Brian Bostian Laird
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PERSONAL DATA

- Born August 16, 1960 in Port Arthur, Texas, USA; married

EDUCATION

- *University of California at Berkeley*
  - Ph.D., Theoretical Chemistry; December 1987
  - Ph.D. Research Advisor: Prof. A.D.J. Haymet
  - Thesis Title: "The Theory of Freezing: prediction of phase diagrams and interfacial structure for monatomic systems"
- *University of Texas at Austin*
  - Bachelor of Science in Chemistry (with special honors); May 1982
  - Bachelor of Science in Mathematics (with honors); August 1982

PROFESSIONAL EXPERIENCE

- Chair of Chemistry Department: July, 2014 - present
- Professor: August, 2004 - present,
- Associate Chair for Graduate Programs: May, 2002 - June, 2013, Department of Chemistry, Univ. of Kansas
- Visiting Scientist, Dept. of Mathematics and Computer Science, Univ. of Leicester, August, 2001 - January, 2002
- Associate Chair for Undergraduate Prgrams: August, 2000 - May, 2002, Department of Chemistry, Univ. of Kansas
- Associate Professor: August, 1998 - July, 2004
- Visting Scientist: May-June, 1997, Institut für Physik, Johannes-Gutenberg Universität, Mainz, Germany
- Visting Scientist: June 1995, Institute for Solid State Physics, Forschungszentrum Jülich, Jülich, Germany
- Assistant Professor: January, 1994 - August, 1998, Department of Chemistry, University of Kansas, Lawrence, KS 66045
- Physical Chemistry Lecturer: January, 1993 - December, 1993, Department of Chemistry, University of Wisconsin, Madison, WI 53703

- ARC Research Fellow: June, 1992 - December,1992, School of Chemistry, University of Sydney, NSW 2006, Australia
- Faculty Intern: January, 1991 - June, 1992, Department of Chemistry, University of Utah, Salt Lake City, UT 84112
- Guest Scientist: August, 1989 - December 1990, Institut für Festkörperforschung des Forschungszentrums, Jülich, GmbH, 5170 Jülich, Germany
- Postdoctoral Research Assistant: January, 1988 - June, 1989, Prof. James L. Skinner, Director Department of Chemistry, Columbia University, New York, NY 10027

CONSULTING

- Expert Technical Consultant for Defendant in the case of Flint Hills Scientific vs. Ruslan Davidchack (2003)

RESEARCH KEYWORDS Computational materials science, computational chemistry, solid-liquid interfaces, algorithms for molecular simulation, phase transitions, properties of glasses and supercooled liquids, general liquid-state theory (equilibrium and non-equilibrium), inhomogeneous fluids

HONOR SOCIETIES, AWARDS and FELLOWSHIPS

- National Science Foundation CAREER Development Award, April, 1995 - April, 1998.
- NATO Postdoctoral Fellowship, August, 1989 - October, 1990.
- American Institute of Chemists Award - Univ. of Texas at Austin, 1982
- Robert A. Welch Foundation Scholarship, 1978-1982
- Phi Beta Kappa, Texas 1982, National Merit Scholarship, 1978-1982

TEACHING EXPERIENCE

- *University of Kansas*
  - Spring 2014: Chemistry 535: Physical Chemistry II
  - Fall 2013: Chemistry 150: Chemistry for Engineers
  - Spring 2013: Chemistry 852: Statistical Thermodynamics
  - Fall 2013: Chemistry 850: Introduction to Quantum Mechanics
  - Spring 2012: Chemistry 852: Statistical Thermodynamics
  - Fall 2011: Chemistry 950/Physics 971: Advanced Statistical Mechanics
  - Spring 2011: Chemistry 752: Statistical Thermodynamics
  - Fall 2010: Chemistry 646: Physical Chemistry I: Quantum Chemistry and Spectroscopy
  - Spring 2010: Chemistry 917/Physics 971: Advanced Statistical Mechanics
  - Spring 2010: Chemistry 696: Jr./Sr. Seminar (with C. Lunte)
  - Fall 2009: Chemistry 750: Quantum Chemistry and Spectroscopy
  - Spring 2009: Chemistry 648: Physical Chemistry II: Thermodynamics and Kinetics
  - Spring 2008: Chemistry 752 - Statistical Thermodynamics

- Fall 2007: Chemistry 750 - Quantum Chemistry and Spectroscopy
- Spring 2007: Chemistry 915 Intermediate Quantum Mechanics
- Fall 2007: Chemistry 917/Physics 971 Advanced Statistical Mechanics
- Spring 2006: Chemistry 648 - Molecular Physical Chemistry
- Fall 2005: Chemistry 646 - Introduction to Physical Chemistry
- Spring 2005: Chemistry 752 - Statistical Thermodynamics
- Fall 2004: Chemistry 646 - Introduction to Physical Chemistry
- Spring 2004: Chemistry 189 - Foundations of Chemistry II, honors (with Craig Lunte)
- Spring 2004: Chemistry 752 - Statistical Thermodynamics (with Carey Johnson)
- Fall 2003: Chemistry 680 - Nanoscience (with Ward Thompson)
- Fall 2003: Chemistry 185 - Foundations of Chemistry I, honors (with Craig Lunte).
- Spring 2003: Chemistry 189 - Foundations of Chemistry II, honors.
- Fall 2002: Chemistry 185 - Foundations of Chemistry I, honors.
- Spring 2002: Chemistry 917 - Advanced Statistical Mechanics
- Spring 2002: Chemistry 696 - Junior-Senior Seminar
- Fall 2001: On Sabbatical Leave
- Spring 2001: Chemistry 752 - Thermodynamics and Kinetics
- Fall 2000: Chemistry 909 - Statistical Thermodynamics
- Fall 2000: Chemistry 185 - Foundations of Chemistry I, honors
- Spring 2000: Chemistry 189 - Foundations of Chemistry II, honors
- Fall 1999: Chemistry 185 - Foundations of Chemistry I, honors
- Spring 1999: Chemistry 125 - College Chemistry
- Fall 1998: Chemistry 750 - Introduction to Quantum Chemistry
- Spring 1998: Chemistry 919 - Techniques in Molecular Simulation
- Fall 1997: Chemistry 646 - Physical Chemistry I
- Spring 1997: Chemistry 917 - Advanced Statistical Mechanics; co-taught Chemistry 649; ran a Chemistry 188 discussion section
- Fall 1996: Chemistry 909 - Statistical Thermodynamics
- Spring 1996: Chemistry 919 - Methods in Chemical Physics
- Fall 1995: Chemistry 750 - Introduction to Quantum Chemistry
- Spring 1995: Chemistry 917 - Statistical Thermodynamics
- Fall 1994: Chemistry 646 - Physical Chemistry I
- Spring 1994: Chemistry 919 - Statistical Mechanics of Liquids

- *University of Wisconsin, Madison*
  - Fall 1993: Chemistry 108 - Chemistry for Non-majors
  - Spring 1993: Chemistry 563&564 - Physical Chemistry Laboratory
- *University of Sydney*
  - October 1992: Third-Year Theoretical Chemistry Workshop
- *University of Utah*

- Winter Quarter 1991: Chemistry 141N - General Chemistry for Nursing Students
- Fall Quarter 1991: Chemistry 123N - Third Quarter General Chemistry

THESIS COMMITTEES CHAIRED

- *Doctoral:* Scott Bembenek (1997)
- *Doctoral:* Ruslan Davidchack, Physics (co-chair) (1998)
- *Doctoral:* Steve Bond, Math (co-chair)(1999)
- *Undergraduate Honors*: Catherine Cronin (1999)
- *Doctoral:* Jess Sturgeon (2001)
- *Doctoral:* Rachel Aga (2002)
- *Doctoral:* Yao Houndonougbo (2002)
- *Doctoral:* Majeed Amini, Physics (2006)
- *Doctoral:* Jesus Pablo Palafox-Hernandez (2011)

PROFESSIONAL SOCIETY MEMBERSHIPS

- American Physical Society (APS)
- Minerals, Metals and Materials Society (TMS)
- Materials Research Society (MRS)
- American Chemical Society (ACS)

NATIONAL AND INTERNATIONAL SERVICE

- Organizer for symposium on "Glasses and Glass Dynamics", American Physical Society March Meeting, Kansas City, MO, March 22-27, 1997
- Co-organizer for symposium on "Density-functional methods in chemistry", American Chemical Society National Meeting, Anaheim, CA, April 2-7, 1995
- Co-organizer for a CECAM workshop on "Advanced Integrators for Molecular Simulation", Lyon, France, May 15-17, 2000
- Co-organizer for a workshop on "Molecular Dynamics" as part of the International Conference on Computational Science, San Francisco, CA, May 28-30, 2001
- Co-organizer for a CECAM workshop on "Crystal-Melt Interfaces: Structure, Thermodynamics and Growth", Lyon, France, June 23-25, 2003
- Reviewer for National Science Foundation, Department of Energy, Research Corporation, Israeli Science Foundation, National Science and Engineering Research Council of Canada and the Petroleum Research Fund Proposals
- Reviewer for Physical Review, Journal of Chemical Physics, Journal of Physical Chemistry, Molecular Physics, Journal of Physics: Condensed Matter

CURRENT DEPARTMENTAL, UNIVERSITY AND LOCAL SERVICE

- *Chemistry*: Chair Advisory Committee, Web Committee
- *University:* Graduate Executive Council

PAST DEPARTMENTAL, UNIVERSITY AND LOCAL SERVICE

- *Chemistry*: Graduate Affairs Committee (Chair, 04-14), Space Committee (94-95), Graduate Recruiting Committee Chair (95-96), Physical Chemistry Lecturer Search Committee (95), Graduate Admissions Committee (99-00), Departmental Space Committee (98-00), Physical Chemistry Faculty Search Committee (chair, 98-99), American Chemical Society Local Chair (00), Analytical Distinguished Faculty Search Committee (00-01), Undergraduate Affairs Committee Chair (00-02), General Chemistry Committee Chair (00-02), General Chemistry Laboratory Director Search Committee (2002), Seminar Coordinator (98 - 04), Joint Chemistry-Physics Space Committee (02-04)

- *Local*: Faculty Co-Advisor $AX\Sigma$ (96-02).

- *University*: Undergraduate Minority Fellowship Committee (95), Physics Faculty Search Committee (96), CUSA (99-00), CUSA Academic Standards Subcommittee (99-00), Graduate Minority Fellowship Committee (00), Committee on Graduate Program Review (03), Faculty Senate Research Committee (04-06), Ad hoc Research Computing Committee (07-08),

- *University*: College Graduate Committee (08-11, Chair 09-11), Provost's task force on Engaged Scholarship (Fall 2011).

CURRENT FUNDING

- National Science Foundation, $450,000, Mar. 1, 2010 - Feb. 28, 2014, "Simulations and Theory of Solid-Liquid Interfaces and Grain Boundaries", B. Laird, PI

- Department of Energy, $750,000 out of $11,500,000 for center, "Energy Frontier Research Center on Molecularly Assembled Material Architectures for Solar Energy Production, Storage, and Carbon Capture", V. Ozolins (UCLA), PI; B. Laird, *et al.*, co-PI's

PREVIOUS FUNDING

- University of Kansas General Research Fund, New Faculty Grant, $5,000 January 1, 1994 - August 31, 1994, "Low-frequency vibrations in glasses"

- Petroleum Research Fund, Type G Starter Grant, $20,000, September 1,1994 - August 31, 1996, "Low-frequency vibrations in glasses"

- Petroleum Research Fund, Type SE Grant to fund a symposium on "Density-functional methods in chemistry" at the ACS National Meeting, Anaheim, CA, 1995, $2,000 February 1,1995 - August 31, 1995.

- Petroleum Research Fund, Type SE Grant to fund two focus sessions on "Dynamics of glasses and supercooled liquids" at the APS March Meeting, Kansas City, MO, 1997, $2,000 February 1,1997 - August 31, 1997.

- National Science Foundation CAREER Development Award, $205,000, April 15, 1995 - March 31, 1998,"Theory and Simulation of Solid-Liquid", B. Laird (PI).

- Petroleum Research Fund, Type AC, $50,000, September 1,1996 - August 31, 1999, "Localization in Glasses and Supercooled Liquids"

- National Institutes of Health, $189,000/year, "Peptide Degradation in Polymer Matrices", August 1,1997 - July 31, 2000, R.L Schowen (PI), R. Borchhart (Co-PI), E.Topp (Co-PI), B. Laird (Collaborator), D. VanderVelde (Collaborator).

- University of Kansas General Research Fund, $11,980 July 1, 1998 - June 30, 1999, "Simulation and Theory of Solid-Liquid Interfaces"
- CECAM, FRF40,000, grant to organize a CECAM symposium on "Advanced Integrators for Molecular Simulation" with B. Leimkuhler, May 2000.
- National Center for Advanced Scientific Computing (NCSA), 10,000 CPU units, grant of computer time to study, Aug. 2000 - Aug. 2001 "the structure and dynamics of crystal-melt interfaces".
- National Science Foundation, $287,000, June 1, 1997 - May 31, 2001, "Stabilized Geometric Integrators with Application to Molecular Simulation", with B.J. Leimkuhler (KU Math, PI) and K. Kuczera (KU Chemistry and Biochemistry)
- National Science Foundation, $260,000 May 15, 1999 - April 30, 2003, "Simulaion and Theory of Crystal-Melt Interfaces", B. Laird (PI).
- Centre Européen de Calcul Atomique et Moléculaire (CECAM), Euro 7,000, proposal to organize a CECAM symposium on "Crystal-Melt Interfaces: Structure, thermodynamics and growth" in Lyon, France - June 23-25,2003
- National Science Foundation, $93,325, July 1, 2003 - June 30, 2005, Integrating Experiment, Computation, Communication, and Independent Inquiry in the Physical Chemistry Laboratory", PI: C. Johnson, CoPI's: C. Berrie, B. Laird ,K. Kuczera, J. Heppert.
- National Science Foundation, $345,000 Aug 1, 2003 - July 31, 2006, "Thermodynamics, Structure and Dynamics of Crystal-Melt Interfaces", B. Laird (PI).
- National Science Foundation, $ 200,000, Oct. 1, 2007 - Sept. 31, 2008, "SBIR PIIR Supplement to CEBC ERC grant", (B.Laird and W.Thompson, co-PI's), grant to work on molecular modelling aspects of ligand based water purification with Crystal Clear Technologies.
- National Science Foundation, $17,000,000, Sept 15, 2003 - Aug 31, 2008, "Center for Environmentally Beneficial Catalysis (CEBC)", PI: B. Subramaniam, Co-PI's: D. Busch, A. Borovik, J. Heppert, B. Laird, D. Lane, R. Givens

INVITED CONFERENCE PRESENTATIONS

- American Chemical Society Meeting, Washington, D.C., August 21-26, 1994, "Low-frequency, localized vibrations in glasses".
- Midwest Thermodynamics and Statistical Mechanics Conference, Madison, WI, May 2-3, 1996, "Simulation of the Binary Hard-Sphere Solid/Liquid Interface".
- American Conference on Theoretical Chemistry, Park City, UT, July 20, 1996, "Localization and the Glass Transition".
- American Crystallographic Association National Meeting, St. Louis, MO, July 20-25, 1997, "Localization in Glasses and Supercooled Liquids".
- American Physical Society March Meeting, Los Angeles, March 9-13, 1998, "Anharmonicities and Barrier Heights in a Model of Amorphous Silica".
- Computational Chemistry Gordon Conference, Tilton School, NH, June 28 - July 3, 1998,"Simulations of the Solid-Liquid Interface".

- CECAM Workshop on Rough Energy Landscapes in Glasses and Supercooled Liquids, CECAM, Lyon, France, May 31-June 3, 1999, "Barriers and Anharmonicities in Amorphous Silica".
- CECAM Workshop on "Proteins at Interfaces", Lyon, France, September, 1999, "Simulations and theory of Crystal-Melt Interfaces".
- CECAM workshop on Advanced Molecular-Dynamics Integration Techniques, May 15-17, 2000, Lyon, France, "A symplectic integrator for isobaric molecular dynamics with a Nosé-Poincaré thermostat"
- Gordon Conference on "Physics Teaching and Research", June 20-25,2000, "Entropy, Disorder and Freezing"
- International Conference on Computational Science, San Francisco, CA, May 28-30, 2001 "A Molecular-Dynamics Algorithm for Mixed Hard-core/Continuous Potentials".
- Fourteenth International Conference on Crystal Growth and Epitaxy, Aug. 9-14, 2002, Seattle, Washington, "Simulations of single-component and binary crystal-melt interfaces".
- Southwest Theoretical Chemistry Conference XIX, November 14-16, 2002, Houston, Texas, "Generalized Distribution Dynamics".
- Annual Meeting of the Metals, Mining and Metalurgy Society, March 2-6, 2003, San Diego, California, "Calculating the crystal-melt interfacial free energy by simulation".
- Fifteenth International Conference on Crystal Growth and Epitaxy, Jul. 20-24, 2003, Keystone, Colorado, "Calculating the crystal-melt interfacial free energy by simulation".
- CECAM/SIMU Workshop on "Algorithms for Accelerated Dynamics", Mar. 23-25, 2004, Lyon, France, "Generalized Distribution Dynamics".
- Prestissimo workshop on Molecular Dynamics Algorithms, December 1-3, 2004, Paris, France, "Direct calculation of the crystal-melt interfacial free energy from molecular-dynamics simulations".
- Midwest Theoretical Chemistry Conference, June 16-18, 2005, Columbia, MO, "Direct calculation of the crystal-melt interfacial free energy from molecular dynamics simulation".
- Southwest Regional ACS meeting, October 20-22, 2006, Houston, TX, "Direct Calculation of the Crystal-Melt Interfacial Free Energy".
- TMS Annual Meeting, Feb 25 - March 1, 2007, Orlando, FL, "SImulation of Crystal-Melt Interfacial Free energies: from hard-spheres to molecules".
- CECAM Workshop on New Frontiers in Liquid Theory, Jul. 2-4, 2007, Lyon, France, "Prefreezing of hard-spheres at a hard wall".
- CECAM Workshop on Fundamental Aspects of Deterministic Thermostats, Jul. 27 - 29, 2009, Lausanne, Switzerland, "MD simulation of mixed continuous/ discontinuous potentials, with and without thermostats".
- CECAM Workshop on Classical Density Functional Theory Methods in Soft and Hard Matter, Oct. 21 - 23, 2009, Lausanne, Switzerland, "Classical DFT calculations of Freezing and Elastic Constants".
- Conference on Computational Physics, Kaoshiung, Taiwan, Dec. 15-19, 2009, "Determination of the Solid-Liquid Interfacial Free Energy by Gibbs-Cahn Integration".

- TMS Annual Meeting, Feb 15 - 19, 2010, Seattle,WA, Symposium on Wetting, "Prefreezing at Chemically Heterogeneous Solid-Liquid Interfaces".
- SIAM Conference on Mathematical Aspects of Materials Modeling, May 20, 2010, "Calculating the solid-liquid interfacial free energy by integration along a coexistence curve.
- TMS Annual Meeting, Feb. 27 - Mar. 3, 2011, San Diego,CA, "Characterization of the Cu/Pb solid-liquid interface by atomic simulation".
- Materials Research Society Spring 2011 Meeting, April 25-30, 2011, San Francisco, CA "Molecular Modeling of the structure, thermodynamics and kinetics of gas adsorption in Zeolitic Imidazolate Frameworks (ZIFs)".
- Materials Research Society Spring 2012 Meeting, April 10-14, 2012, San Francisco, CA, "Topology effects on gas adsorption in zeolitic imidazolate frameworks (ZIFs)".
- ACS Meeting on Solids and Colloids, June 22-26, 2013, Riverside, CA, "Interfacial free energy at curved surfaces".
- 2014 Annual Meeting of the Metals, Mining and Metalurgy Society, Feb 16-20, 2014, San Diego, California, "Prefreezing and premelting at solid-liquid interfaces."
- James Skinner 60th Birthday symposium, May 20-21, 2014, University of Wisconsin-Madison, "Sold-liquid interfacial premelting"
- Workshop on "Structure and Dynamics of Confined Fluids, Oak Ridge National Laboratory, July 16-18, 2014, "Solid-liquid interfacial premelting".

CONTRIBUTED CONFERENCE PRESENTATIONS

- Material Research Society Fall Meeting: Boston, December 1984, "The solid-liquid interface: theory and computer simulations"
- XXVII Midwest Theoretical Chemistry Conference: Columbia, MO, May 19-21, 1994, "Localization in Glasses"
- XXVIII Midwest Theoretical Chemistry Conference: Evanston, IL, May 11-12, 1995, "Determination of hard-sphere elastic constants with density-functional theory
- American Physical Society March Meeting, St. Louis, MO, March 22-26, o 1996, "Localization in Glasses and Supercooled Liquids"
- 3rd European Physical Society Liquid Matter Conference, Norwich, UK, July 6-10, 1996, "Localization and the Glasses Transition"
- 5th Liblice Conference on the Statistical Mechanics of Liquids, Zeledzna Ruda, Czech Republic, June 6-10,1998, "Symplectic Integrators for Molecular Dynamics Simulation".
- Centenial APS National Meeting, March 20-25, 1999, Atlanta, GA, "Symplectic Integrators for Molecular Dynamics Simulation".
- Centenial APS National Meeting, March 20-25, 1999, Atlanta, GA, "Simulations of the Solid-Liquid Interface"
- First Annual KSU-KU Physical Chemistry Symposium, October 30, 2000, Manhattan, KS.

- APS National Meeting, March 12-17, 2001, Seattle, WA, "Direct Calculation of the hard-sphere crystal-melt interfacial free energy" "Symplectic Integrators for Molecular Simulation".
- International Conference on Computational Chemistry, San Francisco, May 28-30, 2001, "Molecular Dynamics Algorithm for mixed hard-core/continuous potentials".
- StatPhys 21, July 15-21, 2001, Cancun, Mexico, "Simulation of the crystal-melt interfacial free energy for the hard-sphere system".
- Workshop on "Liquids and Interfaces", CCCP Annual Meeting, University of Warwick, September 16-18, 2001, "Hard spheres and the crystal-melt interfacial free energy of simple metals"
- Yangtzee conference on interfaces, Nanjing, China, October 12-18, 2002, "Simulations of the crystal-melt interface"
- 3rd International Conference on Computational Materials Science, May 30 - Jun. 4, 2004, Acireale, Italy, "Direct calculation of the crystal-melt interfacial free energy by simulation".
- Southwest Texas Theoretical Chemistry Conference, October 22-23, 2004, "Generalized Distribution Dynamics"
- Computational Materials Science Network workshop, Oct 28-29, 2005, Northwestern University, "Direct calculation of the crystal-melt interfacial free energy from molecular-dynamics simulations"
- Computational Materials Science Network workshop, Nov. 1-2, 2005, Santa Fe, NM, "Calculation of the crystal-melt interfacial free energy of succinonitrile"
- 8th Liblice Conference on the Statistical Mechanics of Liquids, June 13-18, 2010, Brno, CZ, , "Calculation of solid-liquid interfacial free energies from atomistic simulation"
- 5th International Conference on Multiscale Materials Modeling, Oct. 3-8, 2010, Freiburg, Germany, "Calculation of solid-liquid interfacial free energies using Gibbs-Cahn integration".
- 8th Liquid Matter Conference, Vienna, Austria, Sept. 6-10, 2011 "Calculation of solid-liquid interfacial free energies using Gibbs-Cahn integration" (poster).
- 8th Pacific Rim International Congress on Advanced Materials, Aug. 4-9, 2013, Waikoloa, HI, "Premelting at solid-liquid lnterfaces".
- International Soft Matter Conference, Sept. 15-19, 2013, Rome, Italy, "Solid-liquid interfacial free energy of curved surfaces"
- 9th Liblice Conference on the Statistical Mechanics of Liquids, Se? Dam Lake, Czech Republic, June 16-20, 2014, "Premelting at solid-liquid interfaces ".

INVITED LECTURES

- Swarthmore College, Physics Colloquium, March 15, 1989 "The density-functional theory of freezing"
- University of Illinois - Urbana, Chemistry Department, January 18, 1991, "Microscopic theory of pressure effects in hole-burning spectra"
- University of California - Los Angeles, Chemistry Department, January 28, 1991, "Microscopic theory of pressure effects in hole-burning spectra"

- University of Pittsburgh, Chemistry Department, March 6, 1991, "Microscopic theory of pressure effects in hole-burning spectra"
- University of Utah, Chemistry Department, December 11, 1991, "Microscopic theory of pressure effects in hole-burning spectra"
- New York University, Chemistry Department, January 20, 1992, "Microscopic theory of pressure effects in hole-burning spectra"
- Princeton University, Chemistry Department, January 22, 1992 "Microscopic theory of pressure effects in hole-burning spectra"
- Southern Methodist University, Chemistry Colloquium, January 12, 1993, "Entropy and correlation functions"
- University of Wisconsin - Madison, Physical Chemistry Seminar, January 21, 1991, "Entropy and correlation functions"
- Purdue University, Physical Chemistry Colloquim, February 15, 1993, "Entropy and correlation functions"
- University of Kansas, Physical Chemistry Colloquim, March 15, 1993, "Entropy and correlation functions"
- University of Indiana, Physical Chemistry Seminar, April 6, 1993 "Entropy and correlation functions"
- University of Kansas, Physical Chemistry Colloquim, December 2, 1993, "Microscopic theory of reversible pressure broadening in hole-burning spectra"
- Kansas Theory Institute, January 18, 1994, "Low-frequency, localized vibrations in glasses"
- University of Kansas, Physics Colloquim, January 21, 1994 "Entropy and correlation functions"
- Kansas State University, Physics Colloquium, Oct. 5, 1994 "Instantaneous normal modes and the glass transition"
- University of Missouri, Kansas City, Physics Colloquium, Oct. 28, 1994 "Instantaneous normal modes and the glass transition"
- University of Kansas, Physical Chemistry Colloquium, Sept. 6, 1995, "Density-functional theory of freezing"
- University of Nebraska, Materials Science Inst. Colloquium, Oct. 23, 1995, "Localization in glasses and supercooled liquids"
- University of Oklahoma, Physics Colloquium, Nov. 9, 1995, "Localization in glasses and supercooled liquids"
- University of Missouri-Columbia, Chemistry Colloquium, Sept. 6, 1996, "Simulations of solid-liquid interfaces"
- University of Kansas, Physical Chemistry Seminar, Oct. 15, 1996, "Simulations of solid-liquid interfaces"
- University of California at Irvine, Physical Chemistry Seminar, Jan. 28, 1997, "Simulations and theory of solid-liquid interfaces"

- University of Missouri-Kansas City, Chemistry Colloquium, Jan. 31, 1997, "Simulations and theory of solid-liquid interfaces"
- University of Wisconsin-Madison, Chemistry Colloquium, Apr. 8, 1997, "Simulations and theory of solid-liquid interfaces"
- University of Missouri-Kansas City, Physics Colloquium, Apr. 18, 1997, "Syplectic integrators for molecular simulation"
- Institut für Festkörperforschung, Forschungszentrum Jülich, Jülich, Germany, June 11, 1997, "Simulations and Theory of Solid-Liquid Interfaces"
- Institut für Physik, Johannes-Gutenberg Universität, Mainz, Germany, June 26, 1997, "Simulations and theory of solid-liquid Interfaces"
- Pittsburg State University, Chemistry Seminar, March 6, 1998, "Simulation of crystal-melt interfaces".
- University of Nebraska-Kearny, Chemistry Seminar, April 3, 1998, "entropy, disorder and freezing"
- University of Wisconsin-Madison, Physical Chemistry Seminar, September 8,1 998, "Simulation of crystal-melt interfaces".
- Creighton University, Chemistry Seminar, September 17,1998, "Simulation of crystal-melt interfaces".
- Ohio University, Condensed Matter and Surface Science Seminar, October 21, 1998, "Symplectic integrators for molecular-dynamics simulation"
- University of Houston, Physical Chemistry Seminar, November 24, 1998, "Symplectic integrators for molecular-dynamics simulation".
- Kansas State University, Departmental Colloquium, October 28, 1999, "Simulation of crystal-melt interfaces"
- Leicester University, June 3, 2000, Department of Mathematics and Computer Science, "Symplectic integrators for molecular-dynamics simulation"
- University of Kansas, Chemical Engineering Seminar, Jan. 31, 2001, "Simulations of the crystal-melt interface".
- Washington University at St. Louis, April 5, 2001, Department of Chemistry, "Simulation of Crystal-Melt Interfaces"
- Kansas Center for Advanced Scientific Computing, Oct. 5, 2001, "Adventures in Molecular Dynamics Simulation: A new algorithm for mixed hard-core/continuous potentials"
- Oxford University, UK, Physical Chemistry Seminar, Nov. 12, 2001, "Simulations of the crystal-melt interface"
- University of Leicester, UK, Center for Molecular Modelling Seminar, Dec. 12, 2001, "Simulations of the crystal-melt interface"
- University of Bristol, UK , Physics Seminar, Dec. 4, 2001, "Simulations of the crystal-melt interface".

- Iowa State University, Chemistry Colloquim, Apr. 4, 2002, "Simulations of the crystal-melt interface".
- University of Kansas , Physics Colloquim, Mar. 6, 2002, "Deconstructing Newton: modified dynamics in the service of molecular simulation".
- Emporia State University, Chemistry Seminar, Sept. 23rd, 2002 "Studying the crystal-melt interface via simulation"
- Condensed-Matter Physics Seminar, KU, November 2006, "Direct calculation of the crystal-melt interfacial free energy"
- ACS Local Section Awards Banquet Speaker, KU, April, 2007, "When order meets disorder, what is the cost?"
- Chemistry Colloquium, University of Missouri-Columbia, Sept. 5, 2007, "Direct calculation of the crystal-melt interfacial free energy"
- Department of Chemical Engineering Seminar, SUNY at Buffalo, Buffalo, NY, Feb. 6, 2008, "When order meets disorder, what is the cost? The solid-liquid interfacial free energy".
- Department of Chemistry, University of Illinois - Urbana, Physical Chemistry Seminar, April 30, 2008 , "When order meets disorder, what is the cost? The solid-liquid interfacial free energy".
- Materials Science Institute, University of Oregon, May 5, 2008 , "When order meets disorder, what is the cost? The solid-liquid interfacial free energy".
- Department of Physics, Kansas State University, Oct. 16, 2009, "When order meets disorder, what is the cost? The solid-liquid interfacial free energy".
- Research Institute for Solid-State Physics and Optics, Hungarian Academy of Science, Budapest, HU, June 22, 2010, "Calculation of solid-liquid interfacial free energies from atomistic simulation".
- Wichita State University, Chemistry Colloquium, Feb. 16, 2011, Wichita, KS, "Molecular modeling of CO_2 adsorption in zeolitic imidazolate frameworks".
- Department of Mathematics, University of Kansas, Applied Mathematics Seminar, Oct. 12, 2011, "Simulations of solid-liquid interfaces".

BOOKS

1. *Chemical Applications of Density-Functional Theory*, B.B. Laird, R.B. Ross, T. Ziegler, eds., ACS Symposium Series 629, (American Chemical Society, Washington, D.C, 1996).
2. *University Chemistry*, B.B. Laird (McGraw-Hill Higher Ed., Dubuque, IA, 2009).

REFEREED PUBLICATIONS

Undergraduate Research

1. "3-hydroxy-4-nitro-cyclohexanones from ketones and 4-nitrobutanoyl chloride. A ring enlarging five-ring annulation", T. Weller, D. Seebach, R. Davis and B. Laird, Helvectica Chimica Acta **64**, 736–780 (1981).

2. "Octafluorocyclooctatetraene transition-metal chemistry: 1,2-eta and 1,2,3,6-eta complexes of iron and platinum", A. Barefoot III, E. Corcoran Jr., R. Hughes, D. Lemal, W. Sanders, B. Laird and R. Davis, JACS **103**, 970–972 (1981).

3. "Octafluorocyclooctatetraene at 238K", B.B. Laird and R.E. Davis, Acta. Cryst. **B38**, 678–680 (1982).

4. "Octafluorocyclooctatetraene transition-metal complexes: Novel transanular ring closures and a formal intramolecular redox equilibrium between 1,2,5,6-eta and 1,2,3,6-eta ligands", R.Hughes, D. Samkoff, R. Davis and B. Laird, Organometallics **2**, 195–197 (1983).

5. "Calculation of the Green function from high- and low-density series expansions for disordered transport", D. Calef, R. Friesner, G. Korzeniewski, B. Laird and R. Silbey, Phys. Rev. A **29**, 2963-2966 (1984).

Graduate Research

6. "Freezing of the Lennard-Jones liquid", C. Marshall, B. Laird and A.D.J. Haymet, Chem. Phys. Lett. **122**, 320–324 (1985).

7. "The solid-liquid interface: Theory and computer simulation" B.B. Laird and A.D.J. Haymet, Materials Research Society Symposia Proceedings **63**,67–72 (1986).

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