Curriculum Vitæ: FRANCIS W. STARR

ADDRESS:

National Institute of Standards and Technology (NIST) Polymers Division, Center for Computational and Theoretical Materials Science 100 Bureau Drive, MS 8500 Gaithersburg, MD 20899 *e-mail:* fstarr@nist.gov

EDUCATION:

- Ph.D., Physics, 1999; Advisor: H. Eugene Stanley, Boston University, Boston, MA
- M.A., Physics, 1999; Boston University, Boston, MA
- B.S. with University Honors, Physics, 1994; Carnegie Mellon University, Pittsburgh, PA

EMPLOYMENT:

- Deputy Director, Center for Theoretical and Computational Materials Science; Physicist, Polymers Division, N.I.S.T., Gaithersburg, MD, May 2001 present.
- N.R.C. Postdoctoral Associateship, N.I.S.T., Gaithersburg, MD, August 1999 August 2001; Advisor: Sharon C. Glotzer
- Research Assistant, Physics Department, Boston University. Summer 1995 March 1999.
- Lecturer for the College on Computational Physics, International Centre for Theoretical Physics, Trieste (Italy). May-June 1997.
- Teaching Assistant, Physics Department, Boston University. Fall 1994 Spring 1996.
- Research Assistant, Physics Division, Oak Ridge National Lab. Jan. 1994 June 1994.

PUBLICATIONS:

Research Articles

- 1. F.W. Starr, S.T. Harrington, B.M. Boghosian, and H.E. Stanley. "Interface Roughening in a Hydrodynamic Lattice-Gas Model with Surfactant". *Physical Review Letters* **77**, 3363-3366 (1996).
- M. Canpolat, F.W. Starr, M.R.S.-Lahijany, A. Scala, O. Mishima, S. Havlin, and H.E. Stanley. "Local Structural Heterogeneities in Liquid Water under Pressure". *Chemical Physics Letters* 294, 9-12 (1998).
- F.W. Starr, J.K. Nielsen, and H.E. Stanley. "Fast and Slow Dynamics of Hydrogen Bonds in Liquid Water". *Physical Review Letters* 82, 2294-2297 (1999).
- F.W. Starr, S. Harrington, F. Sciortino, and H.E. Stanley "Slow Dynamics of Water under Pressure". *Physical Review Letters* 82, 3629-3632 (1999).
- F.W. Starr, M.-C. Bellissent-Funel, and H.E. Stanley. "Structure of supercooled and glassy water". *Physical Review E* 60, 1084-1087 (1999).
- F.W. Starr, F. Sciortino, and H.E. Stanley "Dynamics of simulated water under pressure". *Physical Review E*, 60, 6757-6768 (1999).
- E. La Nave, A. Scala, F.W. Starr, F. Sciortino, and H.E. Stanley. "Instantaneous Normal Mode Analysis of Supercooled Water". *Physical Review Letters* 84, 4605-4608 (2000).
- 8. F.W. Starr, J.K. Nielsen, and H.E. Stanley. "Hydrogen Bond Dynamics in the extended simple point charge model of water". *Physical Review E* **62**, 579-587 (2000).

- 9. A. Scala, F.W. Starr, E. La Nave, F. Sciortino, and H.E. Stanley. "Configurational Entropy and Diffusivity of Supercooled Water". *Nature* **406**, 166-169 (2000).
- 10. A. Scala, F.W. Starr, E. La Nave, H.E. Stanley, and F. Sciortino. "Free Energy Surface of Supercooled Water". *Physical Review E* 62, 8016-8020 (2000).
- 11. F.W. Starr, S. Sastry, E. La Nave, A. Scala, H.E. Stanley, and F. Sciortino. "Thermodynamic and structural aspects of the potential energy surface of simulated water". *Physical Review E*, **63**, 041201 (2001).
- P.A. Netz, F.W. Starr, H.E. Stanley, and M.C. Barbosa. "Static and dynamic properties of stretched water". *Journal of Chemical Physics* 115, 344-348 (2001).
- F.W. Starr, T.B. Schrøder, and S.C. Glotzer, "Effects of a nanoscopic filler on the structure and dynamics of a simulated polymer melt and the relationship to ultra-thin films". *Physical Review* E, 64, 021802 (2001).
- 14. E. La Nave, A. Scala, F.W. Starr, F. Sciortino, and H.E. Stanley. "Dynamics of Supercooled Water in Configuration Space". *Physical Review E* 64, 036102 (2001).
- 15. Y. Gebremichael, T.B. Schrøder, F.W. Starr, and S.C. Glotzer. "Spatially correlated dynamics in a simulated glass-forming polymer melt: Analysis of clustering phenomena". *Physical Review E* **65**, 051503 (2001).
- N. Giovambattista, F.W. Starr, F. Sciortino, and H.E. Stanley, "Transitions between Inherent Structures in Water". *Physical Review E* 65, 041502 (2002).
- F.W. Starr, T.B. Schrøder, and S.C. Glotzer, "Molecular dynamics simulation of a polymer melt with a nanoscopic particle". *Macromolecules* 35, 4481-4492 (2002).
- 18. F.W. Starr, S. Sastry, J.F. Douglas, and S.C. Glotzer, "What do we learn from the local geometry of glass-forming liquids?". *Physical Review Letters* **89**, 125501 (2002).
- 19. N. Lačević, F.W. Starr, T.B. Schrøder, V.N. Novikov, and S.C. Glotzer, "Growing correlation length on cooling below the onset of caging in a simulated glass-forming liquid". *Physical Review* E 66, 030101 (2002).
- 20. N. Giovambattista, S.V. Buldyrev, F.W. Starr, and H.E. Stanley, "Connection between Adam-Gibbs Theory and Spatially Heterogeneous Dynamics". To appear in *Physical Review Letters*.
- 21. F.W. Starr, C.A. Angell, R.J. Speedy, and H.E. Stanley. "Entropy and dynamic properties of water below the homogeneous nucleation temperature". To appear in *Physica A*.
- 22. F.W. Starr, J.F. Douglas, and S.C. Glotzer. "Clustering mechanism in a simulated polymer nanocomposite". Submitted to *Macromolecules*
- 23. F.W. Starr, J.F. Douglas, and S.C. Glotzer. "Rheological properties of a simulated polymer nanocomposite". Submitted to *Macromolecules*
- 24. M. Aichele, Y. Gebremichael, F.W. Starr, J. Baschnagel, and S.C. Glotzer, "Stringlike correlated motion in the dynamics of supercooled polymer melts". In preparation.
- 25. S. Kumar, J. Douglas, and F.W. Starr. "Equilibrium structural indicator of vitrification in hardcore fluids". In preparation.
- 26. N. Lačević, T.B. Schrøder, F.W. Starr, V.N. Novikov, and S.C. Glotzer, "Growing dynamic correlation length of a simulated glass-forming liquid". In preparation.

Conference Proceedings

- H.E. Stanley, L. Cruz-Cruz, S.T. Harrington, P.H. Poole, S. Sastry, F. Sciortino, F.W. Starr, and R. Zhang. "Cooperative Molecular Motions in Water: The Liquid-Liquid Critical Point Hypothesis" [Proc. International Conf. on "Complex Fluids"]. *Physica A*, 236, 19-37 (1997).
- H.E. Stanley, S.T. Harrington, P.H. Poole, S. Sastry, F. Sciortino, and F.W. Starr. "Cooperative Molecular Motions in Water" [Proc. 1996 Kyoto YKIS Conf], Prog. Theor. Phys. Suppl. 126, 201-206 (1997).

- H.E. Stanley, S.T. Harrington, O. Mishima, P.H. Poole, S. Sastry, F. Sciortino, and F.W. Starr. "The Puzzling Statistical Physics of Liquid Water" [Proc. VIII Spanish Statistical Physics FISES '97], Anales de Física, Monografías RSEF, 4, 21–30 (1998).
- H. E. Stanley, S.V. Buldyrev, M. Canpolat, M. Meyer, O. Mishima, M. R. Sadr-Lahijany, A. Scala, and F.W. Starr. "The Puzzling Behavior of Liquid Water". [Proc. Latin American Workshop on Condensed Matter Physics], *Physica A* 257, 213-222 (1998).
- 5. S. V. Buldyrev, M. Canpolat, S. Havlin, O. Mishima, M. R. Sadr-Lahijany, A. Scala, F. W. Starr, and H. E. Stanley, "Physics of Supercooled Water: Possibility of Two Liquid Phases," in *Slow Dynamics in Complex Systems: Proceedings of the 8th Tohwa University International Symposium*, edited by Michio Tokuyama and Irwin Oppenheim (AIP Conference Series, 1999), 243–256.
- H. E. Stanley, S.V. Buldyrev, M. Canpolat, S. Havlin, O. Mishima, M. R. Sadr-Lahijany, A. Scala, and F.W. Starr. "The puzzle of liquid water: a very complex fluid". [Proc. 18th Annual CNLS Conference on Quantifying Uncertainty in Models of Complex Phenomena] Physica D 133, 453-462 (1999).
- H.E. Stanley, S.V. Buldyrev, O. Mishima, M.R. Sadr-Lahijany, A. Scala, and F.W. Starr, "Unsolved Mysteries of Water in its Liquid and Glassy Phases," [Proc. Intl. Conf. on Liquid Matter] J. Phys. Cond. Mat. **12** A403-A412 (2000).
- H. E. Stanley, S. V. Buldyrev, M. Canpolat, O. Mishima, M. R. Sadr-Lahijany, A. Scala, and F. W. Starr, "The Puzzling Behavior of Water at Very Low Temperature" [Proc. International Meeting on Metastable Fluids, Bunsengesellschaft] Physical Chemistry and Chemical Physics (PCCP), 2, 1551-1558 (2000).
- M. Canpolat, O. Mishima, M. R. Sadr-Lahijany, A. Scala, H. E. Stanley, and F. W. Starr, "The Hypothesized Low-Temperature, High-Pressure Second Critical Point in Liquid Water," in *Steam, Water, and Hydrothermal Systems: Physics and Chemistry Meeting the Needs of Industry* [Proc. 13th Intl. Conf. on the Properties of Water and Steam, Toronto], edited by P. R. Tremaine, P. G. Hill, D. E. Irish, and P. V. Balakrishnan (NRC Research Press, Ottawa, 2000), pp. 494–500.
- F.W. Starr, S. Sastry, F. Sciortino, and H.E. Stanley. "Supercooled Water: Dynamics, Structure and Thermodynamics". Proceedings of the DAE (India) Solid State Physics Symposium 1999, Ed.s R. Mukhopadhyay, B. K. Godwal and S. M. Yusuf (Universities Press, India, 2000) Solid State Physics (India) 42, 77 (1999).
- S.C. Glotzer and F.W. Starr. "Multiscale Modeling of Filled and Nanofilled Polymers". Proc. of Foundations of Molecular Modeling and Simulation (FOMMS 2000), AICHE Symposium Series 97 (2001).
- 12. F.W. Starr and S.C. Glotzer. "Simulation of filled polymer melts on multiple length scales". *Proc.* of Materials Research Society **661** (2001).
- 13. S.C. Glotzer, Y. Gebremichael, N. Lačević, T.B. Schrøder, and F.W. Starr, "Glass-Forming Liquids and Polymers: With a Little Help From Computational Statistical Physics", *Computer Physics Communications* 146, 24-29 (2002).
- H.E. Stanley, S.V. Buldyrev, N. Giovambattista, E. La Nave, A. Scala, F. Sciortino, and F.W. Starr. "Statistical physics and liquid water: 'What matters' ". *Proceedings of StatPhys 21*. Submitted.
- 15. R.L. Jones, C.L. Soles, F.W. Starr, E.K. Lin, J.L. Lenhart, W.-L. Wu, D.L. Goldfarb, M. and Angelopoulos. "Chain conformations in ultrathin polymer resists". *Proceedings of SPIE* (2002).
- 16. H. E. Stanley, M. C. Barbosa, S. Mossa, P. A. Netz, F. Sciortino, F. W. Starr, and M. Yamada, "Water at Positive and Negative Pressures" In Proc NATO Advanced Research Workshop "Liquids Under Negative Pressure", February 23-25, 2002, A. Imre, Ed (Kluwer, Dordrecht, 2002).
- 17. H.E. Stanley, S.V. Buldyrev, N. Giovambattista, E. La Nave, S. Mossa, A. Scala, F. Sciortino, F.W. Starr, and M. Yamada, "Application of Statistical Physics to Understand the Static and Dynamics Anomalies in Liquid Water". In press.

 F.W. Starr, C.A. Angell, E. La Nave, S. Sastry, A. Scala, F. Sciortino, and H.E. Stanley. "Dynamics of deeply supercooled water." Invited paper to appear in a special issue honoring W. Kauzmann.

CONFERENCE AND WORKSHOP ORGANIZATION:

- 1. Co-Organizer for Workshop on Nanofilled Polymers, May 2002 in Gaithersburg, USA.
- 2. Co-Organizer for Workshop on Predicting the Thermophysical Properties of Fluids by Molecular Simulation, June 2001 in Gaithersburg, USA.

INVITED TALKS, CONFERENCE, AND WORKSHOP PARTICIPATION:

- 1. Invited Speaker at the 15th Symposium on Thermophysical Properties, June 2003, Boulder, USA. Title: TBA
- 2. Nanomaterials and the Chemical Industry R&D Roadmap Workshop, October 2002, Baltimore, USA.
- 3. Gordon Conference on Polymer Physics, August 2002 in Newport, Rhode Island. Title: Molecular Dynamics Simulations of a Filled Polymer Melt.
- 4. Invited Speaker at *Workshop on nanofilled materials*, May 2002 in Gaithersburg, USA. Title: Probing nanocomposite structure and properties using computer simulations.
- 5. Invited Speaker at the Air Force Research Lab, Dayton, USA, March 2002.
- 6. Invited Speaker at *Unifying Concepts in Glass Physics*, February 2002 in Roma, Italy. Title: What can we learn from the local geometry of melts and liquids?
- 7. American Institute of Chemical Engineers, November 2001 in Reno, USA. Talks: (1) Simulation of a nanofilled polymer melt and (2) Predicting thermophysical properties of fluids by molecular simulation plenary session, presented by A.M. Chaka.
- 8. Invited Speaker at *The International Association for the Properties of Water and Steam Annual Meeting*, September 2001 in Gaithersburg, USA. (Canceled due to September 11 events.)
- 9. 4th International Discussion Meeting on Relaxations in Complex Systems, June 2001 in Hersonissos, Crete. Title: Local structure and dynamics of a cooled polymer melt.
- 10. Invited Speaker at New kinds of phase transitions: Transformations in disordered substances (NATO-ARW) May 2001 on the Volga River, Russia; could not attend.
- 11. American Physical Society, March 2001 in Seattle, USA. Session Chair: Nanoparticle Filled Systems. Talks: (1) Molecular Dynamics Simulations of a Nanoparticle in a Polymer Melt and (2) Local Structure, Mobility, and Vitrification of a Polymer Melt.
- 12. Invited Speaker at U. Maryland Institute for Physical Science and Technology (IPST), December 2000. Title: Dynamics of Supercooled Liquids: Water as a Model Liquid.
- 13. *Materials Research Society*, November 2000 in Boston, USA. Title: Molecular Dynamics Simulations of a Filled Polymer Melt.
- 14. American Chemical Society, August 2000 in Washington, DC, USA. Title: Dynamics of a Simulated Filled Polymer Melt.
- 15. Gordon Conference on Water and Aqueous Solutions, August 2000 in New Hampshire. Title: Phase Diagram, Energy Landscape, and Dynamics of Simulated Water.
- 16. Gordon Conference on Polymer Physics, August 2000 in New London, Connecticut. Title: Molecular Dynamics Simulations of a Filled Polymer Melt.
- 17. Invited Speaker at NIST Center for Neutron Research, March 2000. Title: Thermodynamics and Dynamics of Supercooled Water.
- 18. American Physical Society, March 2000 in Minneapolis, USA. Session Chair: Classical Fluids and Thermodynamics. Talks: (1) Structure and Dynamics in Simulated Filled Polymers and (2) Dynamics and Energy Landscape of Liquid Water.

- 19. International Bunsen Discussion Meeting on Metastable Water, September 1999 in Nordkirchen, Germany. Title: Dynamics and Energy Landscape of Liquid Water.
- 20. Unifying Concepts in Glass Physics, September 1999 in Trieste, Italy. Title: Dynamics and Energy Landscape of Liquid Water.
- 21. The Instantaneous Normal Mode Approach to Dynamics in Liquids, July 1999 in Lyon, France. Title: Dynamics and Configurational Entropy of Liquid Water.
- 22. Phase space and energy landscapes in disordered systems, June 1999 in Lyon, France.
- 23. Workshop on Non-equilibrium Phenomena in Supercooled Fluids, Glasses, and Amorphous Materials, September 1998 in Pisa, Italy. Title: Dynamics and Inherent Structures of Liquid Water.
- 24. Gordon Conference on Water and Aqueous Solutions, August 1998 in New Hampshire. Titles: (1)Dynamics of Water and the Energy Landscape (2) Continuity of Liquid and Glassy Water: Structural Evidence (3) presented by M. Yamada Effect of Solutes on the Liquid-Liquid Transition of Simulated Water.
- 25. StatPhys 20, July 1998 in Paris. Title: Continuity of Liquid and Glassy Water.
- 26. *Hydration Processes in Biology* (NATO-ASI), May 1998 in Les Houches, France. Title: Continuity of Liquid and Glassy Water: Structural and Dynamic Evidence.
- 27. 78th Statistical Mechanics Conference, December 1997 at Rutgers University. Title: Effect of Pressure on the Local Structure of Liquid Water.
- 28. Provided a simulation for *Super-Computing 97*, November 1997 in San Jose, California. Title: Stretched Liquid Water: Finite Size Effects.
- 29. Gordon Conference on the Chemistry and Physics of Liquids, August 1997 in New Hampshire. Title: Effect of Pressure on Liquid Water.
- 30. Sixth International Conference on Discrete Models for Fluid Mechanics, August 1996 at Boston University. Title: Interface Roughening in a Hydrodynamic Lattice-Gas Model with Surfactant.
- 31. Gordon Conference on Water and Aqueous Solutions, August 1996 in New Hampshire.

HONORS and ACTIVITIES

- Recipient of a NIST/NRC Postdoctoral Associateship, August 1999 August 2001.
- Recipient of a NSF Graduate Research Trainee Fellowship, 1996 1999.
- Computer simulation images featured on the cover of the MRS Bulletin, May 1999
- Recipient of a NSF award to attend CECAM workshop "The Instantaneous Normal Mode Approach to Dynamics in Liquids", July 1999
- Recipient of a NSF award to attend StatPhys 20, July 1998.
- Recipient of a NSF award to attend NATO-ASI "Hydration Processes in Biology", May 1998.
- Member of the American Physical Society since 1999.
- Member of the American Institute of Chemical Engineers since 2001.
- Recipient of the Pugh Undergraduate Scholarship for Physics at Carnegie Mellon University: 1991 and 1992.

REFERENCES:

Provided upon request.