemical Engineering, Rutgers University, March 27, 2003.

"Recent Progress in the Thermodynamics of Supercooled Liquids and Glasses." 2003 Berkeley Lectures in Chemical Engineering. Department of Chemical Engineering, University of California at Berkeley, April 28, 2003.

"Towards the Engineering of Biological Stability in the Amorphous Solid State." 2003 Berkeley Lectures in Chemical Engineering. Department of Chemical Engineering, University of California at Berkeley, May 1, 2003.

"The Kauzmann Paradox Revisited." Chemistry and Dynamics in Complex Environments, Telluride Summer Research Conference. Telluride, Colorado, June 23, 2003.

"Recent Progress in the Theory of Glass-Forming Systems." Area 1a Keynote Lecture, American Institute of Chemical Engineers Annual Meeting, San Francisco, California, November 18, 2003.

2004

"Some Recent Results on the Theory of Glasses and Supercooled Liquids." Symposium on the Occasion of George Stell's Retirement, Chemistry Department, State University of New York at Stony Brook, April 24, 2004.

"Energy Landscape Statistics." 91st Statistical Mechanics Conference, Rutgers University, New Brunswick, New Jersey, May 16st, 2004.

"Some Recent Developments in the Theory of Glasses." Unifying Concepts in Glass Physics III, Jawaharlal Nehru Institute for Advanced Scientific Research, Bangalore, India, July 1, 2004.

"Thermodynamics of Supercooled and Glassy Water." Plenary Lecture. 18^a IUPAC International Conference on Chemical Thermodynamics, Beijing, China, August 17, 2004.

"Thermodynamics of Supercooled and Glassy Water." ISOPOW 2004, 9^a International Symposium on the Properties of Water, Mar del Plata, Argentina, September 26, 2004.

"Supercooled and Glassy Water: Thermodynamics, Transport Phenomena and Relaxation." Workshop on Dynamics and Relaxation in Supercooled Fluids and Glassy Systems, Mar del Plata, Argentina, September 28, 2004.

"New Applications of Thermodynamics in the Life and Material Sciences." Plenary Lecture. Dechema/GVC Annual Meeting, Karlsruhe, Germany, October 12, 2004.

2005

"Why do Liquids Form Glasses?" Inaugural Walker Lecture in Physical Chemistry. Departments of Chemistry and Chemical Engineering, Pennsylvania State University, January 20, 2005.

"Cold Water." Walker Lecture in Physical Chemistry. Departments of Chemistry and Chemical Engineering, Pennsylvania State University, January 21, 2005.

"Applications of Thermodynamics to Molecular Design and Materials Characterization." Donald L. Katz Lectureship, Department of Chemical Engineering, University of Michigan, April 7, 2005.

"Why do Liquids Form Glasses?" Donald L. Katz Lectureship, Department of Chemical Engineering, University of Michigan, April 8, 2005.

"New Results on the Structure of Water Glasses, and on the Thermodynamics of Binary Mixtures of Non-Polar Solutes in Water." Thermo 2005 Symposium in Honor of Sandra Greer, University of Maryland at College Park, April 30, 2005.

"Towards the Engineering of Protein Stability." Distinguished Seminar Series, Department of Chemical Engineering, University of California, Riverside, June 3, 2005.

"Thermodynamics and Dynamics of Supercooling and Vitrification: from Water to Simple Liquids." Opening Plenary Lecture, 6 Liquid Matter Conference, Utrecht University, The Netherlands, July 2, 2005.

"Thermodynamics of Glasses and Supercooled Liquids: from Fundamentals to Applications." Keynote Lecture, 7th World Congress of Chemical Engineering, Glasgow, Scotland, July 11, 2005.

"An Alternative View of Diffusion." Session in Honor of Eli Ruckenstein's 80th Birthday, AIChE Annual Meeting, Cincinnati, Ohio, October 31, 2005.

2006

"Thermodynamics of Confinement, Hydrophobicity and Supercooling. What is Special About Water?" Patten Distinguished Lectureship, Department of Chemical and Biological Engineering, University of

Colorado at Boulder, March 23, 2006.

"Confined Water and Bulk "Water." 7^a Liblice Meeting on the Statistical Mechanics of Liquids, Lednice, Czech Republic, June 15, 2006.

"Liquid and Glassy Water under Hydrophobic, Hydrophilic and 'Patchy' Confinement." Gordon Research Conference on Water and Aqueous Solutions, Holderness School, Plymouth, New Hampshire, August 2, 2006.

"Metastable Thermodynamics of Confined Liquid and Glassy Water." Opening Plenary Lecture, IV Workshop on Nonequilibrium Phenomena in Supercooled Fluids, Glasses and Amorphous Materials, Scuola Normale Superiore, Pisa, Italy, September 18, 2006.

"Thermodynamics of Water in Nanoscale Confinement." Symposium in Celebration of the Life and Work of Robert C. Reid, Department of Chemical Engineering, Massachusetts Institute of Technology, October 13, 2006.

"Structure, Dynamics and Thermodynamics of Water Confined by Surfaces with Patterned Hydrophobicity." Session in Honor of Carol Hall's 60^a Birthday, AIChE Annual Meeting, San Francisco, November 15^a, 2006.

2007

"Water in Confined Spaces." Reilly Lectureship in Chemical and Biomolecular Engineering, Department of Chemical and Biomolecular Engineering, University of Notre Dame, April 3, 2007.

"From Particle Packings to Amino Acid Sequences: Statistical Characterization of Complex Systems." Reilly Lectureship in Chemical and Biomolecular Engineering, Department of Chemical and Biomolecular Engineering, University of Notre Dame, April 4, 2007.

"The Order Map: Towards a Smooth Progression of Liquid Behavior, from Hard Spheres to Water." Princeton Center for Theoretical Physics Symposium on Packing Problems, Classical Ground States and Glasses, Princeton University, April 13, 2007.

"Water in Confined Spaces." Michael M. Abbott Lecture. Department of Chemical and Biological Engineering, Rensselaer Polytechnic Institute, May 16, 2007.

"Water in Confined Spaces." Joe Smith Distinguished Lecture. Department of Chemical Engineering and Materials Science, University of California at Davis, June 5, 2007.

"Water in Confined Spaces." International Conference on Soft, Complex and Biological Matter (Socobim 2007), Citta del Mare, Sicily, July 17, 2007.

2008

"Hydrophobicity: a Theoretical and Computational Perspective." Centenary Seminar, Imperial College, London, March 12, 2008.

"Water in Confinement." Kelly Lecture, School of Chemical Engineering, Purdue University, March 18, 2008.

"Statistical Characterization of Structure in Complex Systems." Kelly Lecture, School of Chemical Engineering, Purdue University, March 19, 2008.

"Water in Confinement." Hunter Henry Lecture, Department of Chemical Engineering, Mississippi State University, March 25, 2008.

"Effect of Sequence on Protein Stability. A Numerical Study Using Water-Explicit Lattice Models." Industrial and Engineering Chemistry Divisional Fellow Award Symposium Honoring Ruben Carbonell,

American Chemical Society National Meeting, New Orleans, April 7, 2008.

"Computational Studies of Confined Water." Joel Henry Hildebrand Award Lecture, Physical Chemistry Awards Symposium, American Chemical Society National Meeting, New Orleans, April 8, 2008.

"Liquid and Glassy Water in Nano-Scale Confinement." International Workshop on Aqueous Solutions and their Interfaces, Crete, June 26, 2008.

"Hydrophobicity and its Consequences: from Nano-Scale Hydration to Protein Phase Diagrams." Plenary Lecture, 20th International Symposium on Chemical Thermodynamics, Warsaw, August 4, 2008.

"Structural and Mechanical Properties of Glassy Water in Nano-Scale Confinement." Faraday Discussion, "Water: From Interfaces to the Bulk", Heriot-Watt University, Edinburgh, United Kingdom, August 29, 2008.

"Water in Confined Spaces." ADVANCE Distinguished Lecturer, Department of Chemical Engineering, Kansas State University, October 8, 2008.

"Some Recent Applications of Thermodynamics and Statistical Mechanics." Symposium in Honor of the 60th Birthday of George Stephanopoulos, AIChE National Meeting, Philadelphia, November 17, 2008.

2009

"Hydrophobic Hydration. Results from Simple, and from Detailed Models." Symposium in Honor of John Finney, University College of London, United Kingdom, January 8, 2009.

"Water: Simple Models of Complex Thermodynamics." Symposium in Honor of C. Austen Angell, American Ceramic Society Meeting, Vancouver, Canada, June 3, 2009.

"Acqua! The Sounds and Science of Water." Entertaining Science Cabaret, Cornelia Street Café, New York, June 7, 2009.

"Structure, Dynamics and Thermodynamics of Water in Nano-Scale Confinement." CECAM Workshop: Modeling and Simulation of Water at Interfaces from Ambient to Supercooled Conditions, Ecole Politechnique Fédérale, Lausanne, Switzerland, June 30, 2009.

"Water-Mediated Interactions. Fundamentals and Applications." Keynote Lecture. 8th World Congress of Chemical Engineering, Montreal, August 24, 2009.

"Computational Studies of the Thermodynamics, Structure and Dynamics of Water in Nano-Scale Confinement." Opening Plenary Lecture. 6th International Discussion Meeting on Relaxations in Complex Systems, Rome, August 29, 2009.

"Hydrophobic Hydration: Insights from Simple and from Detailed Models." Session in Honor of H.E. Stanley, 6th International Discussion Meeting on Relaxations in Complex Systems, Rome, September 3, 2009.

"Computational Studies of the Thermodynamics, Structure and Dynamics of Water in Nano-Scale Confinement." Schlumberger Lecture, D.B. Robinson Distinguished Seminar Speaker, Department of Chemical and Materials Engineering, University of Alberta, Edmonton, September 10, 2009.

"Computational Studies of Interfacial and Confined Water." Office of Naval Research-AMBIO Workshop on Concepts and Strategies for Surface Engineering to Control Biofouling, St. Petersburg, Florida, December 9, 2009.

2010

"Thermodynamic and Kinetic Models for the Appearance and Amplification of Biological Chirality." 103^d Statistical Mechanics Meeting, Rutgers University, May 11, 2010.

"Thermodynamic and Kinetic Models for the Appearance and Amplification of Biological Chirality." Symposium in Honor of Robin Speedy, Victoria University of Wellington, Wellington, New Zealand, July 9, 2010.

"Thermodynamic and Kinetic Models for the Appearance of Biological Homohirality." Passion for Soft Matter Workshop. Passion for Knowledge Symposium in Celebration of the 10^a Anniversary of the Donostia International Physics Center, San Sebastian, Spain, September 29, 2010.

2011

"Thermodynamics, Dynamics and Dimensionality Reduction in Biophysical Simulations." Second New York Theoretical and Computational Chemistry Conference, The Graduate Center, City University of New York, January 14, 2011.

"Thermodynamic and Kinetic Models of the Emergence of Biological Homochirality." HES70, Horizons in Emergence and Scaling, H.E. Stanley Symposium and Gala, Boston University, March 19, 2011.

"The Theory of Hydrophobicity: Some Recent Developments on a Venerable Topic." Eli Ruckenstein Lecture, Department of Chemical and Biological Engineering, University at Buffalo, State University of New York, April 19, 2011.

"Nano-Scale Hydration Phenomena." American Conference on Theoretical Chemistry, Telluride, Colorado, July 22, 2011.

"Desarrollos Recientes en la Teoria de la Hidrofobicidad (Recent Developments in the Theory of Hydrophobicity)." Plenary Lecture. 2nd Joint Meeting of the Argentine and Uruguayan Physical Societies, Montevideo, Uruguay, September 20, 2011.

"Thermodynamics and Kinetics of Water in Hydrophobic Confinement." Sessions in Honor of Jan Sengers' 80th Birthday, Annual Meeting of the American Institute of Chemical Engineers, Minneapolis, October 18, 2011.

2012

"Drying and Hydration of Model and Biological Substrates." Unilever Symposium on Enzymes in Challenging Environments, Liverpool, United Kingdom, February 3, 2012.

"Evaporation Dynamics of Water in Hydrophobic Confinement." Symposium on Water Mediated Chemical Assembly, National Meeting, American Chemical Society, San Diego, March 25, 2012.

"The Liquid-Liquid Transition of ST2 Water, Revisited." Workshop on Structure and Dynamics of Glassy, Supercooled and Nanoconfined Fluids. Centro Atomico Constituyentes, Buenos Aires, Argentina, May 18, 2012.

"The Theory of Hydrophobicity: Some Recent Developments on a Venerable Subject." William G. Lowrie Lecture. Department of Chemical and Biomolecular Engineering, The Ohio State University, May 24, 2012.

"Thermodynamic and Kinetic Models of the Emergence of Biological Homochirality." William G. Lowrie Lecture. Department of Chemical and Biomolecular Engineering, The Ohio State University, May 25, 2012.

"Thermodynamics and Kinetics of Capillary Evaporation in Hydrophobic Confinement." Telluride Science Research Center Workshop on Hydrophibicity: From Theory, Simulation, to Experiment. Telluride, Colorado, June 12, 2012.

"Hydration and Drying of Biological and Model Substrates." Foundations of Molecular Modeling and Simulation (FOMMS) Conference. Mt. Hood, Oregon, July 26, 2012.

"Drying and Hydration of Model and Biological Substrates." Water and Aqueous Solutions Gordon-Kenan Research Seminar. Holderness School, New Hampshire, August 11, 2012.

"Hydration and Drying of Model and Biological Substrates." Fredrickson Lecture, Department of Chemical Engineering and Materials Science, University of Minnesota, October 11, 2012.

"Using Chemical Engineering Tools to Address an Important Puzzle Concerning the Origin of Life." Fredrickson Lecture to Undergraduate Students, Department of Chemical Engineering and Materials Science, University of Minnesota, October 12, 2012.

2013

"Liquid-Liquid Transition in ST2 Water." Focus Session: Supercooled and Nanoconfined Water. American Physical Society Meeting, Baltimore, March 20, 2013.

"Drying and Hydration of Model and Biological Substrates." Julian C. Smith Lecture, School of Chemical and Biomolecular Engineering, Cornell University, March 25, 2013.

"Thermodynamic and Kinetic Models of the Emergence of Biological Homochirality." Julian C. Smith Lecture, School of Chemical and Biomolecular Engineering, Cornell University, March 26, 2013.

"Nanoscale Drying and Hydration Phenomena: Fundamentals and Applications." Opening keynote lecture, 13th International Conference on Properties and Phase Equilibrium for Product and Process Design, Iguazú Falls, Argentina, May 26, 2013.

"Liquid-Liquid Transition in ST2 Water." CECAM Workshop: New Insights on Simulations, Theory and Experiments in Supercooled Water, Ecole Polytechnique Federale, Lausanne, Switzerland, July 3, 2013.

"The Liquid-Liquid Transition in Water: a Computational Perspective." International School of Physics Enrico Fermi. Water: Fundamentals as the Basis for Understanding the Environment and Promoting Technology, Varenna, Italy, July 12, 2013.

"The Liquid-Liquid Transition in ST2 Water." Gordon Research Conference on the Chemistry and Physics of Liquids, Holderness School, Plymouth, New Hampshire, August 6, 2013.

"The Phase Behavior of Supercooled Water: a Computational Perspective." Symposium on Frontiers in Computational Science, Temple University, October 18, 2013.

"The Phase Behavior of Supercooled Water: a Computational Perspective." Chair Lecture, Department of Chemistry, University of Nebraska, Lincoln, November 1, 2013.

"Theory and Computation in Modern Chemical Engineering: a Thermodynamicist's Perspective." 65th Institute Lecture, American Institute of Chemical Engineers, AIChE Annual Meeting, San Francisco, California, November 6, 2013.

2014

"Thermodynamic and Kinetic Models of the Emergence of Biological Homochirality." Warren L. McCabe Lecture, Department of Chemical and Biomolecular Engineering, North Carolina State University, February 3, 2014.

"The Phase Behavior of Supercooled Water: a Computational Perspective." Roger Miller Lecture, Department of Chemistry, University of North Carolina, February 26, 2014.

"The Liquid-Liquid Transition in ST2 Water." International Conference on Water Sciences, Peking University, Beijing, China, April 15, 2014.

"Chiral Symmetry Breaking: From the Origin of Life to Pharmaceutical Processing." Honorary Professorship Lecture, Beijing University of Chemical Technology, Beijing, China, April 16, 2014.

"Thermodynamic and Kinetic Models of the Emergence of Biological Homochirality." Bird, Stewart and Lightfoot Lecture, Department of Chemical and Biological Engineering, University of Wisconsin, May 13, 2014.

"One Substance, Two Liquids? Computational Studies of the Phase Behavior of Supercooled Water." Molecular Physics Lecture, Liblice Conference on the Statistical Mechanics of Liquids, Sec, Czech Republic, June 19, 2014.

"The Phase Behavior of Supercooled Water: a Computational Perspective." Joint European-Japanese Molecular Liquids Group Conference, Molecular Liquids and Soft Matter – From Fundamentals to Applications, University of Rome III, Italy, September 8, 2014.

"Metastable Liquid-Liquid Transition in a Molecular Model of Water." 112th Statistical Mechanics Meeting, Rutgers University, December 15, 2014.

2015

"Computational Investigation of Homogeneous Ice Nucleation and Metastable Phase Behavior in Supercooled Water." Workshop on Fundamental Problems in the Physics and Chemistry of Water, Houston, January 16, 2015.

"Molecular Simulation in Modern Chemical Engineering: a Thermodynamicist's Perspective." 40th Annual David M. Mason Lectures, Department of Chemical Engineering, Stanford University, May 11, 2015.

"Chiral Symmetry Breaking: From the Origin of Life to Pharmaceutical Processing." 40th Annual David M. Mason Lectures, Department of Chemical Engineering, Stanford University, May 13, 2015.

"Thermodynamics and Kinetics of Deeply Supercooled Water: A Computational Perspective." Molecular Physics Lecture, Thermodynamics 2015 Conference, Copenhagen, Denmark, September 15, 2015.

"Thermodynamics and Kinetics of Deeply Supercooled Water: a Computational Perspective." Barnett Dodge Distinguished Lecture in Chemical Engineering, Department of Chemical and Environmental Engineering, Yale University, October 28, 2015.

"Models of Chiral Symmetry Breaking: From the Origin of Life to Pharmaceutical Processing." 17th W.E. Palke Memorial Lectures, Department of Chemistry and Biochemistry, University of California at Santa Barbara, November 4, 2015.

"Thermodynamics and Kinetics of Deeply Supercooled Water: a Computational Perspective." 17th W.E. Palke Memorial Lectures, Department of Chemistry and Biochemistry, University of California at Santa Barbara, November 5, 2015.

"Computational Studies of Biophysical Systems." Invited Lecture at session on New Frontiers of Molecular Thermodynamics, AIChE Annual Meeting, November 10, 2015.

"Thermodynamics and Kinetics of Deeply Supercooled Water: a Computational Perspective." Symposium on Liquids and Glassy Soft Materials: Theoretical and Neutron Scattering Studies, Materials Research Society Fall Meeting, Boston, MA, December 3, 2015.

2016

"Thermodynamics and Kinetics of Deeply Supercooled Water: a Computational Perspective." Greater Boston Area Theoretical Chemistry Lecture Series, Massachusetts Institute of Technology, February 24, 2016.

"Molecular Simulation in Modern Chemical Engineering: a Thermodynamicist's Perspective." John A. Quinn Lecture, Department of Chemical and Biomolecular Engineering, University of Pennsylvania, March 16, 2016.

"Thermodynamics and Kinetics of Deeply Supercooled Water: a Computational Perspective." International School of Neutron Science and Instrumentation. Course on "Water and Water Systems." Ettore Majorana Foundation and Center for Scientific Culture, Erice, Italy. Two lectures, delivered remotely, July 28 and 29, 2016.

"Extreme Environments." Discussion Leader at the Gordon Research Conference on Water and Aqueous Solutions, Holderness School, Plymouth, New Hampshire, August 1, 2016.

"Drying and Hydration Phenomena at the Nanoscale: Implications for Protein Stability and Long-Term Storage." Distinguished Lindsay Speaker, J.D. Lindsay Lecture Series, Artie McFerrin Department of Chemical Engineering, Texas A&M University, November 2, 2016.

"Thermodynamics and Statistical Mechanics of Drying at the Nano-Scale." In Honor of Carol Hall, invited session, AIChE Annual Meeting, San Francisco, November 14, 2016.

2017

"Nano-scale Drying and Hydration Phenomena." Award Symposium Honoring Hildebrand Award Recipient Salvatore Torquato, 253rd ACS National Meeting, San Francisco, April 3, 2017.

"Computational Investigation of the Liquid-Liquid Transition in Deeply Supercooled Water." Congress on Water Under Extreme Conditions, Università degli Studi Roma Tre, Rome, Italy, June 15, 2017.

"Thermodynamics and Kinetics of Hydrophobically Induced Nano-scale Evaporation Transitions." Liquid Theory: Symposium in Honor of Ben Widom's 90th Birthday, 254th ACS National Meeting, Washington, DC, August 21, 2017.

"Thermodynamics and Kinetics of Hydrophobically Induced Nano-scale Evaporation Transitions". Guggenheim Medal Lecture, Thermodynamics 2017, Edinburgh, Scotland, September 5, 2017.

"Metastable Phase Transitions." Session in Honor of Keith Gubbins' 80th Birthday, Annual Meeting of the American Institute of Chemical Engineers, Minneapolis, October 30, 2017.

2018

"Nano-Scale Drying and Hydration Phenomena: Fundamentals and Some Biological Implications." Keynote Lecture, Bioengineering Symposium, Department of Chemical Engineering, University of New Hampshire, May 8, 2018.

II. Seminars

1984

"Molecular Diffusion in Supercritical Fluids." Department of Chemical Engineering, University of Illinois, January 31, 1984.

"Molecular Diffusion in Supercritical Fluids." Department of Chemical Engineering, University of Houston,

February 24, 1984.

"Molecular Diffusion in Supercritical Fluids." Department of Chemical Engineering, California Institute of Technology, March 6, 1984.

"Molecular Diffusion in Supercritical Fluids." Department of Chemical Engineering, University of Wisconsin, March 14, 1984.

"Molecular Diffusion in Supercritical Fluids." Department of Chemical Engineering, Stanford University, March 8, 1984.

"Molecular Diffusion in Supercritical Fluids." Department of Chemical Engineering, Princeton University, March 28, 1984.

"Molecular Diffusion in Supercritical Fluids." Department of Chemical Engineering, University of Delaware, March 29, 1984.

1986

"Sub-Triple Liquids: an Unexplored State of Matter." Department of Chemical Engineering, University of Pennsylvania, April 21, 1986

"From Molecular Chaos to Statistical Order: Some Novel, Predictive Applications of Fluctuation Theory." Department of Chemical Engineering, University of California, Berkeley, December 1, 1986.

"From Molecular Chaos to Statistical Order: Some Novel, Predictive Applications of Fluctuation Theory." Department of Chemical Engineering, University of California, Davis, December 3, 1986.

"From Molecular Chaos to Statistical Order: Some Novel, Predictive Applications of Fluctuation Theory." Department of Chemical Engineering, University of California, Los Angeles, December 5, 1986.

1987

"From Molecular Chaos to Statistical Order: Some Novel, Predictive Applications of Fluctuation Theory." Department of Chemical Engineering, Tufts University, Medford, Massachusetts, April 13, 1987.

"Clustering in Supercritical Mixtures." The Dow Chemical Company, Midland, Michigan, June 23, 1987.

"The Molecular Basis of Supercritical Extraction." AIChE Central Jersey Section, October 20, 1987.

"Sub-Triple Liquids: an Unexplored State of Matter." Department of Chemical Engineering, University of Virginia, Charlottesville, Virginia, December 3, 1987.

"Clustering in Supercritical Solvents and other Topics in Fluctuation Theory." Department of Chemical Engineering, The Johns Hopkins University, Baltimore, Maryland, December 14, 1987.

1988

"Solid Formation and Heterogeneous Catalysis with Near-Critical Fluids." W.R. Grace & Co., Columbia, Maryland, February 10, 1988.

"Thermodynamics and Statistical Mechanics of Near-Critical Mixtures." Department of Chemical Engineering, University of Patras, Patras, Greece, September 8, 1988.

"Thermodynamics of Near-Critical Systems: Theory, Experiments, Simulations, and Applications." Department of Chemical Engineering, University of Pittsburgh, December 9, 1988.

1989

"Thermodynamics of Near-Critical Systems: Theory, Experiments, Simulations, and Applications."

Department of Chemical Engineering, Drexel University, January 23, 1989.

"Solids Formation from Supercritical Fluids." Enzytech, Inc. Cambridge, MA, January 27, 1989.

"Thermodynamics of Cooperative Behavior in Near-Critical Systems: Theory, Simulations, and Applications." Department of Chemical Engineering and the Levich Institute for Physicochemical Hydrodynamics, The City College of the City University of New York, February 13, 1989.

"Thermodynamics of Cooperative Behavior in Dilute Supercritical Systems: Theory, Simulations and Applications." Department of Chemical Engineering, Cornell University, April 4, 1989.

"Toward an Understanding of the Molecular Basis of Solubility in Supercritical Fluids." Department of Chemistry and Chemical Engineering, Stevens Institute of Technology, September 6, 1989.

"Toward an Understanding of the Molecular Basis of Solubility in Supercritical Fluids." Department of Chemical Engineering, University of Arizona, October 24, 1989.

"Tensile Instabilities, Density Anomalies, and Mechanical Stability in Supercooled Liquids: Using Thermodynamics to Understand the Behavior of Liquids Under Tension." Department of Chemical Engineering, University of Rochester, November 29, 1989.

1990

"Particle Formation from Supercritical Fluids." Merck, Sharp & Dohme Research Laboratories, West Point, PA, January 15, 1990.

"Toward an Understanding of the Molecular Basis of Solubility in Supercritical Fluids." Department of Chemical Engineering, University of Notre Dame, January 30, 1990.

"On the Cohesive Strength of Liquids: Some Recent Developments on an Ancient Topic." Department of Chemical Engineering, California Institute of Technology, February 1, 1990.

"Toward an Understanding of the Molecular Basis of Solubility in Supercritical Fluids." Department of Chemical Engineering, Lehigh University, February 14, 1990.

"Toward an Understanding of the Molecular Basis of Solubility in Supercritical Fluids." Department of Chemical Engineering, Yale University, March 22, 1990.

"On the Cohesive Strength of Liquids: Some Recent Developments on an Ancient Topic." Department of Chemical Engineering, University of Delaware, April 5, 1990.

"Toward an Improved Understanding of the Molecular Basis of Solubility in Supercritical Fluids." Department of Chemical Engineering, State University of New York at Buffalo, September 12, 1990.

"Toward an Improved Understanding of the Molecular Basis of Solubility in Supercritical Fluids." Department of Chemical Engineering, Rutgers University, December 13, 1990.

1991

"Stability of Supercooled Liquids." Department of Chemical Engineering, Rensselaer Polytechnic Institute, January 30, 1991.

"Particle Formation with Supercritical Fluids." Merck Pharmaceutical Manufacturing Division, West Point, PA, May 6, 1991.

"Particle Formation with Supercritical Fluids." Lilly Research Laboratories, Indianapolis, IN, June 6, 1991.

"Mechanisms of Solvation and Nucleation in Supercritical Fluids." Advanced Fuels Workshop, Wright-

Patterson Air Force Base, Ohio, September 4, 1991.

"How much can Liquids be Supercooled? Kinetics, Thermodynamics, and some Biological and Technical Implications." Department of Chemical Engineering, Rice University, September 26, 1991.

"How much can Liquids be Supercooled? Kinetics, Thermodynamics, and some Biological and Technical Implications." Department of Chemical Engineering, University of California, Berkeley, November 11, 1991.

1992

"How much can Liquids be Supercooled? Kinetics, Thermodynamics, and some Biological and Technical Implications." Department of Chemistry, Purdue University, February 19, 1992.

"Solvation, Nucleation, and Particle Formation in Supercritical Fluids." Department of Chemical Engineering, Purdue University, February 20, 1992.

"Mechanical Instabilities in Some Supercooled Liquids." Department of Chemical Engineering, University of California, Santa Barbara, March 5, 1992.

"Near-critical Mixtures: Microstructure, Thermodynamics, and Applications." Department of Chemical Engineering, California Institute of Technology, April 13, 1992.

"Mechanical Instabilities in Some Supercooled Liquids." Department of Chemical Engineering, University of California, Los Angeles, April 17, 1992.

"Mechanical Instabilities in Some Supercooled Liquids." Department of Chemical Engineering, Stanford University, April 29, 1992.

"Mechanical Instabilities in Some Supercooled Liquids." Lawrence Livermore National Laboratory, April 30, 1992.

"How Much can Liquids be Supercooled? Kinetics, Thermodynamics, and Some Biological and Technical Implications." Department of Chemical Engineering, Georgia Institute of Technology, May 19, 1992.

"Nucleation, Solvation, and Particle Formation in Supercritical Fluids." Department of Pharmacy and Pharmaceutical Chemistry, University of California, San Francisco, June 16, 1992.

"Applications of Supercritical Fluids in the Production of Controlled Release Devices." Biomedical Polymers Group, SRI International, Menlo Park, California, June 22, 1992.

"Supercritical Fluids as Novel Particle Formation Media: Applications to the Formation of Polymeric and Biological Materials." Exxon Research and Engineering Company, Annandale, NJ, November 18, 1992.

"The Stability of Supercooled Liquids." Department of Chemical Engineering, University of Texas, Austin, December 1, 1992.

1993

"Supercritical Fluids as Particle Formation Media." DuPont Chemicals, Wilmington, Delaware, January 14, 1993.

"Stability of Supercooled Liquids." Department of Chemical Engineering, University of Maine, Orono, February 19, 1993.

"Solvation, Nucleation, and Particle Formation in Supercritical Fluids." Fuel Science Program, Department of Materials Science, Pennsylvania State University, University Park, April 16, 1993.

"Computational Studies of Metastability." Graduate School of Engineering, University of Kyoto, Kyoto, Japan, May 29, 1993.

"Solute-Solute Interactions in Supercritical Solutions: A Molecular Dynamics Investigation." Symposium on Scientific Research on Supercritical Fluids, The University of Tokyo, Tokyo, Japan, May 31, 1993.

1994

"Computer Simulation of Molecular Interactions in Supercritical Solvents." Advanced Fuels Workshop, Wright-Patterson Air Force Base, Ohio, February 7, 1994.

"Thermodynamics of Supercooled and Glassy Water." Department of Chemical Engineering, University of Maryland, February 22, 1994.

"Supercritical Fluids as Particle Formation Media." Department of Chemical Engineering, Yale University, March 28, 1994.

"Supercooled Water: Biological Significance, Thermodynamic Puzzles, and Some General Questions on Metastability in Liquids." Department of Chemical Engineering, Yale University, March 31, 1994.

"Thermodynamics of Supercooled and Glassy Water." Department of Chemical Engineering, Massachusetts Institute of Technology, April 15, 1994.

"Supercritical Fluids as Particle Formation Media." AIChE Central Jersey Section, Princeton University, May 19, 1994.

"Supercritical Fluids as Particle Formation Media." Robert L. Mitchell Technical Center, Hoechst Celanese Corporation, Summit, New Jersey, July 14, 1994.

"Thermodynamics of Supercooled and Glassy Water." Department of Chemical Engineering, City College of the City University of New York, October 31, 1994.

"Supercritical Fluids as Particle Formation Media." Alza Corporation, Palo Alto, California, December 9, 1994.

1995

"Thermodynamics of Supercooled and Glassy Water." Department of Chemical Engineering, Wayne State University, Detroit, Michigan, March 3, 1995.

"Simulation of Structure and Dynamics at Supercritical Conditions." Wright-Patterson Air Force Base, Dayton, Ohio, March 10, 1995.

"Thermodynamics of Supercooled and Glassy Water." Department of Chemical Engineering, Polytechnic University, New York, March 15, 1995.

"Thermodynamics of Supercooled and Glassy Water." School of Chemical Engineering and Materials Science, University of Oklahoma, Norman, Oklahoma, April 27, 1995.

"Thermodynamics of Supercooled and Glassy Water." Department of Chemical Engineering and Petroleum Refining, Colorado School of Mines, April 28, 1995.

"Materials Processing with Supercritical Fluids." Merck Research Laboratories, Rahway, New Jersey, May 1, 1995.

"Computer Simulation of Molecular Interactions in Supercritical Solvents." AFOSR Supercritical Fuels Workshop, Ann Arbor, Michigan, June 15, 1995.

"Materials Processing with Supercritical Fluids." Department of Chemistry and Biochemistry, University of Southern Illinois, Carbondale, Illinois, September 8, 1995.

"Towards an Understanding of Supercooled and Glassy Water." Department of Chemical Engineering, Pennsylvania State University, October 24, 1995.

"Towards an Understanding of Supercooled and Glassy Water." Department of Chemical Engineering, University of Illinois, Urbana, November 7, 1995.

1996

"The Surface Enrichment Problem in Interfacial Thermodynamics." Department of Chemical Engineering, Princeton University, April 22, 1996.

"Phase Behavior of Supercooled and Glassy Water." Department of Chemical Engineering, University of Southern Florida, Tampa, Florida, April 26, 1996.

"Theoretical and Computational Studies of Nucleation in Supercritical Fuels." AFOSR Contractors Meeting, Virginia Beach, Virginia, June 4, 1996.

"Materials Processing with Supercritical Fluids." David Sarnoff Research Center, Princeton, December 4, 1996.

"The Glass Transition." Merck & Co., Inc., West Point, PA, December 12, 1996.

1997

"Materials Processing with Supercritical Fluids." Bristol-Myers Squibb, New Brunswick, NJ, January 3, 1997.

"Thermodynamics of Supercooled and Glassy Water." Department of Chemical Engineering, North Carolina State University, Raleigh, NC, March 3, 1997.

"Thermodynamics of Supercooled and Glassy Water." Department of Chemical Engineering, Ohio State University, Columbus, OH, April 10, 1997.

"Thermodynamics of Supercooled and Glassy Water." Chemistry Division, Brookhaven National Laboratory, Upton, NY, April 23, 1997.

"Materials Processing with Supercritical Fluids." Inhale Therapeutic Systems, Palo Alto, CA, May 21, 1997.

"The Glass Transition: Fundamentals and Applications." Merck Laboratories, Pharmaceutical Research, West Point, PA, May 30, 1997.

"Thermodynamics of Supercooled and Glassy Water." Polymer Science and Engineering Department, University of Massachusetts, Amherst, September 26, 1997.

1998

"Towards an Improved Understanding of Supercooled Liquids and the Glass Transition." Department of Chemical Engineering, Tulane University, February 13, 1998.

"Towards an Improved Understanding of Supercooled Liquids and the Glass Transition." Department of Chemical Engineering, University of Colorado, Boulder, February 26, 1998.

"Statistical Geometry and Energy Landscapes in Liquids and Glasses." Institute for Physical Science and Technology, University of Maryland, College Park, May 12, 1998.

"Water at Extreme Conditions." Department of Chemical Engineering and Materials Science, University of

Minnesota, October 27, 1998.

"Water at Extreme Conditions." Department of Chemical Engineering, McGill University, November 3, 1998.

1999

- "Water at Extreme Conditions: Its Properties and Uses." Department of Chemical Engineering, Texas A&M University, January 29, 1999.
- "Water, water everywhere, nor any drop to drink." Department of Chemical Engineering, University of Pennsylvania, March 15, 1999.
- "Statistical Geometry and Energy Landscapes in Liquids and Glasses." Department of Chemical Engineering, University of California, Santa Barbara, April 15, 1999.
- "Statistical Geometry and Energy Landscapes in Liquids and Glasses." Department of Chemical Engineering, University of California, Los Angeles, April 16, 1999.
- "Statistical Geometry and Energy Landscapes in Liquids and Glasses." Department of Chemical Engineering, Northwestern University, June 3, 1999.
- "Water, water everywhere, nor any drop to drink." Department of Chemical Engineering, Carnegie Mellon University, September 9, 1999.
- "Water, water everywhere, nor any drop to drink." Department of Chemical and Petroleum Engineering, University of Pittsburgh, September 10, 1999.
- "Particle Formation with Supercritical Fluids." Department of Chemical Engineering, Chemistry, and Environmental Science, New Jersey Institute of Technology, October 18, 1999.
- "Water, water everywhere, nor any drop to drink." Department of Chemical Engineering, University of Michigan, December 9, 1999.

2000

- "Water, water everywhere, nor any drop to drink." Department of Chemical Engineering, University of South Carolina, Columbia, February 10, 2000.
- "Towards an Improved Understanding of Supercooled Liquids and Glasses." Department of Chemical Engineering, University of Wisconsin, Madison, May 9, 2000.
- "Relaxation and Dynamics in Supercooled Liquids and Glasses." ExxonMobil Research and Engineering Company, Clinton, September 15, 2000.
- "Towards an Improved Understanding of Water." Department of Chemical Engineering, Rensselaer Polytechnic Institute, November 30, 2000.

2001

- "Ubiquitous but Unusual, Odd but Odered: Recent Developments in Aqueous Thermodynamics." Department of Chemical Engineering, Johns Hopkins University, November 15, 2001.
- "Towards an Improved Understanding of Glasses and Supercooled Liquids." Department of Chemical Engineering, Massachusetts Institute of Technology, November 16, 2001.

2002

"Engineering Pharmaceutical Stability in the Solid State." Baxter Healthcare Corp., Round Lake, IL. May 3, 2002.

"Metastability, Cinfinement and Hydrophobicity: Recent Progress in Aqueous Thermodynamics." Department of Chemical Engineering, City College of the City University of New York. October 28, 2002.

"Recent Progress in the Thermodynamics of Glasses and Supercooled Liquids." Department of Chemical Engineering, University of Texas at Austin, November 26, 2002.

2003

"Metastability, Confinement and Hydrophobicity: Recent Progress in Aqueous Thermodynamics." Department of Chemical Engineering, University of Virginia. April 10, 2003.

2004

"Cold Water." Department of Chemical Engineering, Drexel University, March 8, 2004.

"Recent Developments in the Theory of Glasses and Supercooled Liquids." Department of Chemical Engineering, Ohio State University, April 8, 2004.

"Derivation of Inequalities Using the 2nd Law of Thermodynamics." Friday Lunch Talk, Department of Chemical Engineering, Princeton University, April 16, 2004.

"Recent Developments in the Theory of Glasses: Energy Landscape Statistics." Complex Materials Seminar, Department of Chemical Engineering, Princeton University, April 19, 2004.

"Cold Water." Department of Chemical and Environmental Engineering, Illinois Institute of Technology, Chicago, Illinois, April 21^a, 2004.

"Some Recent Developments in the Theory of Glasses and Supercooled Liquids." Department of Chemical Engineering, University of Massachusetts at Amherst, May 13^a, 2004.

"Recent Developments in the Theory of Glasses and Supercooled Liquids." Pfizer Pharmaceutical Research and Development, Groton, Connecticut, June 18, 2004.

2005

"Biopreservation and Amorphous Glass Characterization." Bend Research, Inc., Bend, Oregon, March 14, 2005.

"Thermodynamic and Kinetic Perspectives on the Glass Transition." Department of Mechanical Engineering, Yale University, October 12^a, 2005.

"Thermodynamics of Supercooled, Glassy and Confined Water." Department of Chemistry, Colorado State University, Fort Collins, November 17^a, 2005.

"Thermodynamics of Supercooled, Glassy and Confined Water." Department of Chemical Engineering, Colorado School of Mines, Golden, November 18^a, 2005.

2006

"Thermodynamics of Supercooled, Glassy and Confined Water." Department of Chemical Engineering, Vanderbilt University, Nashville, Tennessee, January 30^a, 2006.

"Thermodynamics of Supercooled, Glassy and Confined Water." Department of Chemical and Biological Engineering, State University of New York at Buffalo, April 5, 2006.

"Thermodynamics of Confined, Supercooled and Glassy Water." Department of Chemical Engineering and Chemical Technology, Imperial College, London, June 9^a, 2006.

"Thermodynamics of Confined, Supercooled and Glassy Water." Department of Chemical Engineering,

Lehigh University, September 6th, 2006.

2007

"Water in Confined Spaces." Department of Chemical and Biological Engineering, Northwestern University, May 31, 2007.

"Water in Confined Spaces." Department of Chemistry and Biochemistry, Florida State University, September 14, 2007.

"Water in Confined Spaces." Department of Physics, University of Missouri, Rolla, October 11, 2007.

"Water in Confined Spaces." Department of Chemical Engineering, New Jersey Institute of Technology, October 29, 2007.

"Water in Confined Spaces." Department of Chemical and Biomolecular Engineering, University of Houston, November 30, 2007.

2008

"Computational Characterization of Structure in Equilibrium and Non-Equilibrium Materials." Department of Chemical Engineering, Tsinghua University, Beijing, China, January 4, 2008.

"Theory and Simulation of Glasses and Glass-Forming Materials." Department of Chemical Engineering, Tsinghua University, Beijing, China, January 10, 2008.

"Hydrophobicity: Theoretical and Computational Perspectives." School of Chemical Engineering and Materials Science, University of Oklahoma, February 21, 2008.

"Water in Confined Spaces." Chemistry Department, University of Wisconsin, September 23, 2008.

"Water in Confined Spaces." Department of Physics, Yeshiva University, December 2, 2008.

2009

"Phase Behavior and Structure of Water in Nano-Scale Confinement." Geophysical Fluid Dynamics Laboratory, Princeton Forrestal Campus, January 15, 2009.

"Phase Behavior and Structure of Water in Nano-Scale Confinement." Department of Chemical Engineering, University of Rhode Island, April 22, 2009.

"Water in Confined Spaces." Department of Chemical Engineering, University of Washington, April 27, 2009.

2010

"Hydration Phenomena at the Nano-Scale: Theoretical and Computational Perspectives." Department of Chemical Engineering, Carnegie-Mellon University, March 2, 2010.

"Water. A Computational Perspective." Carbon Mitigation Initiative Luncheon Seminar, Princeton University, May 18, 2010.

"Hydration Phenomena at the Nano-Scale: Theoretical and Computational Perspectives." Department of Chemical and Biomolecular Engineering, University of Pennsylvania, September 15, 2010.

2011

"Computational Studies of Mechanical Stresses on Proteins Upon Vitrification (and a Cautionary Note on the Calculation of Fragility via Simulation)." Workshop on Molecular Glasses, Unilever, Colworth, United Kingdom, January 27, 2011.

- "Thermodynamics and Dynamics of Drying Transitions in Nano-Scale Confinement." Workshop on Molecular Glasses, Unilever, Colworth, United Kingdom, January 28, 2011.
- "Nano-scale Hydration Phenomena: Theoretical and Computational Perspectives." Department of Chemical and Biomolecular Engineering, Tulane University, February 18, 2011.
- "Hydration Phenomena at the Nano-Scale: Theoretical and Computational Perspectives." Physical Chemistry Colloquium, Department of Chemistry, University of Utah, April 5, 2011.
- "Thermodynamic and Kinetic Models of the Appearance of Biological Homochirality." Biological Physics Seminar, Arizona State University, April 6, 2011.
- "Hydration Phenomena at the Nano-Scale: Theoretical and Computational Perspectives." Department of Chemistry and Biochemistry, Arizona State University, April 8, 2011.
- "CO2-H2O Phase Behavior and CO2 Hydrate Dynamics." Tenth Annual Carbon Mitigation Initiative (CMI) Meeting, Princeton University, April 12, 2011.
- "Nano-scale Hydration Phenomena: Theoretical and Computational Perspectives." Department of Chemical and Biomolecular Engineering, University of Maryland, May 3, 2011.
- "Desarrollos Recientes en la Teoria de la Hidrofobicidad (Recent Developments in the Theory of Hydrophobicity)." Department of Inorganic, Analytical and Physical Chemistry, Faculty of Exact and Natural Sciences, University of Buenos Aires, Argentina, September 23, 2011.
- "Structural Order and Thermodynamics in Tetrahedral Liquids." Workshop on: Towards Unifying Concepts in the Physics of Aperiodic Systems, Princeton Center for Theoretical Science, Princeton University, October 14, 2011.

2012

- "Computational Studies of Maintenance and Repair of Biological Substrates". Unilever, Port Sunlight, United Kingdom, February 1, 2012.
- "Theoretical and Computational Studies of Nano-Scale Hydration Phenomena". Department of Mechanical Engineering, Villanova University, February 24, 2012.
- "Theoretical and Computational Studies of Nano-Scale Hydration Phenomena". Department of Chemical Engineering, University of Florida, February 27, 2012.
- "Theoretical and Computational Studies of Nano-Scale Hydration Phenomena". School of Chemistry and Biochemistry, Georgia Institute of Technology, March 8, 2012.
- "Polyamorphism in Water: a Computational Perspective." Lunch Seminar Series on Towards Unifying Concepts in the Physics of Aperiodic Systems, Princeton Center for Theoretical Science, Princeton University, April 4, 2012.
- "Hydration and Drying of Biological and Model Substrates." Department of Chemical and Biological Engineering, Iowa State University, October 25, 2012.
- "Hydration and Drying of Biological and Model Substrates." Department of Chemical and Biomolecular Engineering, The Johns Hopkins University, November 8, 2012.

2013

"Thermodynamic and Kinetic Models of the Emergence of Biological Hoochirality." Department of Chemical and Biomolecular Engineering, University of Delaware, September 6, 2013.

2014

"The Phase Behavior of Supercooled Water: a Computational Perspective." Department of Chemistry, Duke University, February 25, 2014.

"Thermodynamic and Kinetic Models of the Emergence of Biological Homochirality." Princeton Center for Theoretical Science, March 13, 2014.

"Thermodynamic and Kinetic Models of the Emergence of Biological Homochirality." Princeton Origin of Life Discussion Group, April 2, 2014.

"One Substance, Two Liquids: Computational Studies of Cold Liquid Water." Princeton Institute for Computational Science and Engineering (PICSciE), Symposium on Data Science, May 16, 2014.

"The Phase Behavior of Supercooled Water: a Computational Perspective." Department of Chemistry, University of Calgary, Canada, October 31, 2014.

2015

"Supercooled Water: a Computational Perspective." Department of Chemistry, Virginia Commonwealth University, January 29, 2015.

"Supercooled Water: a Computational Perspective." Chemistry Division, Naval Research Laboratory, Washington, DC, February 26, 2015.

"Thermodynamic and Kinetic Models of the Emergence of Biological Homochirality." Physical Chemistry Seminar, Chemistry Department, University of California, Berkeley, March 10, 2015.

"Cold Unfolding of Proteins." Princeton Center for Theoretical Science, Princeton University, December 10, 2015.

2016

"The Phase Behavior of Deeply Supercooled Water: a Computational Perspective." The Thomas Young Center for the Theory and Simulation of Materials, London, United Kingdom, January 21, 2016.

"The Phase Behavior of Deeply Supercooled Water: a Computational Perspective." Chemistry Department, Cambridge University, Cambridge, United Kingdom, January 22, 2016.

"Drying and Hydration Phenomena at the Nanoscale: Implications for Stability and Long-Term Storage of Proteins." Department of Chemical Engineering, University of Rochester, September 7, 2016.

2017

"Computational Exploration of the Phase Behavior of Supercooled Water." Department of Chemistry, The Johns Hopkins University, October 10, 2017.

"Computational Investigation of the Phase Behavior of Supercooled Water." Institute for Molecular Science, Okazaki, Japan, October 17, 2017.

"Computational Investigation of the Phase Behavior of Supercooled Water." Institute for Industrial Science, University of Tokyo, Japan, October 20, 2017

"Computational Investigation of the Phase Behavior of Supercooled Water." Vienna Physics Colloquium, University of Vienna, Austria, December 11, 2017.

2018

"Computational Investigation of the Phase Behavior of Supercooled Water." Department of Chemical, Biological and Pharmaceutical Engineering, New Jersey Institute of Technology, January 22, 2018.

"Computational Investigation of the Phase Behavior of Supercooled Water." International Graduate Research Training Group Colloquium, Chemistry Department, Technical University of Berlin, February 13, 2018.

"Computational Investigation of the Phase Behavior of Supercooled Water." Distinguished Seminar Speaker series, Department of Chemical and Environmental Engineering, University of California at Riverside, April 20, 2018.