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Keith E. Gubbins

Biographical Data

Title: W.H. Clark Distinguished University Professor, North Carolina State University
 Address: Department of Chemical & Biomolecular Engineering, EB1, 911 Partners' Way, North Carolina State University, Raleigh, NC 27695-7905
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Education:

B.Sc. Chemistry (First Class Honours), Queen Mary College, University of London, 1958.
 Dipl. Chem. Eng., King's College, University of London, 1959.
 Ph.D. in Chemical Engineering, King's College, University of London, 1962.

Professional Experience:

Postdoctoral Fellow, 1962-64; Assistant Professor, 1964-68; Associate Professor, 1968-72; Professor, 1972-76, University of Florida.
 Endowed Chair (T.R. Briggs Professorship) in Engineering, Cornell University, September 1976-1998.
 Director, School of Chemical Engineering, Cornell University, July 1983-1990.
 Acting Director, School of Chemical Engineering, Cornell University, January-June, 1995.
 Thomas R. Briggs Professor Emeritus, Cornell University, Jan. 1998-present.
 W.H. Clark Distinguished University Professor, North Carolina State University, January 1, 1998-present
 Co-Director, Center for High Performance Simulation, North Carolina State University, July 1, 2004-present
 Director & Founder, Institute for Computational Science and Engineering, North Carolina State University, November, 2008-2012

Visiting Appointments:

Visiting Lecturer, University of London, 1960-62.
 Eppley Foundation Fellow (Sabbatical Leave), September 1971-June 1972 spent at Chemical Engineering Department, Imperial College, London.
 Visiting Consultant, Theoretical Physics Division, United Kingdom Atomic Energy Authority, Harwell, U.K., May-June 1971.
 Visiting Professor, Physics Department, University of Guelph, July-December 1971; June-September 1972; June-August 1973; June-August 1976.
 Visiting Professor of Physics, University of Kent, Canterbury, England,

June-July 1975.
 Visiting Professor of Chemistry, University of Oxford, England, Sept. 1979-July 1980.
 Visiting Professor of Chemical Engineering, University of California, Berkeley, April-August, 1982.
 Visiting Professor of Molecular Engineering, Kyoto University, Kyoto, Japan, March-April, 1987.
 Visiting Professor of Chemistry, University of Oxford, U.K., September 1986-July 1987.
 Olaf Hougen Visiting Professor of Chemical Engineering, University of Wisconsin, Madison, WI, January-June, 1993.
 Visiting Professor of Chemistry, Research School of Chemistry, Australian National University, Canberra, ACT, August 1993-January 1994.
 Visiting Professor of Chemistry, Imperial College of Science, Technology & Medicine, London, January-August 1994.
 Visiting Professor of Chemistry, Chiba University, Chiba, Japan, November-December 1999.
 Visiting Professor of Chemical Physics, Laboratoire de Chimie Physique, Université Paris-Sud, Orsay, France, June 2001 - January 2002.
 Visiting Professor of Chemistry, Imperial College of Science, Technology and Medicine, London, U.K., February-July, 2002.
 Royal Society (London) Visiting Professor, University of Hong Kong, Hong Kong, June-July 2007.
 Royal Academy of Engineering (London) Distinguished Visiting Fellow, visiting and lecturing at University of Manchester, Heriot Watt University, University of Edinburgh, Imperial College London, Oxford University and University College London, U.K, April-May 2009.
 Visiting Professor of Chemical Engineering, Imperial College, London, January-June, 2011.

Awards, Honors: Research

International Awards:

Leverhulme Fellow, King's College London, 1958-1962.
 Annual Award of Canadian Society of Chemical Engineering, best paper published in Canadian Journal of Chemical Engineering, 1973.
 Senior Visiting Fellow (SERC Award), Oxford University, U.K., 1986-87.
 Delegate to the Press, Oxford University Press, 1991-2007
 SERC (Science and Engineering Research Council) Visiting Fellow, Imperial College of Science, Technology & Medicine, London, January-August 1994.
 Chercheur de Haute Niveau, French Ministry of Education, June 2001-February 2002
 Special Issue of *Molecular Physics*, "A Celebration of Statistical Mechanics in Honour of Professor Keith E. Gubbins", Parts 1, 2 and 3, volume **100**, Nos. 13, 14 and 15, eds. Peter T. Cummings and George Jackson (2002)
 Royal Society (London) Kan Tong Po Visiting Professorship, University of Hong Kong, 2007.
 Distinguished Visiting Fellow, Royal Academy of Engineering (London), 2009. Visiting and lecturing at University of Manchester, Heriot Watt University, University of Edinburgh, Imperial College London, Oxford University and University College London, U.K.

Awarded Honorary Professor position, Nanjing University of Technology, China, December 14, 2009.

Royal Society (London) Visiting Scientist, Imperial College London, January-March 2011.

Medal of Merit, Adam Mickiewicz University, Poznan, Poland, December 7, 2011.

Rossini Lecture 2012 Award, International Association for Chemical Thermodynamics, IUPAC, 2012. Presented at the International Conference on Chemical Thermodynamics, Buzios, Brazil, August, 2012.

Foundations of Molecular Modeling and Simulation (FOMMS) Medal 2012 (to honor “profound and lasting contribution by one or more individuals to the development of computational methods and their application to the field of molecular-based modeling and simulation”). Presented at the FOMMS conference, Mount Hood, Oregon, July 2012.

Lennard-Jones Prize and Lectureship, Royal Society of Chemistry, London, 2013. Presented at the Thermodynamics 2013 conference, Manchester, U.K., September 4, 2013

Honorary Director, International Cooperation Center, Nanjing University of Technology, Nanjing, China, October, 2013.

Most Cited in I&EC Research: One of the 15 Greatest Hits among papers in Industrial and Engineering Chemistry Research published by the American Chemical Society since its founding in 1909: “New Reference Equation of State for Associating Liquids”, Walter G. Chapman, Keith E. Gubbins, George Jackson and Maciej Radosz, *I&EC Research*, **29**, 1709-1721 (1990).

National Awards:

Eppley Foundation Fellowship, 1970-71 (for leave at Imperial College, London).

John Simon Guggenheim Memorial Foundation Fellow, 1986-87.

Alpha Chi Sigma Research Award (American Inst. of Chemical Engrs.) 1986.

National Academy of Engineering, elected 1989

Fulbright Senior Scholar, Research School of Chemistry, Australian National University, Canberra, Australia, August 1993-January 1994.

William H. Walker Award of the American Institute of Chemical Engineers, for contributions to the chemical engineering research literature, November 2000.

Fellow, American Institute of Chemical Engineers, elected 2003.

Joel Henry Hildebrand Award in the Theoretical and Experimental Study of Liquids, American Chemical Society, 2007.

Special Issue of *Journal of Physical Chemistry C*, “Keith E. Gubbins Festschrift”, volume **111**, No. 43, eds. Erich A. Müller and Coray M. Colina (2007).

Named one of the "One Hundred Engineers of the Modern Era (Second World War onwards)" who have made significant contributions to the profession and society by the American Institute of Chemical Engineers, June 2008.

Teaching Awards:

Sigma Tau-Tau Beta Pi Award for Excellence in Undergraduate Teaching, College of Engineering, Univ. of Florida, 1968.

Sigma Tau-Tau Beta Pi Award for Excellence in Undergraduate Teaching, College of Engineering, Univ. of Florida, 1974.

Tau Beta Pi Award for Excellence in Undergraduate Teaching, College of Engineering, Cornell University, 1991.

Dean's Award for Excellence in Undergraduate Teaching, Cornell University, 1992.

Class of '79 Honors Award, Cornell University, 1996

Other Awards:

Outstanding Service Award (for Research), University of Florida, 1975.

Alumni Outstanding Research Award, North Carolina State University, 2004.

R.J. Reynolds Award for Excellence in Teaching, Research and Extension, North Carolina State University, 2008

Lectureships:

Reilly Lecturer, Notre Dame University, April 1978.

Lionel A.K. Staveley Lecture, Lisbon, July 15, 1986.

McCabe Lecturer, North Carolina State University, Nov. 10, 1986.

Lindsay Lecturer, Texas A & M University, May 5, 1989.

Gonzalez Lecturer, University of South Florida, April 13, 1990.

B.F. Dodge Lecturer, Yale University, Nov. 8, 1990.

Katz Lecturer, University of Michigan, April 17-20, 1991

Wohl Lecturer, University of Delaware, May 22-24, 1991

Merck Distinguished Lecturer, Rutgers University, April 16-17, 1992

Miles Lecturer, University of Pittsburgh (Chemical Engineering Department), March 2,3, 1995.

Merck Lecturer, University of Puerto Rico (Chemical Engineering Dept.), March 16,17, 1995.

Robb Lecturer, Pennsylvania State University (Chemical Engineering Dept.), January 28, 1997.

James Fair Lecturer, University of Oklahoma (Chemical Engineering Dept.), April 10, 1997.

First Annual Keynote Lecturer in Thermodynamics, Annual American Institute of Chemical Engineers Meeting, Dallas, November 1999.

Keynote Lecturer, International Symposium on Physical Basis of Adsorption, Okayama, Japan, November 10-11, 2000.

Thomas W. Leland Lecturer, Rice University (Chemical Engineering Dept.), March 29, 2001.

Keynote Lecturer, 7th Fundamentals of Adsorption Conference, Nagasaki, Japan, May 23, 2001.

Graduate Association Lecturer for 2004, University of Florida (Chemical Engineering Dept.), March 15, 2004.

Keynote Lecturer, Science and Engineering of Advanced Materials Strategic Workshop, University College Dublin, Ireland, April 25-26, 2005.

Lyman L. Handy Lecturer, Department of Chemical Engineering and Materials Science, University of Southern California, Los Angeles, CA, February 8, 2007.

Thomas Young Distinguished Lecturer, Imperial College London, May 11, 2009.

Taylor & Francis Molecular Physics Lecturer (biannual lectureship award), Imperial College London, September 25, 2009.

Shell Lecturer, Colorado School of Mines, November 18, 2011.

FOMMS Lecturer, FOMMS 2012 Conference, Mt. Hood, Oregon, July 26, 2012.

Rossini Lecturer, International Conference on Chemical Thermodynamics, Buzios, Brazil, August 6, 2012.

Distinguished Seminar Series 2012-2013, The Leader's Forum, Imperial College London, May 1, 2013.

Lennard-Jones Lecturer, University of Manchester, September 4, 2013.

Editorships, Editorial Boards

Editorial Board, Molecular Physics, 1978-1987; 1995-2011.

Editorial Board, Molecular Simulation 1986-.

Regional Editor, North America, Molecular Simulation 1990-2006

Editorial Board, American Institute of Chemical Engineers Journal, 1988-1991

Editor of book series, Topics in Chemical Engineering, Oxford University Press, 1991-2007

Editorial Board, Journal of Chemical Physics, 1996-99

Editorial Board, Adsorption, 1994-2013

Biographies

Who's Who in the World

Who's Who in America

Who's Who in American Education

Who's Who in Finance and Business

Who's Who in Science and Engineering

Invited Lecturer (1975-present) to:

Danish Chemical Society, Copenhagen, March 1975.

Gordon Research Conference on Liquids, 1975.

Fifth Oaxtepec Meeting on Statistical Mechanics, Mexico, 1976.

First International Conference on Fluid Phase Equilibria, Pacific Grove, California, January 1977.

Rutgers Statistical Mechanics Conference, 1978.

Dense Fluids Symposium, Bristol, U.K., April 1979.

Polar Fluids Conference, Aberystwyth, Wales, September 1979.

Second International Conference on Fluid Phase Equilibria, West Berlin, March 1980.

ACS Symposium on Fluid Interfaces, Las Vegas, August 1980.

10th Annual Statistical Physics Conference, Mexico, January 1981.

Lionel Staveley Retirement Meeting, Oxford University, June 1982.

Gordon Research Conference on Chemistry of Interfaces, July 1982.

Chemical Society Symposium on Liquid Mixtures, Hull, U.K., March, 1983.

CCP5 Conference on Molecular Liquids, Hull, U.K., March 1983.

Third International Conference on Fluid Phase Equilibria, Callaway Gardens, Georgia, April, 1983.

Physical Properties Symposium, Chemical Society, Leicester, U.K., January 5, 1984.

Statistical Mechanics of Dense Fluids Meeting, Royal Society of Chemistry, Bristol, U.K., April 10, 1985.

International Chemical Engineering Conference, Coimbra, Portugal, April 15, 1985.

Second Codata Symposium on Critical Evaluation and Prediction of Phase Equilibria in Multicomponent Systems, Paris, September 13, 1985.

- Second Liblice Conference on the Statistical Mechanics of Liquids, Bechyne, Czechoslovakia, May 19, 1986.
- 9th IUPAC Conference on Chemical Thermodynamics, Lisbon, July 15, 1986.
- Conference on Perspectives in Physical Chemistry: The Properties of Molecules in Pores, Imperial College, London, January 15, 1987.
- Conference on Computer Simulation, Kyoto, Japan, March 19, 1987.
- Annual Meeting of the Japanese Chemical Society, Nihon University, Tokyo, April 1, 1987.
- CCP5
- Conference on Industrial Applications of Computer Simulation, Birkbeck College, London, January 7, 1988.
- International Symposium on Thermodynamics in Chemical Engineering and Industry, Beijing, China, May 30-June 2, 1988.
- 6th International Conference on Mixtures of Non-Electrolytes and Intermolecular Interactions, "Carl Schorlemmer" Technical University, Merseburg, German Democratic Republic, August 23-25, 1988.
- 10th IUPAC Conference on Chemical Thermodynamics, Prague, Czechoslovakia, August 29-September 2, 1988.
- Symposium on the Intellectual Foundations of Chemical Engineering, MIT Centennial of Chemical Engineering Education, Brewster, Cape Cod, Massachusetts, Oct 5-7, 1988.
- Fourth International Conference on Thermodynamics of Solutions of Nonelectrolytes, Santiago de Compostela, Spain, Sept. 24-29, 1989.
- IUPAC Symposium on Characterization of Porous Solids, Alicante, Spain, May 6- 9, 1990.
- Third Liblice Conference on Statistical Mechanics of Liquids, Bechyne, Czechoslovakia, May 28-June 1, 1990.
- Fluid Physics Summer School, Aguadulce, Almeria, Spain, August 5-11, 1990.
- Faraday Symposium 26: Molecular Transport in Confined Regions and Membranes, University of Oxford, Dec. 17-18, 1990.
- CCP5 Conference, Molecules in Pores, University of Southampton, UK, April 26, 1991.
- 11th Symposium on Thermophysical Properties, NIST Boulder, June 24-27, 1991.
- Condensed Matter Conference to honor Prof. J.G. Powles, Canterbury, UK, Sept. 5, 1991.
- International Meeting of the Society of Materials Engineering for Resources of Japan, Akita City, Japan, Nov. 5-7, 1991.
- International Symposium on Fractal and Physically Adsorbed Molecular States (Chiba-FP-92), Chemical Society of Japan, Chiba, Japan, May 14-15, 1992.
- IVth International Conference on Fundamentals of Adsorption, Kyoto, Japan, May 17-22, 1992.
- Sixth International Conference on Fluid Properties & Phase Equilibria for Chemical Process Design, Cortina d'Ampezzo, Italy, July 19-24, 1992.
- 12th IUPAC Conference on Chemical Thermodynamics, Snowbird, Utah, August 16-21, 1992.
- AIChE National Meeting, Alpha Chi Award Symposium, Miami Beach, Nov. 2, 1992.
- Materials Research Society Annual Meeting, Symposium on Dynamics in Small Confining Systems, Boston, Nov. 30-Dec. 4, 1992.
- Dense Fluids Meeting, Bristol, U.K., March 25, 1993.
- Conference on Statistical Mechanics of Liquids (in honor of Prof. John Rowlinson's retirement), Oxford, U.K., March 30, 1993.
- Conference on New Directions in Separations, Noordwijkerhout, Netherlands, July 1, 1993.

- International Symposium on Molecular Thermodynamics and Molecular Simulation, Kyoto, January 10-12, 1994.
- Liblice 4 Meeting on Statistical Mechanics of Liquids, Lake Milovoy, Czech Republic, June 6-10, 1994.
- Thermodynamics 95 Conference, Reading, U.K., April 5-7, 1995. [plenary lecture]
- Fifth Fundamentals of Adsorption Conference, Asilomar, CA, May 14-18, 1995.
- CECAM (Centre Européen de Calcul Atomique et Moléculaire) Workshop on Adsorption, Phase Transitions and Transport in Porous Materials, Lyon, France, September 11-15, 1995.
- International Conference on Molecular Modeling in the Oil and Gas Sciences, Institut Français du Pétrole, Paris, France, October 23-24, 1995.
- NATO-ASI Meeting on Physical Adsorption, Nice, France, May 18-30, 1996.
- IUPAC Chemical Thermodynamics Conference, Osaka, Japan, August 26-30, 1996.
- International Conference on Advances in Chemical Engineering, Madras, India, December 11-13, 1996.
- International Symposium on Molecular Thermodynamics and Molecular Simulation (MTMS'97), Hosei University, Japan, Jan. 12-15, 1997.
- Thermodynamics '97 Conference, University of Surrey, U.K., April 16-18, 1997.
- Conference on Physical Chemistry of Surface Phenomena, Polish Chemical Society, Krakow, Poland, June 9-10, 1997.
- "Molecular Modeling of Selective Adsorption from Mixtures", Annual Meeting of the Materials Research Society, Boston, December 4, 1997.
- "Fluid Phase Separation in Controlled Pore Glasses", 78th Statistical Mechanics Conference, Rutgers University, Dec. 14, 1997.
- "Freezing in Pores: Simulation and Experiment", Fifth Liblice Conference on the Statistical Mechanics of Liquids, Zelezná Ruda, Czech Republic, June 8, 1998.
- "Recent Advances in Molecular Simulation Methods: Phase Equilibria in Bulk and Confined Systems", International Conference on Thermal Properties, Kyushu University, Fukuoka, Japan, October 21, 1998.
- "Molecular Modeling: Applications to Chemical Engineering", Conference on Molecular Modelling: A Tool for the Modern Era, St. Bartholomew's Hospital, London, December 14, 1998.
- "Phase Transitions in Pores: Molecular Simulation and Experimental Results", with M. Sliwinska-Bartkowiak, L.D. Gelb and R. Radhakrishnan, Annual Meeting of the American Chemical Society, Anaheim, CA, March 21-25, 1999.
- "Molecular Modeling of Adsorption in Amorphous Nano-Porous Materials", with L.D. Gelb, Annual Meeting of the American Chemical Society, Anaheim, CA, March 21-25, 1999.
- "Molecular Simulation: Phase Equilibria and Confined Systems", International Workshop on Scientific Computing in Chemical Engineering II, Hamburg, Germany, May 26-28, 1999.
- "Density Functional Theory and the Pore Size Distribution", with C. M. Lastoskie, Characterization of Porous Solids V, Heidelberg, Germany, May 30-June 2, 1999.
- "Thermodynamics of Confined Nano-Phases", First Annual Keynote Lecture in Thermodynamics, American Institute of Chemical Engineers Meeting, Dallas, November 1, 1999.
- "Molecular Simulation as a Tool in Modeling Nano-Porous Materials and Adsorption", American Institute of Chemical Engineers Meeting, Dallas, November 1, 1999.
- "Molecular Modeling of Amorphous Nano-Porous Materials", Fourth Annual Materials Modeling Meeting, University of the North, Pietersburg, South Africa April 11, 2000.

- “Improved Molecular Models of Amorphous Nano-Porous Materials for Characterization”, 2nd International Workshop on Characterization of Porous Materials, Princeton, NJ, June 19-21, 2000.
- “Molecular Simulation: Some Recent Applications to Phase and Chemical Equilibria”, First International Conference on Foundations of Molecular Modeling and Simulation (FOMMS 2000), Keystone, Colorado, July 23-28, 2000.
- K.E. Gubbins, R. Radhakrishnan and M. Sliwinska-Bartkowiak, “Understanding Freezing Behavior in Porous Materials: Comparison Between Simulation and Experiment”, International Discussion Meeting on Physical Chemistry in Confining Geometries: From Single Molecules to Mesoscopic Systems, Berlin, Germany, September 20-22, 2000.
- “Improved Molecular Models for Adsorption in Porous Carbons”, International Conference on Colloid and Surface Science, Chemical Society of Japan, Tokyo, November 5-8, 2000.
- “Molecular Modeling of Confined Nano-Phases in Disordered Porous Materials”, International Symposium on Physical Basis of Adsorption, Okayama, Japan, November 10-11, 2000.
- “Applications and Opportunities in Separations and Reaction Equilibria”, American Institute of Chemical Engineers Annual Meeting, Los Angeles, November 13, 2000.
- Keynote Lecturer, 7th Fundamentals of Adsorption Conference, Nagasaki, Japan, May 23, 2001.
- "Freezing Behavior in Porous Materials: Simulation and Experiment", CECAM Workshop on Phase Transitions in Complex Confined Systems, Lyon, France, August 22, 2001.
- “Summary: Phase Transitions in Complex Confined Systems”, CECAM Workshop on Phase Transitions in Complex Confined Systems, Lyon, France, August 24, 2001.
- "Realistic Molecular Models for Porous Carbons", 4th International Symposium on Surface Heterogeneity in Adsorption and Catalysis, Krakow, Poland, August 27, 2001.
- “Chemical Reactions in Pores”, Statistical Mechanics of Adsorption Conference (in honor of the retirement of David Nicholson), Imperial College London, October 3, 2001.
- “Freezing in Narrow Pores”, 5th Liquid Matter Conference of the European Physical Society, Konstanz, Germany, September 14-18, 2002.
- “Phase Transitions and Chemical Reactivity at the Nanoscale: Effects of Confinement”, Plenary Lecture, American Institute of Chemical Engineers Annual Meeting, Indianapolis, November 5, 2002.
- “Improved Molecular Models for Nano-Porous Materials”, American Institute of Chemical Engineers Annual Meeting, Indianapolis, November 6, 2002.
- “Effects of Confinement on Freezing”, JC2003 Conference on Molecular Thermodynamics, Instituto Superior Tecnico, Lisbon, Portugal, January 6, 2003.
- “Molecular Modeling of Confined Nano-Phases in Activated Carbons”, 2nd International Workshop on Dynamics in Confinement, Institut Laue-Langevin, Grenoble, France, January 22-25, 2003.
- “Phase Transitions and Chemical Reactions at the Nano-Scale: Effects of Confinement”, Plenary Lecture, Thermodynamics 2003 Conference, Cambridge, U.K., April 9-11, 2003.
- “Molecular Modeling of Nano-Porous Materials and Confined Fluids”, American Chemical Society Annual Meeting, New York, NY, September 11, 2003.
- “Adsorption and Diffusion in Highly Disordered Microporous Carbons: Molecular Simulation vs. Experiment”, Materials Research Society Annual Meeting, Boston, December 4, 2003.
- “The SAFT Equation: History and Recent Advances”, keynote lecture for the International Symposium “15 Years of SAFT”, Barcelona, December 12, 2003.

- “Phase Transitions and Chemical Reactions at the Nanoscale: Effects of Confinement”, American Chemical Society National Meeting, Anaheim, CA, March 30, 2004.
- “Thermodynamics of Confined Fluids in Porous Carbons”, ISAIE 2004 (Ice, Soot and Aviation International Conference), La Londe, France, May 10-14, 2004
- “Phase Transitions and Chemical Reactions at the Nano-Scale: Effects of Confinement”, European/Japanese Molecular Liquids Group Conference on “Complex Liquids: Fundamental Properties to Industrial Applications”, Sheffield, U.K., September 3-7, 2004.
- “Application of Molecular Simulation to Study Nano-Porous Materials”, First International Symposium on Functional Innovation of Molecular Informatics”, Fukuoka, Japan, October 13-15, 2004.
- “Application of Molecular Simulation to Study Nano-Porous Materials”, Annual Meeting of American Institute of Chemical Engineers, Austin, Texas, November 7-12, 2004 (Plenary Lecture).
- “Effects of Confinement on Phase Transitions and Chemical Reactions”, 14th Ostwald-Kolloquium on Fluids at Interfaces and in Pores: Phase Transitions and Related Phenomena, a colloquium on behalf of the 66th birthday of Gerhard Findenegg, November 22-23, 2004, Berlin, Germany (Plenary Lecture).
- “Phase Transitions and Chemical Reactions at the Nano-Scale: Effects of Confinement”, First Indo-US Joint Meeting in a Global Environment, organized by the Indian Institute of Chemical Engineers and the American Institute of Chemical Engineers, Mumbai, India, December 28-30, 2004 (Plenary Lecture).
- “Molecular Modelling and Simulation of Advanced Materials”, Keynote Lecture, Science and Engineering of Advanced Materials Strategic Workshop, University College Dublin, Ireland, April 25-26, 2005.
- “Effect of Confinement on Chemical Reaction”, 93rd Statistical Mechanics Conference, Rutgers University, May 16th, 2005.
- “Phase Transitions and Chemical Reactions at the Nano-Scale: Effects of Confinement”, First US-China Workshop on Sustainable Resources, Energy and Materials – A Challenge to Chemical Engineers, Beijing, August 10-12, 2005.
- “Effects of Confinement on Chemical Reactivity”, DuftyFest2005: A Celebration to Honor Jim Dufty on his 65th Birthday, University of Florida, September 22-24, 2005.
- “Modeling Porous Carbons by Constrained Reverse Monte Carlo Methods”, S.K. Jain, J.P. Pikunic, R. J-M. Pellenq and K.E. Gubbins, International Conference on Carbon for Energy Storage and Environmental Protection (CESEP), Orléans, France, October 2-6, 2005. (Keynote Lecture).
- “Effects of Confinement on Chemical Reactivity”, Pacificchem, International Chemical Congress of Pacific Basin Societies, Honolulu, Hawaii, December 15-20, 2005 (Keynote Lecture)
- “Structural Modeling of Porous Carbons using a Hybrid Reverse Monte Carlo Method”, 4th Pacific Basin Conference on Adsorption Science & Technology, Tianjin, China, May 23, 2006.
- “Molecular Modeling of Porous Carbons Using Hybrid Reverse Monte Carlo”, TRI Princeton Workshop on Characterization of Porous Solids”, Princeton, NJ, June 21, 2006.
- “Confinement Effects on Chemical Reactions – Toward an Integrated Rational Catalyst Design”, U.S. – Poland Workshop on Nanoscience and Nano-Structured Materials, Poznan, Poland, June 26-28, 2006.

- “Confinement Effects on Chemical Reactions – Towards an Integrated Rational Catalyst Design”, Sixth International Symposium on Surface Heterogeneity Effects in Adsorption and Catalysis on Solids, Zakopane, Poland, August 28-September 2, 2006.
- “Modeling Chemical Reactivity: Effects of Confinement”, Annual Meeting of the American Institute of Chemical Engineers, San Francisco, November 12-17, 2006 [symposium in memory of Professor Koichiro Nakanishi].
- “Effects of Confinement on Freezing and Melting”, Annual Meeting of the American Institute of Chemical Engineers, San Francisco, November 12-17, 2006 [symposium in honor of Carol Hall’s 60th birthday].
- “Effects of Confinement on Freezing and Melting”, International Conference on Frontier Science and Technology of Nanoporous Systems 3, Chiba University, Japan, January 27, 2007 [in honor of Professor Katsumi Kaneko’s 60th birthday]
- “Confinement Effects on Chemical Reactions – Towards an Integrated Rational Catalyst Design”, American Chemical Society Annual Meeting, Chicago, March 27, 2007.
- “Molecular Modeling of Adsorption in Porous Carbons”, International Conference on Adsorption, in honor of Ken Sing, Bristol, U.K., April 12, 2007.
- “Molecular Modeling of Porous Carbons Using Reverse Monte Carlo and Grand Canonical Monte Carlo Simulations”, S.K. Jain, K.E. Gubbins and R-J.M. Pellenq, 9th International Conference on Fundamentals of Adsorption, Giardini Naxos, Sicily, Italy, May 20-25, 2007.
- ”Surface Nanostructure and Catalysis: The Role of Confinement and Surface Chemistry”, Center for Nanophase Materials Sciences 2007 Users’ Meeting, Oak Ridge National Laboratory, October 10, 2007. (Plenary Lecture)
- “Confinement Effects on Chemical Reactions: Towards an Integrated Rational Catalyst Design”, Molecular Modelling 2007, Melbourne, Australia, November 27-30, 2007. (Plenary Lecture)
- ”Surface Nanostructure, Diffusion and Catalysis: The Role of Confinement and Surface Chemistry”, Second NSF US/Poland Workshop, Gdansk, Poland, June 3-6, 2008.
- “Multi-Scale Modeling of Matter: A Graduate Course”, 20th International Conference on Chemical Thermodynamics, Warsaw, Poland, August 3-8, 2008.
- “Molecular Modeling of Matter: Impact and Prospects in Engineering”, Distinguished Lecture Series, Reynolds Award Lecture, College of Engineering, North Carolina State University, November 5, 2008.
- “Molecular Simulation as a Foundation for Engineering Models: Impact and Prospects”, American Institute of Chemical Engineers Annual Meeting, Philadelphia, November 16-21, 2008.
- “Surface Nanostructure, Diffusion and Catalysis: The Role of Confinement and Surface Chemistry”, American Institute of Chemical Engineers Annual Meeting, Philadelphia, November 16-21, 2008.
- “Surface Nanostructure, Diffusion and Catalysis: The Role of Confinement and Surface Chemistry”, Festcollquium: SSNI Symposium “Self-Assembled Soft-Matter Nanostructures at Interfaces”, Technische Universität Berlin, Berlin, Germany, February 20, 2009.

- “Surface Nanostructure, Diffusion and Catalysis: The Role of Confinement and Surface Chemistry”, American Chemical Society Annual Meeting, Salt Lake City, March 22, 2009.
- “Transition from Single-File to Fickian Diffusion in Carbon Nanotube Structures”, 5th Pacific Basin Conference on Adsorption Science & Technology, Singapore, May 25, 2009.
- “Crossover from Single-File to Fickian Diffusion in Carbon Nanotubes and Nanotube Bundles: Pure Components and Mixtures”, Diffusion Fundamentals III, Athens, Greece, August 24, 2009.
- “Molecular Modeling of Disordered Micro-Porous Carbons: Atomistic Models, Adsorption and diffusion”, 8th Torunian Carbon Symposium: Fabrication, Modification and Investigations of Novel Forms of Carbon, Torun, Poland, September 3-6, 2009.
- “The Theory of Non-Electrolyte Solutions: A Recent History”, Taylor & Francis Molecular Physics Lecturer (biannual lectureship award), Imperial College London, September 25, 2009.
- “Transitions between Single-File and Fickian Self-Diffusion for Fluids Confined in Carbon Nanotubes, Bundles and Activated Carbon”, 10th Symposium of Computational Chemistry in China (SCCC2009), Hangzhou, China, October 23-25, 2009.
- “Molecular Modeling of Matter at the Nanoscale: Impact and Prospects”, Hong Kong University, Public Lecture, Hong Kong, December 8, 2009.
- “Transitions between Single-File and Fickian Self-Diffusion for Fluids Confined in Carbon Nanotubes, Bundles and Disordered Carbons”, Advances in Theoretical and Computational Chemistry Workshop, Hong Kong, December 11, 2009.
- “Life in Confinement: Phase Transitions, Diffusion and Reaction in Nano-pores”, NSF Workshop on Molecular Models of Carbon-Neutral Industrialization, University of California at Riverside Palm Desert Graduate Center, Palm Desert, CA, April 9-10, 2010.
- “Life in Confinement: The Role of Molecular Modeling”, 12th International Conference on Properties and Phase Equilibria for Product and Process Design, Suzhou, China, May 16-21, 2010.
- “Under Pressure: High Pressure Effects in Nanopores”, Yun Long, Jeremy C. Palmer, Benoit Coasne, Małgorzata Śliwinska-Bartkowiak and Keith E. Gubbins, 3rd U.S.-Poland Workshop: Nanoscale Phenomena in Materials and at Interfaces, Krakow, Poland, June 6-10, 2010.
- “Under Pressure: High Pressure Effects in Nanopores”, 8th Liblice Conference on the Statistical Mechanics of Liquids, Brno, Czech Republic, June 13-17, 2010.
- “Under Pressure: High Pressure Effects in Nanopores”, IGRTG Second Annual Workshop, Berlin, Germany, July 25-27, 2010.
- “Under Pressure: Quasi-High Pressure Effects in Nano-Pores”, International Materials Research Congress, IMRC XIX, Cancún, México, August 15-20, 2010.
- “The Origin of SAFT”, SAFT 2010 Symposium: 20 Years of the SAFT Equation, Barcelona, Spain, September 19-21, 2010. (Keynote Lecture).
- “Thermodynamics and Dynamics of Confined Nano-Phases”, K.E. Gubbins, American Institute of Chemical Engineers Annual Meeting, Salt Lake City, Utah, November 7-12, 2010. (Plenary Lecture)

- “Quasi-High Pressure Effects in Nanopores”, Y. Long, J.C. Palmer, B. Coasne, M. Sliwinski-Bartkowiak and K.E. Gubbins, American Institute of Chemical Engineers Annual Meeting, Salt Lake City, Utah, November 7-12, 2010.
- “Thermodynamics and Dynamics of Confined Nano-Phases”, International Symposium on Recent and Emerging Advances in Chemical Engineering (REACH), Indian Institute of Technology Madras, Chennai, India, December 2-4, 2010.
- “The Institute for Computational Science & Engineering”, ICSE External Advisory Board Annual Meeting, North Carolina State University, Raleigh, NC, April 14, 2011.
- “Under Pressure: Quasi-High Pressure Effects in Nanopores”, IGRTG Colloquium, Technical University of Berlin, Berlin, Germany, May 17, 2011.
- “High Pressure Effect and Material Deformation due to Confined Nanophases”, Compliant Solids Workshop, Chimie Paris Tech, Paris, June 9-11, 2011.
- “Molecular Simulation: Methods and Applications”, Zhejiang University, Hangzhou, China, November 1, 2011.
- “Pressure Enhancement in Nanopores and Effects on Adsorbent Structure”, Characterization of Porous Materials: From Angstroms to Millimeters, Delray Beach, FL, April 30-May 2, 2012. [Keynote Lecture]
- “High Pressure Effects and Material Deformation due to Confined Nanophases”, Symposium on Recent Advances in Materials Physics, in Honor of Jerzy Bernholc 60th Birthday, North Carolina State University, May 5, 2012.
- “High Pressure Effect and Material Deformation due to Adsorption”, 6th Pacific Basin Conference on Adsorption Science and Technology, Taipei, Taiwan, May 20-23, 2012.
- “Under Pressure: Quasi-High Pressure Effects in Nanopores”, Third Symposium on Future Challenges for Carbon-Based Nanoporous Materials – Adsorption and Energy, Shinshu University, Nagano, Japan, May 26-28, 2012.
- “Pressure Enhancement in Nanopores and Effects on Adsorbent Structure”, 4th U.S.-Poland Workshop on Interfacial Phenomena at the Nanoscale: Fluids and Soft Matter, Poznan, Poland, June 20-24, 2012.
- “Pressure Enhancement in Nanopores and Effects on Adsorbent Structure”, Professor Nick Quirke’s 60th Birthday Symposium, Imperial College London, July 6th, 2012.
- “Molecular Modeling and Simulation of Confined Nano-Phases”, FOMMS Lecture, FOMMS 2012 Conference, Resort at the Mountain, Mount Hood, Oregon, July 26, 2012.
- “Thermodynamics of Confined Nano-Phases”, Rossini Lecture, International Conference on Chemical Thermodynamics, Buzios, Brazil, August 6, 2012.
- “Under Pressure: Quasi-High Pressure Effects in Nano-Pores”, 8th International Symposium on Surface Heterogeneity Effects in Adsorption and Catalysis on Solids, Krakow, Poland, August 27, 2012 (Keynote Lecture).
- “Thermodynamics of Confined Nano-Phases”, Equifase 2012, IX Iberoamerican Conference on Phase Equilibria and Fluid Properties for Process Design, Puerto Varas, Chile, October 8-12, 2012 (Keynote Lecture).
- “Thermodynamics and Dynamics of Confined Nano-Phases: The Role of Molecular Simulation”, Escuela “Giorgio Zgrablich”, Universidad Nacional San Luis, San Luis, Argentina, February 17, 2013.
- “Pressure Enhancement in Nanopores and Effect on Adsorbent Structure”, Quantachrome Instruments Corp., Boynton Beach, Florida, March 27, 2013.

- “The Pressure Tensor in Nanopores and its Effect on Adsorbent Structure”, Workshop on Adsorption in Compliant Solids, Chemie Paris Tech, Paris, France, June 5-7, 2013.
- “Thermodynamics and Dynamics of Confined Nano-Phases: The Role of Molecular Simulation”, Workshop on Molecular Interactions and Nanobiological Applications, University of São Paulo, Ribeirao Preto, São Paulo, Brazil, June 25, 2013.
- “Thermodynamics of Confined Nano-Phases”, Lennard-Jones Lecture, Thermodynamics 2013 Conference, University of Manchester, U.K., September 4, 2013.
- “The Theory of Polar Liquids and their Mixtures: A Historical Review”, Third Poznań Symposium on Quantum Engineering, Information and Non-Linear Optics, Adam Mickiewicz University, Poznań, Poland, October 15-17, 2013. (Keynote Lecture)
- “Thermodynamics of Confined Nanophases”, Discussion Meeting on Molecular Simulation of Fluids at Interfaces”, Indian Institute of Science, Bangalore, April 24, 2014.
- “Wetting at the Nanoscale”, Annual Meeting of IRTG 1524 Group: Self-Assembled Soft-Matter Nanostructures at Interfaces, Potsdam, Germany, June 6-8, 2014.
- “Thermodynamics of Confined Nanophases: The Role of Wetting”, 5th US-Poland Workshop, Thermodynamics of Complex Fluids and Interfaces, Warsaw, Poland, June 11-13, 2014.
- “Theory of the Thermodynamics of Polar and Associating Liquids: A Historical Review”, 9th Liblice Conference on Statistical Mechanics of Liquids, Sec, Czech Republic, June 15-20, 2014.
- “Wetting at the Nano-Scale”, 17th National Symposium on Chemical Thermodynamics and Thermal Analysis, Hangzhou, China, October 18-20, 2014. [Keynote Lecture]
- “Wetting at the Nano-Scale”, Symposium to Honor Peter Cummings, Annual Meeting of the American Institute of Chemical Engineers, Atlanta, GA, November 17, 2014.
- “Theory of the Thermodynamics of Polar and Associating Liquid Mixtures: A Historical Review”, SAFT Houston 2015, 25th Anniversary Celebration of the Statistical Associating Fluid Theory, Rice University, Houston, TX, May 17-19, 2015. [Keynote Lecture]
- “Corresponding States Theory of Adsorbed Films: Influence of Wetting and Wall Roughness”, 9th International Symposium on Surface Heterogeneity Effects in Adsorption and Catalysis on Solids (ISSHAC-9), Wroclaw, Poland, July 18-22, 2015.
- “Corresponding States Theory of Adsorbed Films: Influence of Wetting and Wall Roughness”, 2015 Workshop on the International Research Network GdRi-M2UN. A Joint Micromeritics/M.I.T./CNRS Event, M.I.T., Cambridge, MA, August 26-28, 2015.
- “Corresponding States Theory of Adsorbed Films”, Yun Long, An Rong, Cody K. Addington, Małgorzata Śliwinska-Bartkowiak, Matthias Thommes and Keith E. Gubbins, 7th Pacific Basin Conference on Adsorption Science and Technology, Xiamen, China, 24-27 September, 2015.
- “Corresponding States Theory of Adsorbed Films: Influence of Wetting and Wall Roughness”, Keith E. Gubbins, An Rong, Cody K. Addington, Małgorzata Śliwinska-Bartkowiak and Matthias Thommes, American Institute of Chemical Engineers Annual Meeting, Salt Lake City, UT, November 8-13, 2015.

Invited Seminars (1973-present):

National Bureau of Standards, Boulder, Colorado, Oct. 17, 1973.
 Clarkson College (Chemical Engineering Dept.), Potsdam, New York.
 University of Guelph (Physics Dept.), Ontario, Canada, Dec. 11, 1973.
 Rice University (Chemical Engineering Dept.), Houston, Texas, Feb. 14, 1974.
 University of Houston (Chemical Engineering Dept.), Houston, Texas, Feb. 15, 1974.
 University of Wisconsin (Chemical Engineering Dept.), Madison, March 6, 1974.
 University of Kent (Physics Dept.), Canterbury, England, July 10, 1974.
 Cornell University (Chemical Engineering Dept.), Ithaca, New York, Nov. 11, 1974.
 University of Virginia (Chemical Engineering Dept.), Charlottesville, Dec. 5, 1974.
 Danish Technical University (Chemical Engineering Dept.), Copenhagen, Denmark, March 18, 1975.
 Danish Chemical Society, Oersted Institute, Copenhagen, Denmark, March 20, 1975.
 University of Florida (Chemistry Dept.), Gainesville, April 15, 1975.
 University of Florida (Engineering Science and Mechanics Dept.), May 9, 1975.
 University of California at Los Angeles (Chemistry Dept.), Los Angeles, Nov. 19, 1975.
 University of Oklahoma (Chemical Engineering Dept.), Norman, Nov. 21, 1976.
 Cornell University (Chemical Physics Group), Ithaca, New York, Sept. 28, 1976.
 U.S. Military Academy (Chemistry and Physics Depts.), West Point, Oct. 26, 1976.
 University of Minnesota (Chemical Engineering Dept.), Minneapolis, March 4, 1977.
 University of Guelph (Physics Dept.), Ontario, Canada, March 15, 1977.
 Texas A & M University, College Station, March 22, 1977.
 University of Karlsruhe, Germany, June 20, 1977.
 University of Heidelberg, Germany, June 22, 1977.
 University of Bochum, Germany, June 24, 1977.
 University of Rochester (Chemical Engineering Dept.), Rochester, New York, Sept. 29, 1977.
 University of Pennsylvania (Chemical Engineering Dept.), Philadelphia, Nov. 28, 1977.
 Rennselaer Polytechnic Institute (Chemical Engineering Dept.), Troy, New York, Oct. 29, 1977.
 Purdue University (Chemical Engineering Dept.), West Lafayette, Indiana, Feb. 23, 1978.
 Princeton University (Chemical Engineering Dept.), Princeton, New Jersey, April 12, 1978.
 National Research Council (Chemistry Division), Ottawa, Canada, Aug. 22, 1978.
 Clemson University (Chemical Engineering Dept.), Clemson, South Carolina, Feb. 2, 1979.
 Mobil Research and Development Corporation, Paulsboro, New Jersey, Feb. 22, 1979.
 Massachusetts Institute of Technology (Chemical Engineering Dept.), Cambridge, Feb. 23, 1979.
 Syracuse University (Chemical Engineering Dept.), Syracuse, New York, March 6, 1979.
 University of Guelph (Physics Dept.), Ontario, Canada, July 4, 1979.
 University of Sheffield (Chemistry Dept.), Sheffield, England, Nov. 7, 1979.
 Cambridge University (Dept. of Theoretical Chemistry), Cambridge, England, Jan. 16, 1980.
 Oxford University (Physical Chemistry Laboratory), Oxford, England, Jan. 21, 1980.
 University of Duisburg (Thermodynamics Institute, Duisburg, West Germany, March 13, 1980.
 University of Trento (Physics Dept.), Italy, April 15, 1980.
 Free University of the Ruhr (Joint to Institutes of Applied Thermodynamics and Institute of Physical Chemistry), Bochum, West Germany, April 18, 1980.
 Instituto Superior Tecnico, Lisbon, Portugal, June 30, 1980.
 University of Coimbra, Portugal, July 3, 1980.
 University of Kent (3 lectures, Physics Dept.), Canterbury, England, July 10, 11, 1980.

University of Bristol (Physics Dept.), Bristol, England, July 15, 1980.

University of Illinois at Chicago Circle (Dept. of Energy Engineering), Chicago, Illinois, Feb. 6, 1981.

University of Florida (Chemical Engineering Dept.), Gainesville, Feb. 27, 1981.

Union Carbide Corporation, Charleston, West Virginia, Sept. 24, 1981.

University of California (Chemical Engineering Dept.), Berkeley, May 3, 1982.

Stanford University (Chemical Engineering Dept.), Stanford, California, May 23, 1982.

University of California (Chemical Engineering Dept.), Berkeley, California, May 19, 1982.

IBM, San Jose, California, May 24, 1982.

University of California (Chemical Engineering Dept.), Los Angeles, May 26, 1982.

California Institute of Technology (Chemical Engineering Dept.), Pasadena, May 27, 1982.

Process Simulation International, Fullerton, California, May 28, 1982.

University of Bristol (Physics Dept.), Bristol, U.K., July 2, 1982.

Pennsylvania State University (Chemical Engineering Dept.), College Park, Oct. 19, 1982.

University of California at San Diego (Chemistry Dept.), Jan. 20, 1983.

University of Southern California (Chemical Engineering Dept.), Los Angeles, Jan. 21, 1983.

Universite Libre de Bruxelles, (Physics Dept.) Belgium, March 25, 1983.

State University of New York at Buffalo (Chem. Eng. Dept.), April 27, 1983.

National Bureau of Standards, Boulder, May 12, 1983.

University of Massachusetts (Chemical Engineering Dept.), Oct. 6, 1983.

Clarkson College of Technology (Chemical Engineering Dept.), Oct. 25, 1983.

Instituto Superior Tecnico, Lisbon (Chemical Engineering Dept.), Nov. 11, 1983.

Universidade de Coimbra, Portugal (Chemical Engineering Dept.), Nov. 17, 1983.

Universidade de Coimbra, Portugal (Chemistry Dept.), Nov. 18, 1983.

University of Guelph (Physics Dept.), Feb. 14, 1984.

Johns Hopkins University (Chemical Engineering Dept.), April 16, 1984.

Ecole des Mines, Paris, June 19, 1984.

University of Virginia (Chemical Engineering Dept.), October 18, 1984.

Rennselaer Polytechnic Inst. (Chemical Engineering Dept.), Nov. 14, 1984.

Cornell University (Materials Science and Engineering Department), Feb. 21, 1985.

Universidad Autonoma, Madrid (Institute for Solid State Physics), April 19, 1985.

Exxon Research and Engineering Co., Clinton, NJ, Oct. 25, 1985.

Massachusetts Institute of Technology (Chemical Engineering Dept.), Nov. 22, 1985.

Unilever Research, Port Sunlight Laboratory, U.K. Dec. 11, 1985.

University of Southampton, U.K., Chemistry Department, Dec. 13, 1985.

Princeton University (Chemical Engineering Dept.) Jan. 8, 1986.

Instituto Superior Tecnico (Chemistry Dept.), Lisbon, Feb. 25, 1986.

University of Dortmund (Chemical Engineering), Dortmund, West Germany, Oct. 17 & 18, 1986.

North Carolina State University (Chemical Engineering Dept.), Nov. 10, 1986.

Imperial College (Chemical Engineering Dept.), Dec. 3, 1986.

University of Kent (Physics Dept.), Canterbury, U.K., Jan. 21, 1987.

University of Bristol (Chemistry Dept.), Bristol, U.K., Feb. 10, 1987.

University of Cambridge (Chemistry Dept.), Cambridge, U.K., Feb. 18, 1987.

University of Oxford (Physical Chemistry Laboratory), Oxford, U.K., March 2, 1987.

Kyoto University (Dept. of Molecular Engineering), Kyoto, Japan, March 21, 1987.

Institute for Molecular Science, Okazaki, Japan, March 23, 1987.
 University of Karlsruhe (Institute for Physical Chemistry), Karlsruhe, West Germany, May 11, 1987.
 Ruhr University (Institute for Physical Chemistry), Bochum, West Germany, May 12, 1987.
 Leningrad State University (Chemistry Dept.), Leningrad, USSR, June 3, 1987.
 Institute for Low Temperature Physics & Engineering, Academy of Sciences of the Ukr SSR, Kharkov, USSR, June 10, 12, 1987.
 University of Bradford (School of Chemical Engineering), Bradford, U.K., June 26, 1987.
 University of Wisconsin (Chemical Engineering Dept.), Madison, Wisconsin, November 11, 1987.
 University of Minnesota (Chemical Engineering Dept.), Minneapolis, Minn., Feb. 9, 1988.
 McGill University (Chemical Engineering Dept.), Montreal, Feb. 19, 1988.
 University of Pennsylvania (Chemical Engineering Dept.), Philadelphia, April 11, 1988.
 University of Hokkaido (Chemistry Dept.), Sapporo, Japan, May 27, 1988.
 Tsinghua University (Chemical Engineering Dept.), Beijing, China, May 31, 1988.
 Linde Division, Union Carbide, Tonawanda, NY, Nov. 23, 1988.
 Institute for Low Temperature Physics & Engineering, Academy of Sciences UkrSSR, Kharkov, USSR, Dec. 14, 1988.
 Purdue University (Chemical Engineering Dept.), West Lafayette, IN, Feb. 9, 1989.
 University of Maryland (Joint to Statistical Physics and Chemical Engineering), Feb. 14, 1989.
 Simon Bolivar University, (Chemical Engineering Dept.), Caracas, Venezuela, March 17, 1989.
 Instituto Venezolano Investigaciones Cientificas (Centro de Fisica), Caracas, Venezuela, March 21, 1989.
 University of Texas, Austin (Chemical Engineering Dept.), April 18, 1989.
 Rice University (Chemical Engineering Dept.), Houston, TX, April 20, 1989.
 Shell Development Company, Westhollow Lab., Houston, TX, April 21, 1989.
 Texas A&M University (Chemical Engineering Dept.), College Station, TX (Lindsay Lecture), May 5, 1989.
 University of Duisburg (Thermodynamics Institute), Duisburg, West Germany, May 12, 1989.
 Tokyo Metropolitan University (Dept. of Industrial Chemistry), Tokyo, Japan, June 29, 1989.
 Brunel University (Chemistry Dept.), Uxbridge, Middx., UK, Sept. 20, 1989.
 Exxon Research & Engineering, Clinton, NJ, October 18, 1989.
 BP Research, Sunbury-on-Thames, UK, December 15, 1989.
 Rennselaer Polytechnic Institute (Chemical Engineering Dept.), Troy, NY, Jan. 31, 1990.
 Kyoto University (Industrial Chemistry Dept.), Kyoto, Japan, March 19, 1990.
 Kyushu University (Chemical Engineering Dept.), Fukuoka, Japan, March 22, 1990.
 Hong Kong University (Chemistry Dept.), Hong Kong, March 29, 1990.
 University of South Florida (Juan O. Gonzalez Lecture, Chemical Engineering Dept.), April 13, 1990.
 Australian National University (Chemistry Dept.), June 29, 1990.
 University of Queensland (Chemical Engineering Dept.), July 4, 1990.
 Yale University (Chemical Engineering Dept.), Nov. 8, 1990.
 Instituut voor Atoom-en Molecuulfysica, Amsterdam, Dec. 10, 1990.
 Koninklijke Shell Laboratorium, Amsterdam, Dec. 11, 1990.
 University of Amsterdam (Department of Chemistry), Dec. 11, 1990.

Institute for Low Temperature Physics & Engineering, Academy of Sciences Ukr. SSR, Kharkov, USSR, January 8, 1991.
 Institute for Theoretical Physics, Academy of Sciences Ukr SSR, Kiev, USSR, January 10, 1991.
 Hokkaido University (Chemistry Department), Sapporo, Japan, March 19, 1991.
 Chiba University (Chemistry Department), Chiba, Japan, March 20, 1991.
 University of Michigan (Katz Lectures in Chemical Engineering), April 18 & 19, 1991.
 Notre Dame University (Chemical Engineering Dept.), May 7, 1991.
 Iowa State University (Chemical Engineering Dept.), May 9, 1991.
 University of Delaware (Wohl Lectures in Chemical Engineering), May 23, 24, 1991.
 Mobil Central Research Laboratory, Princeton, June 10, 1991.
 Exxon Chemical Co., Baton Rouge, LA, Oct. 14, 1991.
 National University, Singapore (Chemical Engineering Dept.), Nov. 11, 1991.
 Chiba University (Chemistry Dept.), Japan, Jan. 9, 1992.
 Chiba University (Chemistry Dept.), Japan, Jan. 10, 1992.
 University of Rochester (Chemical Engineering Dept.), Jan. 29, 1992.
 University of California, San Diego (Dept. of Applied Mechanics and Engineering Sciences), Feb. 5, 1991.
 University of California, Santa Barbara (Chemical Engineering Dept.), Feb. 6, 1991.
 University of California, Los Angeles (Chemical Engineering Dept.), Feb. 7, 1991.
 University of California, Berkeley (Chemical Engineering Dept.), Feb. 10, 1991.
 Rutgers University (Chemical Engineering Dept.), Merck Lecture, April 16, 1992.
 Hong Kong University (Chemistry Dept.), May 25, 1992.
 Tulane University (Chemical Engineering Dept.), Oct. 2, 1992.
 University of Illinois at Chicago Circle, January 15, 1993.
 University of Wisconsin, Madison (Chemical Engineering Dept.), First Hougen Lecture, January 28, 1993.
 University of Wisconsin, Madison (Chemical Engineering Dept.), Second Hougen Lecture, February 4, 1993.
 University of Illinois, Urbana (Chemical Engineering Dept.), February 16, 1993.
 Imperial College of Science, Technology and Medicine (Chemical Engineering Department), London, March 24, 1993.
 Australian National University (Research School of Chemistry), Canberra, April 6, 1993.
 University of Wisconsin, Madison (Chemical Engineering Dept.), Third Hougen Lecture, April 22, 1993.
 University of Wisconsin, Madison (Chemical Engineering Dept.), Fourth Hougen Lecture, April 29, 1993.
 Poznan University, Poland (Institute of Physics), May 17, 1993.
 Institute of Catalysis, Polish Academy of Sciences, Krakow, May 20, 1993.
 Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, May 21, 1993.
 University of Technology, Delft, Netherlands (Chemical Engineering Department), July 2, 1993.
 Sydney University (Chemistry Department), Sydney, Australia, September 22, 1993.
 Sydney University (Chemical Engineering Department), Sydney, Australia, September 24, 1993.
 BHP Research, Melbourne, Australia, October 6, 1993.
 Swinburne University of Technology (Computer Science Department), Melbourne, Australia, October 7, 1993.

University of Adelaide (Chemical Engineering Department), Adelaide, Australia, October 22, 1993.

University of Queensland (Chemical Engineering Department), Brisbane, Australia, Nov. 8, 1993.

Keimyung University (Chemical Engineering Department), Taegu, South Korea, Jan. 14, Jan. 15, 1994.

University of Reading (Chemistry Department), Reading, U.K., February 21, 1994.

University of Cambridge (Chemical Engineering Department), Cambridge, March 9, 1994.

Technical University, (Physical Chemistry Institute), Berlin, Germany, June 3, 1994.

King's College, University of London (Chemistry Department), London, U.K., June 21, 1994.

Johnson Matthey Technology Centre, Sonning Common, U.K., June 22, 1994.

University of Pittsburgh (Chemical Engineering Department), Miles Lectures, March 2,3, 1995.

University of Puerto Rico (Chemical Engineering Dept.), Merck Lectures, March 16,17, 1995.

State University of New York at Buffalo (Chemical Engineering Dept.), March 29, 1995.

Chevron Research & Technology, Richmond, CA, May 12, 1995.

Chiba University (Chemistry Department), Chiba, Japan, December 29, 1995

University of Hong Kong (Chemistry Department), Hong Kong, January 8, 1996.

Sogang University (Chemical Engineering Department), Seoul, South Korea, January 10, 1996.

Oak Ridge National Laboratory, Oak Ridge, Tennessee, April 8, 1996.

University of Tennessee (Chemical Engineering Dept.), Knoxville, TN, April 9, 1996.

University of Gdansk (Institute of Physics), Poland, June 12, 1996.

University of Poznan (Institute of Physics), Poland, June 14, 1996.

Universitat Rovira i Virgili (Chemical Engineering Dept.), Tarragona, Spain, June 16-24, 1996.
[Series of 2 lectures]

Rensselaer Polytechnic Institute (Chemical Engineering Dept.), Troy, NY, October 16, 1996.

North Carolina State University (Chemical Engineering Dept.), Raleigh, NC, November 4, 1996.

Chiba University (Chemistry Department), Chiba, Japan, January 15, 1997.

Pennsylvania State University (Chemical Engineering Dept.), Robb Lecture, January 28, 1997.

Exxon Chemical Co., Baton Rouge, LA, February 27, 1997.

University of Oklahoma (Chemical Engineering Dept.), April 10, 1997.

University of Poznan (Institute of Physics), Poland, June 6, 1997.

Technical University of Berlin (Stranski Institute of Physical Chemistry), June 13, 1997.

University of Nebraska (Chemistry Dept.), Lincoln, October 10, 1997.

King's College London, University of London (Chemistry Dept.), January 28, 1998.

University of Minnesota (Chemical Engng. Dept.), Minneapolis, MN, February 17, 1998.

Chiba University (Chemistry Dept.), Chiba, Japan, February 23, 1998.

National Institute of Materials Chemistry, Tsukuba, Japan, February 26, 1998.

Northwestern University (Chemical Engng. Dept.), March 5, 1998.

Simon Bolivar University, Caracas, Venezuela, March 16, 1998

Simon Bolivar University (Dept. of Thermodynamics and Transport Phenomena), Caracas, Venezuela, March 18, 1998.

City College of New York (Chemistry Dept.), CUNY, New York, April 8, 1998.

"A New Molecular Simulation Model for Adsorption in Controlled Pore Glass", University of Paris-Sud, Orsay, France, May 22, 1998.

"Phase Transitions in Confined Systems", University of Poznan (Institute of Physics), Poland, August 6, 1999.

- “Phase Separation in Nano-Porous Materials”, University of California, Santa Barbara (Chemical Engineering Dept.), November 5, 1998.
- “Phase Separation in Nano-Porous Materials”, University of California, Los Angeles (Chemical Engineering Dept.), November 6, 1998.
- “Phase Separation in Nano-Porous Materials”, Louisiana State University (Chemical Engineering Dept.), December 4, 1998.
- “Molecular Modeling of Adsorption in Amorphous Nano-Porous Materials”, University of Surrey (Chemical Engineering Dept.), December 10, 1998.
- “Molecular Modeling of Adsorption and Phase Transitions in Amorphous Nano-Porous Materials”, Imperial College of Science & Technology, London, U.K. (Chemistry Dept.), December 17, 1998.
- “Thermodynamics of Confined Nanophases: Fluids in Amorphous Nano-Porous Materials”, Simon Bolivar University (Thermodynamics and Transport Phenomena Dept.), March 8, 1999.
- “Molecular Simulation: Applications in Chemical Engineering”, Simon Bolivar University (Thermodynamics and Transport Phenomena Dept.), March 9, 1999.
- “Improved Molecular Models for Adsorption in Amorphous Nano-Porous Materials”, Princeton University (Chemical Engineering Dept.), April 7, 1999.
- “Thermodynamics of Confined Nano-Phases: Fluids in Amorphous Nano-Porous Materials”, Adam Mickiewicz University (Institute of Physics), Poznan, Poland, Sept. 10, 1999.
- “Thermodynamics of Confined Nano-Phases: Fluids in Amorphous Nano-Porous Materials”, Marie Curie Sklodowska University (Theoretical Chemistry Department), Lublin, Poland, Sept. 13, 1999.
- “Thermodynamics of Confined Nano-Phases: Fluids in Amorphous Nano-Porous Materials”, University of North Carolina at Chapel Hill (Chemistry Department), Chapel Hill, NC, Oct. 21, 1999.
- “Molecular Simulation Methods and Some Recent Applications”, Frontier Science Lecture, Chiba University, Japan, Nov. 26, 1999.
- “Thermodynamics of Confined Nano-Phases”, Center for Frontier Electronics and Photonics, Chiba University, Japan, Dec. 20, 1999.
- “Modeling and Characterization of Amorphous Nano-Porous Materials”, Centre de Recherche sur la Matière Divisée, CNRS-Université d’Orléans, France, Feb. 9, 2000.
- “Freezing in Pores”, Institute of Physical Chemistry, Université Paris-Sud, Orsay, France, Feb. 11, 2000.
- “Thermodynamics of Confined Nano-Phases”, University of South Carolina (Chem. Eng. Dept.), March 3, 2000.
- “Melting and Freezing in Pores”, Universidad Nacional de Mexico, Cuernavaca, March 10, 2000.
- “Applications of Molecular Simulation in Chemical Engineering”, Simon Bolivar University, Caracas, March 15, 2000.
- “Confined Nano-Phases: Fluids in Amorphous Nano-Porous Materials”, National Institute of Standards and Technology, Gaithersburg, MD, June 22, 2000.
- “Freezing and Melting Phenomena in Pores”, Institute of Physics, Adam Mickiewicz University, Poznan, Poland, August 9, 2000.
- “Structural Morphology of Carbons by Reverse Monte Carlo”, Westvaco Technical Center, Charleston, SC, October 27, 2000.

- “Molecular Modeling of Nano-Porous Materials”, Universidad de los Andes, Merida, Venezuela, December 14, 2000.
- “Molecular Modeling of Nano-Porous Materials”, Venezuelan Institute for Scientific Research (IVIC), Caracas, Venezuela, December 18, 2000.
- “Molecular Modeling of Confined Nano-Phases in Disordered Porous Materials”, Universidad de Alicante, Alicante, Spain, March 15, 2001.
- “Some Recent Applications of Molecular Simulation: Phase and Chemical Equilibria in Nano-Scale Systems”, Rice University (Chemical Engineering), March 29, 2001. [Leland Lecture]
- “Molecular Simulation of Confined Nano-Phases”, Osaka University, May 18, 2001.
- “Effects of Confinement on Phase Transitions and Chemical Reactions”, Institute of Physics, Adam Mickiewicz University, Poznan, Poland, Sept. 3, 2001.
- “Phase Transitions and Chemical Reactions at the Nano-Scale: Effects of Confinement”, Laboratoire Chimie Physique, Université Paris-Sud, Orsay, France, October 12, 2001.
- “Phase Transitions and Chemical Reactions at the Nano-Scale: Effects of Confinement”, Army Research Laboratory, Aberdeen, MD, November 14, 2001.
- “Molecular Modeling of Adsorption”, Army Research Laboratory, Edgewood, MD, November 15, 2001.
- “Phase Transitions and Chemical Reactions at the Nano-Scale: Effects of Confinement”, Technical University, Berlin, November 22, 2001.
- “Phase Transitions and Chemical Reactions at the Nano-Scale: Effects of Confinement”, Institut Leon Brillouin, Saclay, France, December 11, 2001.
- “Phase Transitions and Chemical Reactions at the Nano-Scale: Effects of Confinement”, Oxford University, U.K., February 18, 2002.
- “Phase Transitions and Chemical Reactions at the Nano-Scale: Effects of Confinement”, Cambridge University, U.K., March 6, 2002.
- “Phase Transitions and Chemical Reactions at the Nano-Scale: Effects of Confinement”, Centre de Thermodynamique et Microcalorimétrie de CNRS, MADIREL (Matériaux Divisés, Revêtements, Electrocéramiques), Marseille, France, March 12, 2002.
- “Phase Transitions and Chemical Reactions at the Nano-Scale: Effects of Confinement”, Loughborough University, U.K., March 19, 2002.
- “Effects of Confinement on Phase Transitions and Chemical Reactions”, Imperial College of Science, Technology and Medicine (Chemistry Department), London, April 16, 2002.
- “Some Recent Advances in Molecular Simulation: Thermophysical Properties in Bulk and Confined Systems”, Dow Chemical Co., Midland, MI, April 23, 2002.
- “Phase Transitions and Chemical Reactions at the Nano-Scale: Effects of Confinement”, University of Delaware, April 24, 2002.
- “Freezing in Narrow Pores”, Oak Ridge National Laboratory, April 29, 2002.
- “Freezing in Narrow Pores”, Oxford University, Colloquium in Soft Matter, Biomaterials and Interfaces, May 1, 2002.
- “Molecular Simulation: Some Recent Applications in Phase Separations and Reacting Systems”, Imperial College of Science, Technology and Medicine (Joint Centre for Process Systems Engineering & Chemical Engineering Department Seminar), London, May 16, 2002.
- “Phase Transitions and Chemical Reactions at the Nano-Scale: Effects of Confinement”, University of Kent, Canterbury, U.K., May 29, 2002.

- “Freezing in Nano-Porous Materials”, Queen’s University, Belfast, June 6, 2002.
- “Phase Transitions and Chemical Reactions at the Nano-Scale: Effects of Confinement”, Colorado School of Mines, December 6, 2002.
- “Molecular Simulation of Confined Nano-Phases: Adsorption, Phase Changes and Chemical Reactions in Nano-Porous Materials”, Vanderbilt University, Nashville, TN, February 24, 2003.
- “Phase Transitions and Chemical Reactions at the Nano-Scale: Effects of Confinement”, University of Edinburgh, Scotland, April 7, 2003.
- “Phase Transitions and Self-Assembly at the Nano-Scale: Effects of Confinement”, Institute of Physics, Adam Mickiewicz University, Poznan, Poland, June 4, 2003.
- “Molecular Simulation of Confined Nano-Phases: Adsorption, Phase Changes and Chemical Reactions in Nano-Porous Materials”, University of Wyoming, Laramie, WY, October 9, 2003.
- “Phase Transitions and Chemical Reactions at the Nano-Scale: Effects of Confinement”, University of California, Riverside, CA, November 14, 2003.
- “Phase Transitions and Chemical Reactions at the Nano-Scale: Effects of Confinement”, University of Florida, Gainesville, FL, March 15, 2004.
- “Phase Transitions and Chemical Reactions at the Nano-Scale: Effects of Confinement”, University of Missouri, Rolla, April 9, 2004.
- “Phase Transitions and Chemical Reactions at the Nano-Scale: Effects of Confinement”, University of California Santa Barbara, April 29, 2004.
- “Effects of Confinement on Chemical Reactions”, Adam Mickiewicz University, Institute of Physics, August 26, 2004.
- “Phase Transitions and Chemical Reactions at the Nano-Scale: Effects of Confinement”, Hong Kong University of Science and Technology, Chemical Engineering Department, October 5, 2004.
- “Phase Transitions and Chemical Reactions at the Nano-Scale: Effects of Confinement”, Chiba University, Department of Chemistry, Chiba, Japan, October 12, 2004.
- “Phase Transitions and Chemical Reactions at the Nano-Scale: Effects of Confinement”, University of Buffalo, Department of Chemical Engineering, December 8, 2004.
- “Phase Transitions and Chemical Reactions at the Nano-Scale: Effects of Confinement”, Indian Institute of Science, Chemical Engineering Department, Bangalore, India, January 4, 2005.
- “Molecular Modeling of Nano-Porous Materials and Confined Fluids”, Colorado School of Mines, Department of Chemical Engineering, February 4, 2005.
- “Molecular Modeling of Nano-Porous Materials and Confined Fluids”, Quantachrome Instruments, March 7, 2005.
- “Phase Transitions and Chemical Reactions at the Nano-Scale: Effects of Confinement”, University of Maryland, Chemical and Biomolecular Engineering Department, April 19, 2005.
- “Phase Transitions and Chemical Reactions at the Nano-Scale: Effects of Confinement”, University of Washington, Department of Chemical Engineering, May 9, 2005.
- “Phase Transitions and Chemical Reactions at the Nano-Scale: Effects of Confinement”, Institut Européen des Membranes, University of Montpellier, France, May 24, 2005.
- “Effect of Confinement on Chemical Reactivity”, Institute of Physics, Adam Mickiewicz University, Poznan, Poland, May 31, 2005.

- “Effects of Confinement on Chemical Reactivity”, Technisches Universität Hamburg-Harburg, Department of Chemical Engineering, Hamburg, Germany, April 13, 2006.
- “Modeling Chemical Reactivity: Effects of Confinement”, National University of Singapore, Department of Chemical and Biomolecular Engineering, May 18, 2006.
- “Molecular Modeling of Nano-Porous Materials and Adsorption”, Nanjing University of Technology, Chemical Engineering Department, May 27, 2006.
- “Effects of Confinement in Nano-Pores on Chemical Reactions”, Nanjing University, Chemistry Department, May 28, 2006.
- “Modeling Chemical Reactivity: Effects of Confinement”, Lecture Series on Computational Physics and Numerical Methods, Physics Department, University of Hong Kong, June 1, 2006.
- “Molecular Simulation of Gas Adsorption in Mesoporous Silica SBA-15”, Chemistry Department, University of Hong Kong, June 1, 2006.
- “Phase Change and Chemical Reactions at the Nanoscale: Effects of Confinement”, Joint Chemistry & Chemical Engineering Departments, East China University of Science & Technology, Shanghai, October 13, 2006.
- “Phase Change and Chemical Reactions at the Nanoscale: Effects of Confinement”, Joint Chemistry & Chemical Engineering Departments, Zhejiang University, October 16, 2006.
- “Confinement Effects on Chemical Reactions – Toward an Integrated Catalyst Design”, Chemistry Department, Chiba University, Japan, October 20, 2006.
- “Multi-Scale Modeling in Chemical Engineering Research”, Nanjing University of Technology, Nanjing, China, Chemical Engineering Department, December 13, 2006.
- “Confinement Effects on Chemical Reactions: Towards an Integrated Catalyst Design”, Department of Chemistry and Chemical Engineering, Yangzhou University, Yangzhou, China, December 14, 2006.
- “Phase Change and Chemical Reactions at the Nanoscale: Effects of Confinement”, A*STAR Institute of Bioengineering and Nanotechnology, Singapore, January 25, 2007.
- “Phase Change and Chemical Reactions at the Nanoscale: Effects of Confinement”, Lyman L. Handy Colloquium, Department of Chemical Engineering and Materials Science, University of Southern California, Los Angeles, CA, February 8, 2007.
- “Multi-Scale Modeling in Chemical Engineering Research”, Department of Chemical Engineering, University of California at Riverside, Riverside, CA, February 9, 2007.
- “Confinement Effects on Chemical Reactions: Towards an Integrated Catalyst Design”, Physics Department, University of Rome La Sapienza, Rome, Italy, May 15, 2007.
- “Molecular Modeling of Matter: What Can We Do Now, and in the Near Future?”, Nanjing University of Technology, general lecture, June 30, 2007.
- “Molecular Modeling of Matter: What Can We Do Now, and in the Near Future?”, University of Hong Kong, Public Lecture, July 4, 2007.
- “Confinement Effects on Chemical Reactions: Towards an Integrated Catalyst Design”, Hong Kong University of Science and Technology, Chemical Engineering Department, July 11, 2007.
- “Confinement Effects on Chemical Reactions: Towards an Integrated Catalyst Design”, Zhejiang University, Chemistry Department, July 14, 2007.
- ”Surface Nanostructure and Catalysis: The Role of Confinement and Surface Chemistry”, Adam Mickiewicz University, Institute of Physics, October 25, 2007.

- "Surface Nanostructure and Catalysis: The Role of Confinement and Surface Chemistry", South China University of Technology, Department of Chemical & Energy Engineering, Guangzhou, China, December 19, 2007.
- "Surface Nanostructure and Catalysis: The Role of Confinement and Surface Chemistry", Imperial College London, Department of Chemical Engineering, London, U.K., January 28, 2008.
- "Surface Nanostructure, Diffusion and Catalysis: The Role of Confinement and Surface Chemistry", Quantachrome Instruments, Boynton Beach, FL, April 3, 2008.
- "Surface Nanostructure, Diffusion and Catalysis: The Role of Confinement and Surface Chemistry", Chiba University, Chemistry Department, April 28, 2008.
- "Surface Nanostructure, Diffusion and Catalysis: The Role of Confinement and Surface Chemistry", Chinese University of Hong Kong, May 2, 2008.
- "Adsorption and Diffusion in Nano-Porous Materials: The Role of Confinement and Surface Chemistry", Zhejiang University, Chemistry Department, Hangzhou, China, May 7, 2008.
- "Surface Nanostructure, Diffusion and Catalysis: The Role of Confinement and Surface Chemistry", Adam Mickiewicz University, Institute of Physics, Poznan, Poland, June 9, 2008.
- "Surface Nanostructure, Diffusion and Catalysis: The Role of Confinement and Surface Chemistry", Kyoto University, Department of Chemical Engineering, Kyoto, Japan, August 13, 2008.
- "Thermodynamics and Dynamics of Confined Nano-Phases", University of California at Berkeley, Department of Chemical Engineering, October 29, 2008.
- "Thermodynamics and Dynamics of Confined Nano-Phases", Beijing University of Chemical Technology, Department of Chemical Engineering, December 9, 2008.
- "Molecular Modeling of Matter: Impact and Prospects in Engineering", Beijing University of Chemical Technology, Department of Chemical Engineering, December 9, 2008.
- "Molecular Simulation as a Foundation for Engineering Models: Impact and Prospects", Nanjing University of Technology, Department of Chemical Engineering, Nanjing, China, December 18, 2008.
- "Molecular Modeling of Matter: Impact and Prospects in Engineering", University of Manchester, Department of Chemical Engineering, Manchester, U.K., April 29, 2009.
- "Surface Nanostructure, Diffusion and Catalysis: The Role of Confinement and Surface Chemistry", University of Manchester, Department of Chemical Engineering, Manchester, U.K., May 1, 2009.
- "Surface Nanostructure, Diffusion and Catalysis: The Role of Confinement and Surface Chemistry", Heriot-Watt University, Department of Chemical Engineering, Edinburgh, U.K., May 6, 2009.
- "Surface Nanostructure, Diffusion and Catalysis: The Role of Confinement and Surface Chemistry", Imperial College London, Department of Chemical Engineering, London, U.K., May 11, 2009.
- "Surface Nanostructure, Diffusion and Catalysis: The Role of Confinement and Surface Chemistry", Oxford University, Physical & Theoretical Chemistry Laboratory, Oxford, U.K., May 13, 2009.
- "Molecular Modeling and Simulation of Titanium Carbide Derived Carbons", University of Hong Kong, Chemistry Department, June 1, 2009.

- “Molecular Modeling of Matter: Impact and Prospects in Physical Sciences and Engineering”, Adam Mickiewicz University, Institute of Physics, July 13, 2009.
- “Transitions between Single-File and Fickian Self-Diffusion for Fluids Confined in Carbon Nanotubes, Bundles and Activated Carbons”, Xi’an Jiaotong University, School of Energy & Power Engineering, October 27, 2009.
- “Molecular Modeling of Matter: Impact and Prospects in Engineering”, Xi’an Jiaotong University, School of Energy & Power Engineering, October 28, 2009.
- “Molecular Modeling of Matter at the Nanoscale: Impact and Prospects”, Nanjing University of Technology, Chemical Engineering Department, December 14, 2009.
- “Molecular Modeling of Matter at the Nanoscale: Impact and Prospects”, Chiba University, Chemistry Department, December 17, 2009.
- “Thermodynamics and Dynamics of Confined Nano-Phases”, Quantachrome Instruments, Boynton Beach, FL, April 20, 2010.
- “Under Pressure: High Pressure Effects in Nanopores”, Institute of Physics, Adam Mickiewicz University, Poznan, Poland, June 11, 2010.
- “Under Pressure: Quasi-High Pressure Effects in Nanopores”, Department of Chemistry, University of Hong Kong, September 6, 2010.
- “Molecular Modeling of Matter by Atomistic Simulation. 1. Molecular Dynamics”, Department of Chemistry, Zhejiang University, Hangzhou, October 18, 2010.
- “Molecular Modeling of Matter by Atomistic Simulation. 2. Monte Carlo Simulation”, Department of Chemistry, Zhejiang University, Hangzhou, October 20, 2010.
- “Thermodynamics and Dynamics of Confined Nano-Phases”, Department of Chemical and Biological Engineering, Beijing University of Chemical Technology, Beijing, October 22, 2010.
- “Thermodynamics and Dynamics of Confined Nano-Phases”, Department of Chemical Engineering, University of Waterloo, Waterloo, Ontario, Canada, October 28, 2010.
- “Under Pressure: Quasi-High Pressure Effects in Nanopores”, Shinshu University, Nagano, Japan, December 14, 2010.
- “Under Pressure: Quasi-High Pressure Effects in Nanopores”, Department of Chemistry, Cambridge University, February 9, 2011.
- “Under Pressure: Quasi-High Pressure Effects in Nanopores”, Department of Physics, University College Dublin, Dublin, Ireland, March 14, 2011.
- “Thermodynamics and Dynamics of Confined Nano-Phases”, Basque Centre for Applied Mathematics, Bilbao, Spain, March 28, 2011.
- “Under Pressure: Quasi-High Pressure Effects in Nanopores”, IGRTG Colloquium, Technical University of Berlin, Berlin, Germany, May 17, 2011.
- “High Pressure Effects and Material Deformation due to Confined Nanophases”, Imperial College London, Chemistry Department, June 23, 2011.
- “High Pressure Effects and Material Deformation due to Confined Nanophases”, Chemistry Department, Zhejiang University, Hangzhou, China, November 3, 2011.
- “Thermodynamics and Dynamics of Confined Nano-Phases”, Department of Chemical & Biological Engineering, Colorado School of Mines, November 18, 2011.
- “Thermodynamics and Dynamics of Confined Nano-Phases”, Adam Mickiewicz University, Poznan, Poland, December 7, 2011. Lecture in connection with the award of the Medal of Merit of Adam Mickiewicz University.

- “Multi-Scale Modeling of Matter”, Nanjing University of Technology, December 16, 2011.
- “High Pressure Effects and Material Deformation due to Confined Nanophases”, Chemistry Department, University of North Carolina at Chapel Hill, January 26, 2012.
- “Thermodynamics of Confined Nano-Phases”, Chemistry & Chemical Engineering Departments, Zhejiang University, September 11, 2012.
- “Pressure Enhancement in Nanopores and Effects on Adsorbent Structure”, Chemistry & Chemical Engineering Departments, Zhejiang University, September 13, 2012.
- “Pressure Enhancement in Nanopores and Effects on Adsorbent Structure”, Chemical Engineering Department, East China University of Science & Technology (ECUST), September 15, 2012.
- “Molecular Modeling and Simulation of Confined Nano-Phases: Adsorption, Diffusion and Reaction”, Babcock & Wilcox Co., Akron, Ohio, November 12, 2012.
- “Thermodynamics of Confined Nano-Phases”, Jiang Nan University, Department of Chemical Engineering, Wuxi, China, November 30, 2012.
- “The Role of Nanoscale Wetting in Confinement Effects”. Nanjing University of Technology. Chemical Engineering Department, December 1, 2012.
- “Pressure Enhancement in Nanopores and Effects on Adsorbent Structure”, Quantachrome Instruments, Boynton Beach, FL, March 27, 2013.
- “Molecular Modelling and Simulation of Confined Nano-Phases”, Distinguished Seminar Series 2012-2013, The Leader’s Forum, Imperial College London, May 1, 2013.
- “Thermodynamics of Confined Nano-Phases”, MatGas, Universidad Autonoma de Barcelona, Barcelona, Spain, September 9, 2013.
- “Molecular Modeling and Simulation of Confined Nano-Phases”, Institute for Process Engineering, Chinese Academy of Sciences, Beijing, China, October 27, 2013.
- “Thermodynamics of Confined Nano-Phases”, Nanjing University of Technology. Chemical Engineering Department, October 29, 2013.
- “Thermodynamics of Confined Nano-Phases”, Zhejiang University. Chemistry Department, October 31, 2013.
- “Thermodynamics of Confined Nano-Phases”, University of Pennsylvania, Chemical Engineering Department, November 13, 2013.
- “Thermodynamics of Confined Nano-Phases”, Hong Kong University, Chemistry Department, December 9, 2013.
- “Thermodynamics of Confined Nano-Phases”, Shinshu University, Japan, Chemistry Department, December 12, 2013.
- “Thermodynamics of Confined Nano-Phases”, National University of Singapore, Chemical Engineering Department, December 18, 2013.
- “Wetting at the Nano-Scale”, Institute of Physics, Adam Mickiewicz University, Poznan, Poland, June 9, 2014.
- “Wetting at the Nano-Scale”, Nanjing Tech University, Nanjing, China, Chemical Engineering Department, September 14, 2014.
- “Wetting at the Nano-Scale”, Sechuan University, Chengdu, China, Chemical Engineering Department, September 14, 2014.
- “Wetting at the Nano-Scale”, East China University of Science & Technology, Shanghai, China, Chemical Engineering Department, October 21, 2014.

- “Corresponding States Theory for Thin Adsorbed Films”, Institute of Physics, Adam Mickiewicz University, Poznan, Poland, July 13, 2015.
- “Corresponding States Theory for Thin Adsorbed Films”, Center for Microelectronics and Nanotechnology, Uniwersytetu Rzeszowskiego (University of Rzeszów), Rzeszów, Poland, July 13, 2015.
- “Confinement-Induced High Pressure Phases in Nanopores. Can the Pressure be in the Megabar Range?”, Department of Chemistry, Zhejiang University, October 27, 2015.
- “Corresponding States Theory of Adsorbed Films”, Department of Chemical Engineering, East China University of Science & Technology, Shanghai, China, October 30, 2015.
- “Confinement-Induced High Pressure Phases in Nanopores. Can the Pressure be in the Megabar Range?”, International Center for Science and Innovation, Shinshu University, Nagano, Japan, December 14, 2015.

Papers Presented at National and International Conferences (1973 - present):

- Mo, K.C., Dufty, J.W. and Gubbins, K.E., "Transport Coefficients for Dense Fluids," presented at Washington, D. C. Meeting of the American Physical Society, April 1973.
- Mo, K.C., Gubbins, K.E. and Dufty, J.W., "Perturbation Theory for Dense Fluid Transport Properties," presented at the Sixth American Society of Mechanical Engineers Symposium on Thermophysical Properties, Atlanta, August, 1973. (Published in Proceedings.)
- Mo, K.C. and Gubbins, K.E., "Conformal Solutions Approach for Transport Properties of Mixtures," Annual AIChE Meeting, Nov. 15, 1973, Philadelphia.
- Gubbins, K.E., "Equilibrium Properties of Polyatomic Liquids," Canadian Association of Physics Meeting on Machine Calculations of Structure of Molecular Liquids, University of Guelph, Dec. 8, 1973. (Invited review paper.)
- Gubbins, K.E., "A New Perturbation Expansion for Molecular Liquids," 31st Statistical Mechanics Meetings, Yeshiva University, New York, May 15, 1974.
- Twu, C.H., Stephanopoulos, M. and Gubbins, K.E., "Theory of Solutions Composed of Polar and Quadrupolar Molecules," 78th National Meeting of AIChE, Salt Lake City, Aug. 21, 1974.
- Twu, C.H. and Gubbins, K.E., "Theory of Polyatomic Liquids and Their Mixtures," ACS Meeting, Orlando, May 9, 1975.
- Haile, J.M. and Gubbins, K.E., "Theory of Surface Tension of Polyatomic Fluids," ACS Meeting, Orlando, May 9, 1975.
- Haile, J.M. and Gubbins, K.E., "Viscosity of Cryogenic Liquid Mixtures," Cryogenic Engineering Conference, Kingston, Ontario, July 22, 1975.
- Haile, J.M., Mo, K.C. and Gubbins, K.E., "Viscosity of Cryogenic Liquid Mixtures, Including LNG," Cryogenic Engineering Conference, Kingston, Ontario, July 22, 1975.

- Dufty, J.W. and Gubbins, K.E., "Many-time Correlation Functions and Non-Linear Transport," International Union of Pure and Applied Physics Conference on Statistical Physics, Budapest, Hungary, Aug. 26, 1975.
- Gubbins, K.E. and Haile, J.M., "Surface Tension of Polar Liquids," Annual AIChE Meeting, Chicago, Dec. 1, 1976.
- Gubbins, K.E., "Polar and Quadrupolar Fluid Mixtures," Engineering Foundation Conference on the Estimation and Correlation of Phase Equilibria and Fluid Properties in the Chemical Industry, Pacific Grove, California, Jan. 18, 1977. (Invited paper.)
- Twu, C.H. and Gubbins, K.E., "Theory of Phase Equilibria in Mixtures with Polar and Quadrupolar Constituents," 83rd National AIChE Meeting, Houston, March 23, 1977.
- Gubbins, K.E., "Prospects for Improved Predictive Techniques," NBS Symposium on "Estimation of the Properties of Fluid Mixtures," National Bureau of Standards, Gaithersburg, Maryland, April 19, 1977. (Invited paper.)
- Haile, J.M., Gubbins, K.E. and Streett, W.B., "Computer Simulation of Dense Fluids," 7th Symposium on Thermophysical Properties, American Society of Mechanical Engineers, NBS, Gaithersburg, Maryland, May 10, 1977.
- Gubbins, K.E., "Thermodynamics of Polar and Quadrupolar Fluid Mixtures," Guelph-Waterloo Symposium on Liquids, Guelph, Ontario, May 27, 1977. (Invited paper.)
- Gubbins, K.E., "Theory of Molecular Liquids and Liquid Mixtures," Symposium on Molecular Motion in Liquids," 2nd Joint American Chemical Society - Canadian Institute of Chemistry Conference, Montreal, May 30, 1977. (Invited paper.)
- Murad, S. and Gubbins, K.E., "Molecular Dynamics Simulation of Methane Using a Singularity-Free Algorithm," American Chemical Society Meeting, Anaheim, California, March 14, 1978.
- Thompson, S. and Gubbins, K.E., "On the Computer Simulation of the Liquid-Vapor Surface of Molecular Fluids," American Chemical Society Meeting, Anaheim, California, March 14, 1978.
- Clancy, P. and Gubbins, K.E., "Thermodynamics of Polar Liquid Mixtures," Sixth International Conference on Non-Aqueous Solutions, University of Waterloo, Waterloo, Ontario, Aug. 7-11, 1978.
- Dufty, J.W. and Gubbins, K.E., "Comments on the Self-Diffusion Coefficient for a Square-Well Fluid," American Chemical Society Meeting, Miami Beach, Sept. 11, 1979.
- Clancy, P., Gubbins, K.E., and Gray, C.G., "Thermodynamics of Polar Liquid Mixtures," Faraday Discussion 66, Structure and Motion in Molecular Liquids, University of Kent, Canterbury, U.K., Sept. 13-15, 1979.
- Gubbins, K.E., "The Role of Statistical Mechanics in Phase Equilibria," 40th Annual Statistical Mechanics meeting, Rutgers University, Dec. 14, 1978. (Invited review paper.)
- Clancy, P. and Gubbins, K.E., "Molecular Thermodynamics of Liquid Mixtures at Low Temperatures," Annual Meeting of American Institute of Chemical Engineers, Miami Beach, Nov. 12-16, 1978.
- Gubbins, K.E., "Theory of Liquid Mixtures: The Role of Anisotropic Intermolecular Forces," Annual Chemical Congress, The Chemical Society, Bristol, U.K., April 6, 1979. (Invited review paper.)
- Gubbins, K.E., "Theory of Polar Liquid Mixtures," Symposium on Polar Liquids, Chemical Society (London), Aberystwyth, Wales, Sept. 13, 1979. (Invited review.)

- Clancy, P., Gubbins, K.E., Machado, J.R.S., Lobo, L.Q. and Staveley, L.A.K., "Excess Properties and Phase Equilibria in Cryogenic Mixtures: Experiment and Theory," Annual AIChE Meeting, San Francisco, Nov. 29, 1979.
- Gubbins, K.E., "Some Use of Statistical Thermodynamics," 2nd International Conference on Phase Equilibria and Fluid Properties in the Chemical Industry, West Berlin, March 19, 1980.
- Gubbins, K.E., "Molecular Orientation Effects at Liquid Surfaces," Second North American Chemical Congress, Las Vegas, Aug. 26, 1980. (Invited review lecture.)
- Streett, W.B., Tsang, C., Dieters, U., Clancy, P. and Gubbins, K.E., "Phase Equilibria in the Systems H_2/CH_4 , H_2/CO and H_2/CO from 70 to 290K and Pressures to 2,000 Atmospheres," Annual American Institute of Chemical Engineering Meeting, Chicago, Nov. 17, 1980.
- Gubbins, K.E., "Molecular Orientation Effects Near Surfaces," X Reunion de Fisica Estadistica, Cocoyoc, Mexico, Jan. 7, 1981.
- Gubbins, K.E., "Computer Simulation and Molecular Theory Studies of Natural Gas Properties," Gas Research Institute Physical Properties Project Review, San Antonio, March 26, 1981.
- Gray, C.G., Sullivan, D.E. and Gubbins, K.E., "Structure of Molecular Liquids at Solid Interfaces," Conference on the Structure of Molecular Liquids, Royal Society of Chemistry, Cambridge, U.K., April 7, 1981.
- Shing, K.S. and Gubbins, K.E., "The Chemical Potential in Dense Fluid Mixtures via Computer Simulation," poster paper presented at the Gordon Conference on Liquids, Plymouth, N.H., Aug. 11, 1981.
- Streett, W.B. and Gubbins, K.E., "Experimental and Theoretical Studies of Dense Fluid Mixtures," 8th Symposium on Thermophysical Properties, National Bureau of Standards, Gaithersburg, June 15-18, 1981.
- Jonah, D.A., Shing, K.S. and Gubbins, K.E., "Theory of Dilute Solutions," 8th Symposium on Thermophysical Properties, National Bureau of Standards, Gaithersburg, June 15-18, 1981.
- Shing, K.S., Jonah, D.A., Venkatasubramanian, V. and Gubbins, K.E., "Molecular Thermodynamics of Dilute Solutes in Supercritical Solvents," Annual Meeting of American Institute of Chemical Engineers, New Orleans, Nov. 10, 1981.
- Gubbins, K.E., "The Impact of Dr. Staveley's Work on Theory of Liquid Mixtures," The Lionel Staveley Retirement Meeting, Oxford University, June 25, 1982.
- Shing, K.S. and Gubbins, K.E., "Fluid Phase Equilibria for Nonideal Mixtures: Computer Simulation and Perturbation Theory," Annual Meeting of American Institute of Chemical Engineers, Los Angeles, Nov. 15, 1982.
- Gubbins, K.E., "Fluid Structure Near an Interface," Gordon Research Conference on Chemistry at Interfaces, Meriden, N.H., July 29, 1982.
- Gubbins, K.E., "The Application of Perturbation Theory to Liquids and Liquid Mixtures," Royal Society of Chemistry Conference on Liquids and Liquid Mixtures, University of Hull, Hull, U.K., March 28, 1983.
- Gubbins, K.E., "Computer Simulation and Perturbation Theory Studies of Molecular Liquids," CCP5 Conference on the Computer Simulation of Molecular Liquids and Liquid Mixtures, Hull, U.K., March 29, 1983.
- Gubbins, K.E., "Equations of State--New Theories," Third International Conference on Fluid Phase Equilibria, Callaway Gardens, Ga., April 11, 1983.

- Monson, P.A. and Gubbins, K.E., "Molecular Theory of Fluids with Gaussian Overlap Potentials," Third International Conference on Fluid Phase Equilibria, Callaway Gardens, Ga., April 11, 1983.
- Naik, C.D., Gubbins, K.E., Clancy, P. and Thompson, S.M., "The Use of Computer Graphics to Teach Phase Diagrams," Annual AIChE Meeting, Washington D.C., Nov. 1, 1983.
- Gubbins, K.E., "Predicting Fluid Properties," Chemical Society Symposium, Leicester, U.K., January 5, 1984.
- Gubbins, K.E., "Molecular Studies of Gas Properties," GRI Thermophysical Properties Workshop, New Orleans, March 22, 1984.
- Wojcik, M. and Gubbins, K.E., "Computer Simulation Studies of Model Fluids and Fluid Mixtures," Can-Am Chemical Congress, Montreal, June 4-5, 1984.
- Telo da Gama, M.M. and Gubbins, K.E., "A Mean Field Theory for a Model of a Surfactant at an Oil/Water Interface," Can-Am Chemical Congress, Montreal, June 4, 1984.
- Sullivan, D.E., Gray, C.G., Thompson, S.M. and Gubbins, K.E., "Structure of Molecular Fluids Near Surfaces," Can-Am Chemical Congress, Montreal, June 4, 1984.
- Joslin, C.G., Gray, C.G., Gubbins, K.E., and Venkatasubramanian, V., "Induction Effects in Polar-Polarizable Liquids," Can-Am Chemical Congress, Montreal, June 5, 1984.
- Gubbins, K.E., "Theory and Computer Simulation Studies of Fluid Mixtures," Staveley Lecture, Third International Conference on Thermodynamics of Solutions of Nonelectrolytes, Clermont-Ferrand, France, July 2, 1984.
- Gubbins, K.E., Maher, Z. and Wojcik, M.C., "New Developments in the Theory of Liquid Solutions," Annual Meeting of the American Institute of Chemical Engineers, San Francisco, November 29, 1984.
- Gubbins, K.E., "Molecular Studies of Gas Properties," GRI Thermophysical Properties Workshop, Rice University, Houston, March 21, 1985.
- Eggebrecht, J., Gubbins, K.E., Shreve, A., Thompson, S.M., and Walton, J.P.B.R., "The Vapour-Liquid Interface for a Stockmayer Fluid," Statistical Mechanics of Dense Fluids Meeting, Royal Society of Chemistry, Bristol, U.K., April 10, 1985.
- Lee, D.J., Gubbins, K.E., and Telo da Gama, M.M., "Surface Activity at the Liquid-Vapour Interface of Binary Mixtures," Statistical Mechanics of Dense Fluids Meetings, Royal Society of Chemistry, Bristol, U.K., April 10, 1985.
- Gubbins, K.E., "Computer Simulation and Theoretical Studies of Liquid Mixtures: Brute Force vs. Insight," Chem. Por. '85, International Chemical Engineering Conference, Coimbra, Portugal, April 15, 1985.
- Telo da Gama, M.M. and Gubbins, K.E., "A Microscopic Model for the Interfacial Properties of Mixtures of Oil, Water and Non-Ionic Surfactants, Chem. Por. '85, International Chemical Engineering Conference, Coimbra, Portugal, April 16, 1985.
- Eggebrecht, J., Gubbins, K.E., Shreve, A., Thompson, S.M. and Walton, J.P.B.R., "The Vapour-Liquid Interface for a Stockmayer Fluid," 9th Thermophysical Properties Conference, Boulder, June 24, 1985.
- Peterson, B.K., Walton, J.P.B.R., "Computer Simulation of Fluids in Pores," 9th Thermophysical Properties Conference, Boulder, June 24, 1985.
- Telo da Gama, M.M. and Gubbins, K.E., "Adsorption and Orientation of Amphiphilic Molecules at a Liquid-Liquid Interface," 9th Thermophysical Properties Conference, Boulder, June 24, 1985.

- Gubbins, K.E., "Computer Simulation and Theoretical Studies of Liquid Mixtures," Second Codata Symposium on Critical Evaluation and Prediction of Phase Equilibria in Multicomponent Systems, Paris, Sept. 13, 1985.
- Thurtell, J.H., Telo da Gama, M.M. and Gubbins, K.E., "Theoretical Studies of Surfactants at Liquid-Liquid and Liquid-Vapor Interfaces," Royal Society of Chemistry Conference on Multicomponent Mixtures, University of East Anglia, Norwich, U.K., Sept. 18, 1985.
- Gubbins, K.E., Lee, D.J., Telo da Gama, M.M. and Thurtell, J.H., "Surface Activity at the Vapor-Liquid Interface of Binary Mixtures," Annual Meeting of the American Institute of Chemical Engineers, Chicago, Nov. 11, 1985.
- Peterson, B.K., Walton, J.P.R.B. and Gubbins, K.E., "Fluid Behavior in Narrow Pores," Faraday Symposium No. 20, Royal Society of Chemistry, Oxford, U.K., Dec. 18, 1985.
- Gubbins, K.E., "Molecular Theory and Computer Simulation Studies of Fluid Mixtures," GRI Thermophysical Properties Workshop, San Antonio, March 14, 1986.
- Chapman, W.G., Gubbins, K.E., Joslin, C.G. and Gray, C.G., "Theory and Simulation of Associating Liquid Mixtures," Fourth International Conference on Fluid Properties and Phase Equilibria for Chemical Process Design, Helsingor, Denmark, May 12, 1986.
- Thurtell, J.H. and Gubbins, K.E., "Theoretical and Simulation Studies of Surfactants at Liquid Interfaces," 4th Army Conference on Applied Mathematics and Computing, Cornell University, Ithaca, NY, May 27-30, 1986.
- Peterson, B.K., Gubbins, K.E. and Walton, J.P.R.B., "Fluids in Narrow Pores: Computer Simulation and Mean Field Theory," 4th Army Conference on Applied Mathematics and Computing, Cornell University, Ithaca, NY, May 27-30, 1986.
- Peterson, B.K., Walton, J.P.R.B., and Gubbins, K.E., "Fluid Behavior in Micropores", Second International Conference on Fundamentals of Adsorption, Santa Barbara, May 4-9, 1986.
- Gubbins, K.E., "Theory of Liquid Mixtures," Second Liblice Conference on the Statistical Mechanics of Liquids, Bechyne, Czechoslovakia, May 19, 1986 (plenary lecture).
- Gubbins, K.E., "Mixtures of Polar and Associating Molecules," 9th IUPAC Conference on Chemical Thermodynamics, Lisbon, July 15, 1986.
- Peterson, B.K., Gubbins, K.E., and Walton, J.P.R.B., "Fluid Phase Transitions and Adsorption in Micropores", Annual Meeting of the American Institute of Chemical Engineers, Miami Beach, November 3-7, 1986.
- Chapman, W.G., Gubbins, K.E., Gray, C.G., and Joslin, C.G., "Theory of Mixtures with Molecular Association or Solvation", Annual Meeting of the American Institute of Chemical Engineers", Miami Beach, November 3-7, 1986.
- Gubbins, K.E., "Lennard-Jones Fluids and Fluid Mixtures in Pores", Conference on Perspectives in Physical Chemistry: The Properties of Molecules in Pores, Imperial College, London, January 15, 1987.
- Gubbins, K.E., "Computer Simulation and Theory of Liquid Mixtures", Conference on Computer Simulation, Kyoto University, Kyoto, Japan, March 18-19, 1987.
- Gubbins, K.E., "Computer Simulation and Theory of Liquid Mixtures", Annual Meeting of the Japanese Chemical Society, Nihon University, Tokyo, April 1-2, 1987.
- Gubbins, K.E., Heffelfinger, G.S., Peterson, B.K., and van Swol, F., "Liquid-Vapour Phase Transitions in a Cylindrical Pore", Conference on the Thermodynamics and Statistical Mechanics of Small Systems, Royal Society of Chemistry, University of York, York, U.K., Sept. 24-25, 1987.

- Chapman, W.G., Jackson, G., Gubbins, K.E., and Radosz, M., "A Statistical Mechanical Equation of State for Associating Fluids", Annual Meeting of the American Institute of Chemical Engineers, New York, Nov. 15-20, 1987.
- Gubbins, K.E., "Application of Statistical Mechanics to Engineering Problems: Computer Simulation and Perturbation Theory", Annual Meeting of the American Institute of Chemical Engineers, New York, Nov. 15-20, 1987. (Alpha Chi Sigma Award Lecture).
- Tan, Z., van Swol, F., and Gubbins, K.E., "Phase Equilibria of Mixtures in Capillaries", Annual Meeting of the American Institute of Chemical Engineers, New York, Nov. 15-20, 1987.
- Chan, K.Y., Gubbins, K.E., Henderson, D., and Blum, L., "Monte Carlo Simulations of Ion-Dipole Mixtures", Annual Meeting of the American Institute of Chemical Engineers, New York, Nov. 15-20, 1987.
- Gubbins, K.E., "The Role of Computer Simulation in Studying Phase Equilibria", CCP5 Meeting on Industrial Applications of Molecular Simulation, Birkbeck College, London, Jan. 6-8, 1988.
- Gubbins, K.E., Heffelfinger, G.S., Marini Bettolo Marconi, U., Tan, Z., and van Swol, F., "Fluid Mixtures in Narrow Capillary Pores", CCP5 Meeting on Industrial Applications of Molecular Simulation, Birkbeck College, London, Jan. 6-8, 1988.
- Jackson, G., Chapman, W.G., and Gubbins, K.E., "Phase Equilibria of Associating Fluids", 67th Annual GPA Convention, Dallas, Texas, March 14-16, 1988.
- Jackson, G., Chapman, W.G., and Gubbins, K.E., "Phase Equilibria of Associating Fluids: Spherical and Chain Molecules", International Symposium on Thermodynamics in Chemical Engineering and Industry, Beijing, China, May 31, 1988.
- Gubbins, K.E., "Capillary Condensation of Pure Fluids and Binary Mixtures in Narrow Pores", International Symposium on Thermodynamics in Chemical Engineering and Industry, Beijing, China, May 30, 1988.
- Jackson, G., Chapman, W.G., Gubbins, K.E., "Phase Equilibria of Associating Fluids", Tenth Symposium on Thermophysical Properties, National Bureau of Standards, Gaithersburg, Maryland, June 20, 1988.
- Gubbins, K.E., Heffelfinger, G.S., Marconi, U.M.B., Tan, Z., and van Swol, F., "Fluid Mixtures in Narrow Cylindrical Pores", Tenth Symposium on Thermophysical Properties, National Bureau of Standards, Gaithersburg, Maryland, June 21, 1988.
- Gubbins, K.E., "Mixtures of Polar and Associating Fluids: Theory and Simulation", 6th International Conference on Mixtures of Non-Electrolytes and Intermolecular Interactions, "Carl Schorlemmer" Technical University, Merseburg, German Democratic Republic, August 23-25, 1988.
- Gubbins, K.E., "Statistical Thermodynamics of Polar Fluid Mixtures", 10th IUPAC Conference on Chemical Thermodynamics, Prague, Czechoslovakia, August 9-Sept. 2, 1988.
- Chalam, M.K., Gubbins, K.E., and van Swol, F., "Simulation of a Nematogen in a Narrow Pore", Dense Fluids Conference, Cambridge, England, September 14-16, 1988.
- Gubbins, K.E., "Thermodynamics", A Century of Chemical Engineering: Intellectual Foundations of an Academic Discipline, a symposium by the MIT Department of Chemical Engineering in celebration of its 100th anniversary, Brewster, Cape Cod, MA, October 5-7, 1988.
- Gubbins, K.E., "Fluid Behavior in Narrow Capillary Pores", GRI Review Meeting, Chicago, Oct 25, 1988.

- Gubbins, K.E., "Associating Fluids and Mixtures", GRI Annual Review Meeting, San Antonio, Texas, March 15, 1989.
- Gubbins, K.E., "Fluid Behavior in Micropores", GRI Annual Review Meeting, San Antonio, Texas, March 15, 1989.
- Chapman, W.G., Gubbins, K.E., Jackson, G., Radosz, M., "SAFT: Equation-of-State Solution Model for Associating Fluids", Fifth International Conference on Fluid Properties and Phase Equilibria for Chemical Process Design, Banff, Canada, May 1-5, 1989.
- Tan, Z., van Swol, F., Gubbins, K.E., and Marini Bettolo Marconi, U., "Mixtures Confined to Narrow Pores: Computer Simulation and Theory", Third International Conference on Fundamentals of Adsorption, Sonthofen, Bavaria, FRG, May 9, 1989.
- Gubbins, K.E., "Theory and Simulation of Associating Liquids", Symposium on Computer Simulation of Associating Liquid Mixtures, Kyoto University, June 26, 1989.
- Johnson, J.K., Jackson, G., and Gubbins, K.E., "Thermodynamic Properties of Alkanol + Alkane Mixtures from a Theoretically Based Equation of State", Fifth International IUPAC Workshop on Vapor-Liquid Equilibria in 1-Alkanol and n-Alkane Mixtures, Gradisca, Italy, September 7-8, 1989.
- Tan, Z. and Gubbins, K.E., "Adsorption and Phase Equilibria in Carbon Micropores: Computer Simulation and Statistical Thermodynamics", 4th International Conference on Thermodynamics of Solutions of Nonelectrolytes, Santiago de Compostela, Spain, Sept. 24, 1989.
- Tan, Z. and Gubbins, K.E., "Fluid Mixture Behavior in Micropores", Annual Meeting of the American Institute of Chemical Engineers, San Francisco, Nov. 6, 1989.
- Chalam, M.K., Gubbins, K.E., and van Swol, F., "Liquid Crystal Phase transitions in a Narrow Pore", Annual Meeting of the American Institute of Chemical Engineers, San Francisco, Nov. 7, 1989.
- Gubbins, K.E., "Associating Fluids: Fluids in Micropores", GRI Fluid Properties Contract Review Meeting, Phoenix, AR, March 14, 1990.
- Tan, Z. and Gubbins, K.E., "Theory of Adsorption in Carbon Micropores", IUPAC Symposium on Characterization of Porous Solids (COPS-II), Alicante, Spain, May 7, 1990.
- Gubbins, K.E., "The Behavior of Fluids in Micropores", Third Liblice Conference on the Statistical Mechanics of Liquids, Bechyne, Czechoslovakia, May 28-June 1, 1990.
- E. de Miguel, L.F. Rull, M. Chalam, and K.E. Gubbins, "Computer Simulation of Liquid Crystals: Gay-Berne Model", First Liquid Matter Conference, European Physical Society, Lyon, France, July 7-11, 1990.
- K.E. Gubbins, "Statistical Mechanical Treatment of Inhomogeneous Fluids: Simulation and Density Functional Theory", Fluid Physics Summer School, Aguadulce, Almeria, Spain, August 6, 1990. [Invited main lecture]
- K.E. Gubbins, "Behavior of Fluids in Micropores", Fluid Physics Summer School, Aguadulce, Almeria, Spain, August 6, 1990. [Invited paper]
- Walsh, J.M. and Gubbins, K.E., "Statistical Thermodynamics of Simple Associating Fluids", 11th IUPAC Conference on Chemical Thermodynamics, Como, Italy, Aug. 26-31, 1990.
- Tan, Z., Rhykerd, C. and Gubbins, K.E., "Adsorption, Diffusion and Phase Transitions for Simple Fluids and Mixtures in Carbon Micropores", Annual AIChE Meeting, Chicago, Nov. 14, 1990.

- Walsh, J.M., Johnson, J.K. and Gubbins, K.E., "Simulation and Theory for Polyatomic Associating Fluids", Annual AIChE Meeting, Chicago, Nov. 14, 1990.
- Chalam, M.K., Gubbins, K.E., De Miguel, E. and Rull, L., "Molecular Simulation of a Model Liquid Crystal", Annual AIChE Meeting, Chicago, Nov. 15, 1990.
- Rhykerd, C., Tan, Z., Pozhar, L.A. and Gubbins, K.E., "Properties of Simple Fluids in Carbon Micropores", Faraday Symposium 26: Molecular Transport in Confined Regions and Membranes, Oxford, U.K., Dec. 17-18, 1990. [Invited paper]
- Walsh, J. and Gubbins, K.E., "Properties and Phase Behavior of Associating Fluids: Theory and Simulation", Conference on Molecular Simulation, Kyoto, Japan, March 22, 1991. [Invited paper]
- Gubbins, K.E. "Research in Molecular Simulation and Theory at Cornell University", Conference on Molecular Simulation, Kyoto, Japan, March 22, 1991.
- Gubbins, K.E., "Theory and Simulation of Fluids in Pores", CCP5 Conference on Computer Simulation of Pores, Southampton, UK, April 26, 1991. [Invited paper]
- Gubbins, K.E., "Applications of Statistical Mechanics and Simulation to Some Engineering Problems", Seminar on Molecular Fluids and Materials, School of Chemical Engineering, Cornell University, May 21, 1991.
- Walsh, J.M. and Gubbins, K.E., "Fluids of Small Associating Molecules", 11th Symposium on Thermophysical Properties, Boulder, June 23-27, 1991
- Balbuena, P. and Gubbins, K.E., "Classification of Adsorption Behavior: Simple Fluids in Pores of Cylindrical and Slit-Shaped Geometry", 11th Symposium on Thermophysical Properties, Boulder, June 23-27, 1991 [Invited paper].
- Gubbins, K.E., "Fluid Behavior in Porous Materials: Molecular Simulation", Condensed Matter Conference in honor of Professor J.G. Powles, University of Kent, Canterbury, UK, Sept. 5, 1991.
- Gubbins, K.E., "Behavior of Fluids and Fluid Mixtures in Microporous Materials: Computer Simulation", International Conference on Materials Engineering for Resources, Akita City, Japan, November 6, 1991 [Invited paper].
- Balbuena, P.B., Lastoskie, C., Gubbins, K.E. and Quirke, N., "Theoretical Interpretation and Classification of Adsorption Isotherms for Simple Fluids", Annual AIChE Meeting, Los Angeles, Nov. 20, 1991.
- Cracknell, R. and Gubbins, K.E., "Molecular Simulation of Adsorption and Diffusion in VPI-5", Annual AIChE Meeting, Los Angeles, Nov. 20, 1991.
- Jiang, S., Rhykerd, C., Balbuena, P.B. Pozhar, L.A. and Gubbins, K.E., "Adsorption and Diffusion of Methane in Carbon Pores at Low Temperature", Annual AIChE Meeting, Los Angeles, Nov. 21, 1991.
- Johnson, K., Walsh, J.M. and Gubbins, K.E., "Phase Equilibria for Associating Fluids: Molecular Simulation, Theory and Experiment", Annual AIChE Meeting, Los Angeles, Nov. 20, 1991.
- Gubbins, K.E. and Koh, C.K., "Associating Fluid Theory and Modeling", Gas Research Institute Fluid Properties Contract Review Meeting, Anaheim, CA, March 12-13, 1992.
- R.F. Cracknell, K.E. Gubbins, S. Jiang and S.M. Thompson, "Molecular Simulation Studies of Adsorption of Simple Gases in Microporous Materials", International Symposium on Fractal and Physically Adsorbed Molecular States (Chiba-FP-92), Chemical Society of Japan, Chiba, Japan, May 14-15, 1992. [Invited Paper].

- R.F. Cracknell and K.E. Gubbins, "Molecular Simulation of Adsorption and Diffusion in VPI-5", International Symposium on Fractal and Physically Adsorbed Molecular States (Chiba-FP-92), Chemical Society of Japan, Chiba, Japan, May 14-15, 1992.
- P.B. Balbuena, D. Berry and K.E. Gubbins, "Theoretical Interpretation and Classification of Adsorption Isotherms and Solvation Forces for Simple Fluids", International Symposium on Fractal and Physically Adsorbed Molecular States (Chiba-FP-92), Chemical Society of Japan, Chiba, Japan, May 14-15, 1992.
- R.F. Cracknell and K.E. Gubbins, "Molecular Simulation of Adsorption and Diffusion in VPI-5 and Other Aluminophosphates", IVth International Conference on Fundamentals of Adsorption, Kyoto, Japan, May 17-22, 1992. [Invited Paper].
- P.B. Balbuena, C. Lastoskie, K.E. Gubbins and N. Quirke, "Theoretical Interpretation and Classification of Adsorption Isotherms for Simple Fluids", IVth International Conference on Fundamentals of Adsorption, Kyoto, Japan, May 17-22, 1992.
- S. Jiang, C. Rhykerd, P.B. Balbuena, L.A. Pozhar and K.E. Gubbins, "Adsorption and Diffusion of Methane in Carbon Pores at Low Temperatures", IVth International Conference on Fundamentals of Adsorption, Kyoto, Japan, May 17-22, 1992.
- C. Lastoskie, K.E. Gubbins and N. Quirke, "Pore Size Distribution Analysis of Microporous Carbons Using a Density Functional Theory Approach", International Symposium on Effects of Surface Heterogeneity in Adsorption and Catalysis on Solids, Kazimierz Dolny, Poland, July 12-18, 1992.
- K.E. Gubbins, "Applications of Molecular Simulation", 6th International Conference on Fluid Properties & Phase Equilibria for Chemical Process Design, Cortina d'Ampezzo, Italy, July 19-24, 1992.
- C.A. Koh, H. Tanaka, K.E. Gubbins and J.A. Zollweg, "Thermodynamic and Structural Properties of Methanol-Water Mixtures: Experiment, Theory and Molecular Simulation", 6th International Conference on Fluid Properties & Phase Equilibria for Chemical Process Design, Cortina d'Ampezzo, Italy, July 19-24, 1992.
- K.E. Gubbins, "Molecular Simulation of Fluid Phase Equilibria", 12th IUPAC Conference on Chemical Thermodynamics, Snowbird, Utah, August 16-21, 1992.
- C.A. Koh, H. Tanaka, K.E. Gubbins and J.A. Zollweg, "Thermodynamic and Structural Properties of Methanol-Water Mixtures: Experiment, Theory and Molecular Simulation", 12th IUPAC Conference on Chemical Thermodynamics, Snowbird, Utah, August 16-21, 1992.
- J.K. Johnson and K.E. Gubbins, "Phase Equilibria for Strongly Associating Fluids from Theory and Computer Simulation", 12th IUPAC Conference on Chemical Thermodynamics, Snowbird, Utah, August 16-21, 1992.
- S. Jiang and K.E. Gubbins, "Methane on Graphite: Adsorption, Isosteric Heat and Phase Transitions", American Institute of Chemical Engineers Annual Meeting, November 1-6, 1992, Miami Beach.
- C. Lastoskie, K.E. Gubbins and N. Quirke, "Pore-Size Distribution Analysis and Networking Effects for Microporous Carbons", American Institute of Chemical Engineers Annual Meeting, November 1-6, 1992, Miami Beach.
- P.B. Balbuena, D. Berry and K.E. Gubbins, "Adsorption and Solvation Pressure for Methane/X Mixtures in Slit-Like Pores", American Institute of Chemical Engineers Annual Meeting, November 1-6, 1992, Miami Beach.

- C.A. Koh, H. Tanaka, K.E. Gubbins and J.A. Zollweg, "Thermodynamic and Structural Properties of Water-Methanol Mixtures: Experiment, Theory and Molecular Simulation", American Institute of Chemical Engineers Annual Meeting, November 1-6, 1992, Miami Beach.
- C.A. Koh, K.E. Gubbins and J.A. Zollweg, "The Application of FTIR and FT Raman Spectroscopy to the Study of the Thermophysical Properties and Kinetics of Formation of Gas Hydrates", American Institute of Chemical Engineers Annual Meeting, November 1- 6, 1992, Miami Beach.
- D.E. Ulberg and K.E. Gubbins, "Monte Carlo Simulation of Bulk and Confined Water on the Connection Machine", American Institute of Chemical Engineers Annual Meeting, November 1-6, 1992, Miami Beach.
- R. Cracknell, C.A. Koh, S.M. Thompson and K.E. Gubbins, "Molecular Simulation of Adsorption of Simple Gases in Aluminophosphates and Pillared Clays", Materials Research Society Annual Meeting, Nov. 30-Dec. 4, 1992, Boston.
- S. Jiang and K.E. Gubbins, "Computer Simulation Study of Adsorption, Isothermic Heat and Phase Transition of Methane on Graphite", Materials Research Society Annual Meeting, Nov. 30-Dec. 4, 1992, Boston.
- K.E. Gubbins, "Applications of Molecular Theory and Simulation in Natural Gas-Related Physical Property Research", Gas Processors Association Annual Convention, San Antonio, March 15, 1993.
- K.E. Gubbins, "Molecular Simulation of Phase Equilibria", Conference on Dense Fluids, Bristol, U.K., March 25, 1993.
- K.E. Gubbins, "Liquids and Liquid Mixtures", Symposium on Statistical Mechanics of Fluids (to mark the retirement of Prof. John S. Rowlinson), Physical Chemistry Laboratory, Oxford, U.K., March 30, 1993.
- P.B. Balbuena and K.E. Gubbins, "The Effect of Pore Geometry on Adsorption Behavior", IUPAC Symposium on Characterization of Porous Solids (COPS-III), Marseille, France, May 9-12, 1993.
- C. Lastoskie, K.E. Gubbins and N. Quirke, "Pore-Size Distribution Analysis and Networking: Studies of Microporous Sorbents", IUPAC Symposium on Characterization of Porous Solids (COPS-III), Marseille, France, May 9-12, 1993.
- C.A. Koh, J.A. Zollweg and K.E. Gubbins, "FTIR Spectroscopic Study of Adsorption of Simple Gases, Methanol and Water on Aluminophosphates", IUPAC Symposium on Characterization of Porous Solids (COPS-III), Marseille, France, May 9-12, 1993.
- K.E. Gubbins, "Molecular Theory of Adsorption", Conference on New Directions in Separation Technology, Noordwijkerhout, Netherlands, July 1, 1993.
- L.F. Vega, A.Z. Panagiotopoulos and K.E. Gubbins, "Adsorption of Polymers between Walls: Monte Carlo Simulation", Annual Meeting of the American Institute of Chemical Engineers, St. Louis, November 7-12, 1993.
- C.M. Lastoskie, K.E. Gubbins and N. Quirke, "Air Separation in Model Sieve Carbons", Annual Meeting of the American Institute of Chemical Engineers, St. Louis, November 7-12, 1993.
- L.A. Pozhar, E.V. Akhmatskaya, D.E. Ulberg and K.E. Gubbins, "Transport Coefficients of Dense Inhomogeneous Fluids Confined in Narrow Capillary Pores", Annual Meeting of the American Institute of Chemical Engineers, St. Louis, November 7-12, 1993.

- S. Jiang, K.E. Gubbins and J.A. Zollweg, "Vapor-Liquid Equilibrium of Methane on Graphite by Gibbs Ensemble Simulation", Annual Meeting of the American Institute of Chemical Engineers, St. Louis, November 7-12, 1993.
- C.M. Lastoskie, K.E. Gubbins and N. Quirke, "Sorbent Pore Size Distributions from Density Functional Analysis", Annual Meeting of the American Institute of Chemical Engineers, St. Louis, November 7-12, 1993.
- S. Jiang, J.A. Zollweg and K.E. Gubbins, "High Pressure Adsorption of Methane and Ethane on Activated Carbons and Carbon Fibers", Annual Meeting of the American Institute of Chemical Engineers, St. Louis, November 7-12, 1993.
- S. Jiang, P.B. Balbuena, S. Sowers and K.E. Gubbins, "Selectivity at Infinite Dilution for Methane/X Mixtures in Slit Pores", Annual Meeting of the American Institute of Chemical Engineers, St. Louis, November 7-12, 1993.
- M. Maddox, D. Ulberg and K.E. Gubbins, "Molecular Simulation of Simple Fluids and Water in Porous Carbons", International Symposium on Molecular Thermodynamics and Molecular Simulation, Kyoto, Japan, Jan. 10-12, 1994.
- K.E. Gubbins, M. Maddox and D. Ulberg, "Molecular Simulation of Simple Fluids and Water in Well-Characterized Pores", Fourth Liblice Conference on the Statistical Mechanics of Liquids, Lake Milovoy, Czech Republic, June 6-10, 1994.
- J.K. Johnson, E.A. Muller and K.E. Gubbins, "Equation of State for Lennard-Jones Model Polymer", Annual American Institute of Chemical Engineers' Meeting, San Francisco, Nov. 13-18, 1994.
- E.A. Muller and K.E. Gubbins, "Theory and Molecular Simulation for a New Model of Water", Annual American Institute of Chemical Engineers' Meeting, San Francisco, Nov. 13-18, 1994.
- S.L. Sowers, M.W. Maddox and K.E. Gubbins, "Selective Removal of Trace Pollutants in Gaseous Streams by Adsorption in Micropores", Annual American Institute of Chemical Engineers' Meeting, San Francisco, Nov. 13-18, 1994.
- C. Lastoskie, K.E. Gubbins and N. Quirke, "Pore Size and Connectivity Studies of Microporous Sorbents", Annual American Institute of Chemical Engineers' Meeting, San Francisco, Nov. 13-18, 1994.
- C.A. Koh, R.I. Nooney, M. Maddox, S. Sowers and K.E. Gubbins, "Spectroscopic and Simulation Studies of the Removal of Trace Gases by Adsorption in Novel Materials: MCM-41, Buckytubes, VPI-5", Annual American Institute of Chemical Engineers' Meeting, San Francisco, Nov. 13-18, 1994.
- S. Jiang and K.E. Gubbins, "On Estimating Optimal Operating Conditions for Trace Removal by Adsorption", Annual American Institute of Chemical Engineers' Meeting, San Francisco, Nov. 13-18, 1994.
- M.W. Maddox, S.L. Sowers and K.E. Gubbins, "Molecular Simulation of Binary Mixture Adsorption in Buckytubes and MCM-41", Annual American Institute of Chemical Engineers' Meeting, San Francisco, Nov. 13-18, 1994.
- S. Jiang, K.E. Gubbins and J.A. Zollweg, "Pore Size Distribution of Activated Carbon AC610 Determined from High Pressure Adsorption Data", Annual American Institute of Chemical Engineers' Meeting, San Francisco, Nov. 13-18, 1994.

- L.F. Vega, E.A. Muller, K.E. Gubbins and L.F. Rull, "Monte Carlo Simulation of Associating Chains in Slit-Like Pores - Adsorption Isotherms", Annual American Institute of Chemical Engineers' Meeting, San Francisco, Nov. 13-18, 1994.
- K.E. Gubbins, E.A. Müller, S. Sowers, L.F. Vega and L. Rull, "Selective adsorption from Mixtures in Model Porous Systems", Fourteenth Experimental Thermodynamics Conference (joint with Statistical Mechanics & Thermodynamics Group of the RSC), Reading, U.K., April 5-7, 1995.
- S.L. Sowers and K.E. Gubbins, "Removal of Trace Pollutants by Adsorption: Density Functional Theory and Monte Carlo Simulation", Fifth International Conference on Fundamentals of Adsorption, Asilomar, CA, May 13-18, 1995.
- C.M. Lastoskie, M.W. Maddox, K.E. Gubbins and N. Quirke, "Simulation Studies of Pore Blocking Hysteresis in Model Porous Carbon Networks", Fifth International Conference on Fundamentals of Adsorption, Asilomar, CA, May 13-18, 1995.
- M.W. Maddox, S.L. Sowers and K.E. Gubbins, "Molecular Simulation of Binary Mixture Adsorption in Buckytubes and MCM-41", Fifth International Conference on Fundamentals of Adsorption, Asilomar, CA, May 13-18, 1995.
- L.F. Vega, E.A. Müller and K.E. Gubbins, "Adsorption Isotherms of Associating Chains in Slit-Like Pores: a Monte Carlo Simulation Study", Fifth International Conference on Fundamentals of Adsorption, Asilomar, CA, May 13-18, 1995.
- M. Sliwinska-Bartkowiak, S.L. Sowers and K.E. Gubbins, "Effect of Confinement on Solubility and Liquid-Liquid Phase Transitions", International Symposium on the Effects of Surface Heterogeneity in Adsorption and Catalysis on Solids, Zakopane, Poland, September 4-9, 1995.
- K.E. Gubbins, "Molecular Simulation of Phase Transitions in Pores", CECAM (Centre Européen de Calcul Atomique et Moléculaire) Workshop on Adsorption, Phase Transitions and Transport in Porous Materials, Lyon, France, September 11-15, 1995.
- K.E. Gubbins, "Molecular Simulation of Fluid Phase Equilibria and Adsorption", International Conference on Molecular Modeling in the Oil and Gas Sciences, Institut Français du Pétrole, Paris, France, October 23-24, 1995.
- M. Maddox and K.E. Gubbins, "Molecular Simulation of the Freezing of Adsorbed Fluids in Buckytubes and MCM-41", American Institute of Chemical Engineers Annual Meeting, Miami Beach, November 13-17, 1995.
- C.L. Rhykerd, T.M. Duncan and K.E. Gubbins, "Improved Resolution of Pore Size Distribution of Microporous Carbons", American Institute of Chemical Engineers Annual Meeting, Miami Beach, November 13-17, 1995.
- M. Sliwinska-Bartkowiak, S.L. Sowers and K.E. Gubbins, "Selective Adsorption, Solubility and Liquid-Liquid Phase Transitions in Pores", American Institute of Chemical Engineers Annual Meeting, Miami Beach, November 13-17, 1995.
- E.A. Müller, T. Kraska and K.E. Gubbins, "Application of the LJ-SAFT Equation of State to Water, n-Alkanes, 1-Alkanols and their Mixtures", American Institute of Chemical Engineers Annual Meeting, Miami Beach, November 13-17, 1995.
- E.A. Müller and K.E. Gubbins, "Estudio de la Adsorción de Metano y Vapor de Agua en Carbones Activados Porosos por Simulación Molecular", Equifase 95, December 5-8, 1995.

- K.E. Gubbins, "Theory and Simulation of Adsorption in Micropores", NATO Advanced Summer Institute on Physical Adsorption: Experiment, Theory and Application, Nice, France, May 19-31, 1996.
- K.E. Gubbins and E.A. Müller, "Molecular Simulation of Water and Water-Hydrocarbon Mixtures in Activated Carbons", 1996 International Workshop on Molecular Simulation and its Application", Keimyung University, Taegu, Korea, August 20, 1996.
- K.E. Gubbins, E.A. Müller, L.F. Rull and L.F. Vega, "Adsorption of Water and Water/Methane Mixtures on Activated Carbons", International Symposium on Nanopore Fluid Chemistry and its Application, Makuhari, Chiba, Japan, August 22, 1996.
- K.E. Gubbins and S.L. Sowers, "Fluid Behavior in Well-Characterized Porous Materials: Theory and Simulation", Conference on Catalysis and Reactions in Supercritical Fluids, Ngoya, Japan, August 24, 1996.
- K.E. Gubbins and E.A. Müller, "Molecular Simulation of Fluids in Pores: Adsorption and Phase Transitions", 14th IUPAC Conference on Chemical Thermodynamics, Osaka, Japan, August 25-30, 1996.
- M. Sliwinska-Bartkowiak, R. Sikorski, S.L. Sowers, L.D. Gelb, M.W. Maddox and K.E. Gubbins, "Phase Separation for Mixtures in Well-Characterized Porous Materials: Liquid-Liquid and Freezing Transitions", 14th IUPAC Conference on Chemical Thermodynamics, Osaka, Japan, August 25-30, 1996.
- M.W. Maddox, N. Quirke and K.E. Gubbins, "Simulation Studies of Pore Blocking Phenomena in Model Porous Carbon Networks", 4th International Symposium on the Characterization of Porous Solids, September 15-18, Bath, U.K.
- K. Kiyohara, K.E. Gubbins and A.Z. Panagiotopoulos, "Monte Carlo Simulations of Stockmayer Fluids and Water", 1996 Annual Meeting of the American Institute of Chemical Engineers, Chicago, November 10-15, 1996.
- E.A. Müller and K.E. Gubbins, "Molecular Simulation of Adsorption of Water-Methane Mixtures in Activated Carbons", 1996 Annual Meeting of the American Institute of Chemical Engineers, Chicago, November 10-15, 1996.
- M.W. Maddox, K.E. Gubbins and N. Quirke, "Simulation Studies of Pore Blocking Phenomena in Model Porous Carbon Networks", 1996 Annual Meeting of the American Institute of Chemical Engineers, Chicago, November 10-15, 1996.
- S.L. Sowers, L.D. Gelb and K.E. Gubbins, "A Theoretical and Simulation Study of Liquid-Liquid Phase Equilibria in Porous Materials", 1996 Annual Meeting of the American Institute of Chemical Engineers, Chicago, November 10-15, 1996.
- K.E. Gubbins, "Molecular Modeling of Adsorption Processes", International Conference on Advances in Chemical Engineering 1996, Indian Institute of Technology, Madras, India, December 11-13, 1996.
- K.E. Gubbins, "Molecular Simulation of Adsorption and Phase Equilibria in Porous Media", International Symposium on Molecular Thermodynamics and Molecular Simulation, Hosei University, Tokyo, Japan, January 12-15, 1997.
- K.E. Gubbins, "Phase Separation in Narrow Pores", Thermodynamics '97, University of Surrey, U.K., April 16-18, 1997.
- F. Jimenez Blas, L.F. Vega and K.E. Gubbins, "Modeling New Adsorbents for Ethylene/Ethane Separation by Adsorption via π -Complexation", Thirteenth Symposium on Thermophysical Properties, Boulder, CO, June 22-27, 1997.

- J.R. Errington, K. Kiyohara, K.E. Gubbins and A.Z. Panagiotopoulos, "Monte Carlo Simulation of High Pressure Phase Equilibria", Thirteenth Symposium on Thermophysical Properties, Boulder, CO, June 22-27, 1997.
- L.A. Pozhar and K.E. Gubbins, "Transport Properties of Inhomogeneous Fluid Mixtures", Thirteenth Symposium on Thermophysical Properties, Boulder, CO, June 22-27, 1997.
- F. Jimenez Blas, K.E. Gubbins and L.F. Vega, "Modeling of New Adsorbents by Monte Carlo Simulations", Fisica Estadística 97, Madrid, Sept. 24-27, 1997.
- L. Gelb, M. Miyahara, R. Radhakrishnan, K. Gubbins and M. Sliwinska-Bartkowiak, "Phase Separation in Narrow Pores", Conference on Physical Chemistry of Surface Phenomena, Polish Chemical Society, Krakow, Poland, June 9-10, 1997.
- K.E. Gubbins, "Molecular Simulation Overview", NSF Workshop on Future Directions in Molecular Modeling and Simulation: Fundamentals and Applications, The National Science Foundation, Arlington, VA, November 3-4, 1997.
- K.E. Gubbins, "Molecular Modeling of Adsorption", 1997 Annual Meeting of the American Institute of Chemical Engineers, Los Angeles, Nov. 19, 1997.
- R. Radhakrishnan and K.E. Gubbins, "Phase Transitions in Nanoporous Materials", 1997 Annual Meeting of the American Institute of Chemical Engineers, Los Angeles, Nov. 19, 1997.
- T.J. Bandosz, K.E. Gubbins, F.J. Blas, C.L. McCallum, S.L. Sowers and L.F. Vega, "Molecular Modeling of Selective Adsorption from Mixtures", Annual Meeting of the Materials Research Society, Boston, December 4, 1997.
- L.D. Gelb, M. Sliwinska-Bartkowiak and K.E. Gubbins, "Fluid Phase Separation in Controlled Pore Glasses", 78th Statistical Mechanics Conference, Rutgers University, Dec. 14, 1997.
- J.K. Button and K.E. Gubbins, "SAFT Prediction of Vapour-Liquid Equilibria of Mixtures Containing Carbon Dioxide and Aqueous Monoethanolamine or Diethanolamine", 8th International Conference on Properties and Phase Equilibria for Product and Process Design, April 29, 1998.
- L.D. Gelb and K.E. Gubbins, "Characterization of Porous Glasses by Adsorption: Models, Simulations and Data Inversion", International Conference on Fundamentals of Adsorption FOA6, Presqu'île de Giens, France, May 24-28, 1998.
- K.P. Travis and K.E. Gubbins, "Transport Diffusion of a Mixture of Oxygen and Nitrogen in a Carbon Slit via Dual Control Volume Grand Canonical Molecular Dynamics", International Conference on Fundamentals of Adsorption FOA6, Presqu'île de Giens, France, May 24-28, 1998.
- T.J. Bandosz, K.E. Gubbins, C.L. McCallum, S.C. McGrother, E.A. Müller and S.L. Sowers, "An Improved Model for Adsorption of Water and Aqueous Mixtures on Activated Carbons", International Conference on Fundamentals of Adsorption FOA6, Presqu'île de Giens, France, May 24-28, 1998.
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- M. Sliwinska-Bartkowiak, J. Gras, G. Dudziak, L.D. Gelb, R. Radhakrishnan and K.E. Gubbins, "Phase Transitions in Pores: Molecular Simulation and Experimental Results", Third

- International Symposium on Effects of Surface Heterogeneity in Adsorption and Catalysis on Solids, Toruń, Poland, August 9-16, 1998.
- K.P. Travis and K.E. Gubbins, "The Effect of Confinement on Transport Diffusion in Binary Liquid Mixtures: A Non-Equilibrium Molecular Dynamics Study", Third International Symposium on Effects of Surface Heterogeneity in Adsorption and Catalysis on Solids, Toruń, Poland, August 9-16, 1998.
- K.E. Gubbins, "Recent Advances in Molecular Simulation Methods: Phase Equilibria in Bulk and Confined Systems", International Conference on Thermal Properties, Kyushu University, Fukuoka, Japan, October 21, 1998.
- R. Radhakrishnan and K.E. Gubbins, "Freezing in Slit Pores: An Order Parameter Study using Monte Carlo Simulation", Annual Meeting of the American Institute of Chemical Engineers, Miami Beach, November 15-20, 1998.
- L.D. Gelb and K.E. Gubbins, "Adsorption in Glasses: Realistic Models", Annual Meeting of the American Institute of Chemical Engineers, Miami Beach, November 15-20, 1998.
- K.E. Gubbins, F.J. Blas and L.F. Vega "Selective Adsorption from Mixtures: Grand Canonical Monte Carlo and Density Functional Theory", Annual Meeting of the American Institute of Chemical Engineers, Miami Beach, November 15-20, 1998.
- K.P. Travis and K.E. Gubbins, "Computer Simulation of Liquid Flow in Porous Materials", Annual Meeting of the American Institute of Chemical Engineers, Miami Beach, November 15-20, 1998.
- K.E. Gubbins, "Molecular Modeling: Applications to Chemical Engineering", Conference on Molecular Modeling: A Tool for the Modern Era, St. Bartholomew's Hospital, London, December 14, 1998.
- M. Sliwinska-Bartkowiak, L.D. Gelb, R. Radhakrishnan and K.E. Gubbins, "Phase Transitions in Pores: Molecular Simulation and Experimental Results", Annual Meeting of the American Chemical Society, Anaheim, CA, March 21-25, 1999.
- L.D. Gelb and K.E. Gubbins, "Molecular Modeling of Adsorption in Amorphous Nano-Porous Materials", with L.D. Gelb, Annual Meeting of the American Chemical Society, Anaheim, CA, March 21-25, 1999.
- K.E. Gubbins, M. Sliwinska-Bartkowiak and R. Radhakrishnan, "Experimental and Simulation Studies of Melting and Freezing in Porous Materials", Thermodynamics 99 Conference, Imperial College of Science & Technology, London, April 15, 1999.
- K.E. Gubbins, "Molecular Simulation: Phase Equilibria and Confined Systems", International Workshop on Scientific Computing in Chemical Engineering II, Hamburg, Germany, May 26-28, 1999.
- K.E. Gubbins and C.M. Lastoskie, "Density Functional Theory and the Pore Size Distribution", Characterization of Porous Solids V, Heidelberg, Germany, May 30- June 2, 1999.
- M. Miyahara, H. Kanda, K. Higashitani and K.E. Gubbins, "Molecular Simulation Study on Freezing in Nano-Pores", Characterization of Porous Solids V, Heidelberg, Germany, May 30-June 2, 1999.
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- S.A. Gavalda, R. Radhakrishnan, S.C. McGrother, K. Kaneko, M. Sliwinska-Bartkowiak and K.E. Gubbins, "Remarkable Freezing Behavior in Activated Carbon Fibers: Comparison Between Simulation and Experiment", Carbon '99, Charleston, SC, July 11-16, 1999.
- C.H. Turner and K.E. Gubbins, "Molecular Modeling of Chemical Reaction Equilibria in Pores: Effects of Confinement on Equilibrium Yield", Carbon '99, Charleston, SC, July 11-16, 1999.
- K.T. Thomson and K.E. Gubbins, "Improved Molecular Model of Activated Carbons Using Molecular Simulation", Carbon '99, Charleston, SC, July 11-16, 1999.
- M. Sliwinska-Bartkowiak, K. Kaneko, K.E. Gubbins and R. Radhakrishnan, "Understanding Freezing Behavior in Porous Materials: Comparison between Simulation and Experiment", American Institute of Chemical Engineers Annual Meeting, Dallas, October 31-November 5, 1999.
- S. Jiang, A.V. Shevade and K.E. Gubbins, "Molecular Simulation Studies of Adsorption of Water-Methanol Mixtures in Activated Carbons", American Institute of Chemical Engineers Annual Meeting, Dallas, October 31-November 5, 1999.
- K.E. Gubbins, C.H. Turner and J.K. Johnson, "Molecular Modeling of Chemical Reaction Equilibria in Narrow Pores: Effect of Confinement on Equilibrium Yield", American Institute of Chemical Engineers Annual Meeting, Dallas, October 31-November 5, 1999.
- K.E. Gubbins and R. Radhakrishnan, "Novel Phase Behavior in Activated Carbon Micropores: A Monte Carlo Study of the Breaking of the Rotational and Translational Symmetry", American Institute of Chemical Engineers Annual Meeting, Dallas, October 31-November 5, 1999.
- K.E. Gubbins, J.P. Pikunic and K.T. Thomson, "Molecular Simulation Methods for Modeling Pore Morphology of Activated Carbons", American Institute of Chemical Engineers Annual Meeting, Dallas, October 31-November 5, 1999.
- R. Radhakrishnan, K.E. Gubbins, M. Sliwinska-Bartkowiak and K. Kaneko, "Understanding Freezing Behavior in Pores", 2nd Pacific Basin Conference on Adsorption Science and Technology, Brisbane, Australia, May 14-18, 2000.
- K. Thomson, J. Pikunic and K.E. Gubbins, "An Improved Model of Microporous Carbon Morphology Using Molecular Simulation", 2nd Pacific Basin Conference on Adsorption Science and Technology, Brisbane, Australia, May 14-18, 2000.
- C. H. Turner, J. Brennan, K.E. Gubbins and J.K. Johnson, "Effects of Confinement on Chemical Reaction Equilibrium", 2nd Pacific Basin Conference on Adsorption Science and Technology, Brisbane, Australia, May 14-18, 2000.
- K.E. Gubbins, M. Sliwinska-Bartkowiak, J. Gras, R. Sikorski and R. Radhakrishnan, "Understanding Freezing Behavior in Porous Materials", 2nd International Workshop on Characterization of Porous Materials, Princeton, NJ, June 19-21, 2000.
- J. Brennan, K.E. Gubbins and T.J. Bandosz, "Review Article: Water in Porous Carbon", 2nd International Workshop on Characterization of Porous Materials, Princeton, NJ, June 19-21, 2000.
- K.E. Gubbins, "Molecular Simulation: Some Recent Applications to Phase and Chemical Equilibria", First International Conference on Foundations of Molecular Modeling and Simulation (FOMMS 2000), Keystone, Colorado, July 23-28, 2000.
- J.K. Brennan, K.T. Thomson and K.E. Gubbins, "Water in Porous Carbon: Simulation Study", First International Conference on Foundations of Molecular Modeling and Simulation (FOMMS 2000), Keystone, Colorado, July 23-28, 2000.
- L.D. Gelb and K.E. Gubbins, "Simulations of Capillary Condensation in Porous Glasses", First International Conference on Foundations of Molecular Modeling and Simulation (FOMMS 2000), Keystone, Colorado, July 23-28, 2000.

- S.F. Gerstenmaier, L.F. Vega, F.J. Blas and K.E. Gubbins, "Molecular Model of Gamma-Alumina: Nitrogen Adsorption and Pore Size Distribution", First International Conference on Foundations of Molecular Modeling and Simulation (FOMMS 2000), Keystone, Colorado, July 23-28, 2000.
- K.E. Gubbins, R. Radhakrishnan and M. Sliwinska-Bartkowiak, "Understanding Freezing Behavior in Porous Materials: Comparison Between Simulation and Experiment", International Discussion Meeting on Physical Chemistry in Confining Geometries: From Single Molecules to Mesoscopic Systems, Berlin, Germany, September 20-22, 2000.
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- K.T. Thomson, J. Pikunic and K.E. Gubbins, "Improved Molecular Models for Adsorption in Porous Carbons", International Conference on Colloid and Surface Science, Chemical Society of Japan, Tokyo, November 5-8, 2000.
- M. Sliwinska-Bartkowiak, J. Gras, R. Sikorski, R. Radhakrishnan and K.E. Gubbins, "Freezing Behavior in Porous Materials: Simulation vs. Experiment", International Conference on Colloid and Surface Science, Chemical Society of Japan, Tokyo, November 5-8, 2000.
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- K.E. Gubbins, "Applications and Opportunities in Separations and Reaction Equilibria", American Institute of Chemical Engineers Annual Meeting, November 13, 2000.
- C.H. Turner, J.K. Brennan, J.K. Johnson and K.E. Gubbins, "Effect of Confinement on Chemical Reaction Equilibria: Simulation of NO Dimerization and NH_3 Synthesis in a Carbon Pore", American Institute of Chemical Engineers Annual Meeting, November 13, 2000.
- R. Radhakrishnan and K.E. Gubbins, "An Attempt to Nucleate the Ice Phase in Computer Simulations", American Institute of Chemical Engineers Annual Meeting, November 13, 2000.
- C.M. Colina and K.E. Gubbins, "Solubility of PFOA and PDMS in Supercritical Carbon Dioxide Using SAFT", American Institute of Chemical Engineers Annual Meeting, November 13, 2000.
- R. Radhakrishnan, K.E. Gubbins and M. Sliwinska-Bartkowiak, "A Free Energy Study of the Lower-Dimensional Phase Behavior Using the Landau-Ginzburg Formalism", American Institute of Chemical Engineers Annual Meeting, November 13, 2000.
- S. Figueroa Gerstenmaier, L.F. Vega, F.J. Blas, L.D. Gelb and K.E. Gubbins, "Pore Size Distribution Analysis of Model Porous Glasses by Molecular Simulation and Density Functional Theory", American Institute of Chemical Engineers Annual Meeting, November 13, 2000.
- K.T. Thomson and K.E. Gubbins, "Characterizing Adsorption, Diffusion and Freezing in Activated Carbons Using the Reverse Monte Carlo Method", American Institute of Chemical Engineers Annual Meeting, November 13, 2000.
- S.A. Gavalda, K.T. Thomson, K. Kaneko and K.E. Gubbins, "Molecular Modeling of Carbon Aerogels", American Institute of Chemical Engineers Annual Meeting, November 13, 2000.

- J.G. Pikunic, K.T. Thomson, K.E. Gubbins, R. Pellenq, P. Levitz and J.-N. Rouzaud, "Realistic Molecular Models for Porous Carbons from Radiation Scattering Data", American Institute of Chemical Engineers Annual Meeting, November 13, 2000.
- K.E. Gubbins, J.K. Brennan and K.T. Thomson, "Simulation of Water and Water/Methane Mixtures in Microporous Carbon", American Institute of Chemical Engineers Annual Meeting, November 13, 2000.
- R. Radhakrishnan, K.E. Gubbins and M. Sliwinska-Bartkowiak, "Do Molecules Freeze in Confined Spaces: A Comparative Study of Simulations and Experiment", American Institute of Chemical Engineers Annual Meeting, November 13, 2000.
- K.E. Gubbins, "Molecular Modeling of Confined Nano-Phases in Amorphous Materials", Fundamentals of Adsorption 7, Nagasaki, Japan, May 20-25, 2001.
- K.E. Gubbins, R. Radhakrishnan, K. Kaneko and M. Sliwinska-Bartkowiak, "Understanding Freezing Behavior in Porous Materials: Comparison between Simulation and Experiment", Fundamentals of Adsorption 7, Nagasaki, Japan, May 20-25, 2001.
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- J.K. Brennan, K.T. Thomson and K.E. Gubbins, "Water in Porous Carbon: Simulation Study", Fundamentals of Adsorption 7, Nagasaki, Japan, May 20-25, 2001.
- C.H. Turner and K.E. Gubbins, "Monte Carlo Simulations of Chemical Reaction Equilibria in Carbon Micropores: $2\text{NO} = (\text{NO})_2$ and $\text{N}_2 + 3\text{H}_2 = 2\text{NH}_3$ ", Fundamentals of Adsorption 7, Nagasaki, Japan, May 20-25, 2001.
- M. Lisal, C.K. Hall, K.E. Gubbins and A.Z. Panagiotopoulos, "Micellar Behavior in Supercritical Solvent-Surfactant Systems from Lattice Monte Carlo Simulations", 9th International Conference on Properties and Phase Equilibria for Product and Process Design, Kurashiki, Japan, May 20-25, 2001.
- C.M. Colina, C.K. Hall and K.E. Gubbins, "Phase Behavior of PVAC-PTAN Block Copolymer in Supercritical Carbon Dioxide Using SAFT", 9th International Conference on Properties and Phase Equilibria for Product and Process Design, Kurashiki, Japan, May 20-25, 2001.
- M. Sliwinska-Bartkowiak, A.G. Dudziak, R. Gras, R. Radhakrishnan and K.E. Gubbins, "Understanding Freezing Behavior in Porous Materials: Comparison Between Simulation and Experiment", 4th International Symposium of Effects of Surface Heterogeneity in Adsorption and Catalysis, Krakow, Poland, August 27-31, 2001.
- C.H. Turner, J.K. Brennan, J. Pikunic and K.E. Gubbins, "Simulation of Chemical Reaction Equilibria in Heterogeneous Carbon Micropores", 4th International Symposium of Effects of Surface Heterogeneity in Adsorption and Catalysis, Krakow, Poland, August 27-31, 2001.
- M. Sliwinska-Bartkowiak, R. Radhakrishnan and K.E. Gubbins, "Freezing in Pores", Statistical Mechanics of Adsorption Conference (in honor of the retirement of Dr. David Nicholson), Imperial College London, October 3, 2001.

- F. Siperstein and K.E. Gubbins, "Mimetic Synthesis and Characterization of Templated Mesoporous Materials Using Molecular Simulation", American Institute of Chemical Engineers Annual Meeting, Reno, NV, November 4-9, 2001.
- L.F. Turens, L.F. Vega, C.G. Olivera-Fuentes, C.M. Colina and K.E. Gubbins, "Joule-Thomson Inversion Curves from the Soft-SAFT Equation of State", American Institute of Chemical Engineers Annual Meeting, Reno, NV, November 4-9, 2001.
- J.K. Brennan, C.H. Turner and K.E. Gubbins, "Approximate Treatment of Reaction Equilibria in Porous Materials", American Institute of Chemical Engineers Annual Meeting, Reno, NV, November 4-9, 2001.
- J. Pikunic, R.J. Pellenq and K.E. Gubbins, "Modeling Porous Carbons by Simultaneous Reverse Monte Carlo and Energy Minimization", American Institute of Chemical Engineers Annual Meeting, Reno, NV, November 4-9, 2001.
- C.H. Turner, J. Pikunic and K.E. Gubbins, "Enhancement of the Ammonia Synthesis Reaction in Heterogeneous Microporous Carbon Models Predicted from Monte Carlo Simulation", American Institute of Chemical Engineers Annual Meeting, Reno, NV, November 4-9, 2001.
- J.K. Brennan, K.T. Thomson and K.E. Gubbins, "Adsorption Simulations of Water-Methane Mixtures in Activated Carbons", American Institute of Chemical Engineers Annual Meeting, Reno, NV, November 4-9, 2001.
- C.M. Colina, C.K. Hall and K.E. Gubbins, "Modeling Surfactant Aggregation and Solubility of Block Copolymers in Supercritical Carbon Dioxide using SAFT", American Institute of Chemical Engineers Annual Meeting, Reno, NV, November 4-9, 2001.
- L.H. Fillous, F.R. Siperstein, M. Lisal and K.E. Gubbins, "Phase Behavior of Water/Oil/Surfactant Systems Using Lattice Monte Carlo: Determination of Optimum Formulation", American Institute of Chemical Engineers Annual Meeting, Reno, NV, November 4-9, 2001.
- C.H. Turner, J.K. Brennan and K.E. Gubbins, "Chemical Reaction Kinetics in Non-Ideal Environments Predicted from Reactive Monte Carlo Simulations: The Reaction $2\text{HI} = \text{H}_2 + \text{I}_2$ ", American Institute of Chemical Engineers Annual Meeting, Reno, NV, November 4-9, 2001.
- K.E. Gubbins, R. Radhakrishnan, M. Sliwinska-Bartkowiak and C.H. Turner, "Effects of Confinement on Phase Transitions and Chemical Reactions", Statistical Mechanics Mini-Symposium, Imperial College of Science, Technology and Medicine, April 16, 2002.
- M. Sliwinska-Bartkowiak, R. Radhakrishnan and K.E. Gubbins, "Freezing and Melting Phenomena in Nano-Pores", Sixth Liblice Conference on the Statistical Mechanics of Liquids, Špindlerův Mlýn, Czech Republic, June 9-14, 2002.
- C.M. Colina, M. Lisal, F. Siperstein and K.E. Gubbins, "Accuracy of Joule-Thomson Inversion Curves by Molecular Simulation", Sixth Liblice Conference on the Statistical Mechanics of Liquids, Špindlerův Mlýn, Czech Republic, June 9-14, 2002.
- J.K. Brennan, C.H. Turner and K.E. Gubbins, "Effect of Confinement in Porous Materials on Chemical Reaction Kinetics", Sixth Liblice Conference on the Statistical Mechanics of Liquids, Špindlerův Mlýn, Czech Republic, June 9-14, 2002.
- M. Sliwinska-Bartkowiak, R. Radhakrishnan and K.E. Gubbins, "Freezing in Narrow Pores", 5th Liquid Matter Conference of the European Physical Society, Konstanz, Germany, September 14-18, 2002.

- F.R. Hung, F.R. Siperstein, M. Sliwinska-Bartkowiak, C. Alba-Simionesco and K.E. Gubbins, "Freezing/Melting Behavior of Fluids Confined in Carbon Nanotubes and MCM-41", American Institute of Chemical Engineers Annual Meeting, Indianapolis, November 3-8, 2002.
- J. Pikunic, R. Pellenq and K.E. Gubbins, "Properties of Simple Fluids Confined in Realistic Models of Nano-Porous Carbons", American Institute of Chemical Engineers Annual Meeting, Indianapolis, November 3-8, 2002.
- A. Striolo, K.E. Gubbins, A.A. Chialvo and P.T. Cummings, "Water Adsorption in Porous Carbon", American Institute of Chemical Engineers Annual Meeting, Indianapolis, November 3-8, 2002.
- F.R. Siperstein and K.E. Gubbins, "Liquid Crystal Self-Assembly of Surfactant-Inorganic Oxide Systems using Monte Carlo Simulations", American Institute of Chemical Engineers Annual Meeting, Indianapolis, November 3-8, 2002.
- L.F. Scanu, K.E. Gubbins and C.K. Hall, "Phase Behavior of scCO_2 /Surfactant/Water Systems using Lattice Monte Carlo Simulation", American Institute of Chemical Engineers Annual Meeting, Indianapolis, November 3-8, 2002.
- C.M. Colina, C.G. Olivera-Fuentes, M. Lisal, F.R. Siperstein and K.E. Gubbins, "Thermal Properties of Carbon Dioxide in the Single Phase Region by Monte Carlo Simulations", American Institute of Chemical Engineers Annual Meeting, Indianapolis, November 3-8, 2002.
- S. Figueroa-Gerstenmaier, J. Bonet Avalos, L.D. Gelb, K.E. Gubbins and L.F. Vega, "Pore Size Distribution of Model Porous Glasses by Adsorption of Nitrogen using Density Functional Theory", 9th Mediterranean Conference in Chemical Engineering, Barcelona, Spain, November 26-29, 2002.
- F. Siperstein, K.E. Gubbins, C. Alba-Simionesco, "Realistic Simulations of Solid-Liquid Transitions of a Molecular Liquid in Regular Mesoporous Matrices", 2nd International Workshop on Dynamics in Confinement, Grenoble, France, January 22-25, 2003.
- M. Sliwinska-Bartkowiak, F. Hung, R. Radhakrishnan and K.E. Gubbins, "Freezing Behavior in Porous Carbons", 2nd International Workshop on Dynamics in Confinement, Grenoble, France, January 22-25, 2003.
- K.E. Gubbins, "Phase Transitions and Chemical Reactions at the Nano-Scale: Effects of Confinement", Thermodynamics 2003 Conference, Cambridge, U.K., April 9-11, 2003.
- C. Colina and K.E. Gubbins, "Molecular Modeling of Long-Chain Hydrocarbons: Polymers and Surfactants in Supercritical Carbon Dioxide using SAFT", Thermodynamics 2003 Conference, Cambridge, U.K., April 9-11, 2003.
- L.F. Scanu, C.K. Hall and K.E. Gubbins, "Phase Separation and Micellization in Supercritical CO_2 /Surfactant Systems using Lattice Monte Carlo Simulations", Thermodynamics 2003 Conference, Cambridge, U.K., April 9-11, 2003.
- J. Pikunic, R. Pellenq and K.E. Gubbins, "Molecular Simulation of Adsorption and Diffusion of Simple Fluids Confined in Realistic Models of Nanoporous Carbons", Thermodynamics 2003 Conference, Cambridge, U.K., April 9-11, 2003.
- M. Sliwinska-Bartkowiak, R. Radhakrishnan and K.E. Gubbins, "Freezing in Narrow Pores", Thermodynamics 2003 Conference, Cambridge, U.K., April 9-11, 2003.
- H. Bock and K.E. Gubbins, "Lattice Gas Theory for Adsorption of Surfactants from Aqueous Solutions", Thermodynamics 2003 Conference, Cambridge, U.K., April 9-11, 2003.

- Striolo, A., Colina, C.M., Gubbins, K.E., Elvassore, N. and Lue, L., "The Depletion Attraction between Pairs of Colloids in Polymer Solution", FOMMS 2003, Keystone Resort, Colorado, July 6-11, 2003.
- Striolo, A., Gubbins, K.E., Chialvo, A.A. and Cummings, P.T., "Simulated Water Adsorption Isotherms in Carbon Nanopores", FOMMS 2003, Keystone Resort, Colorado, July 6-11, 2003.
- Bock, H., Siperstein, F. and Gubbins, K.E., "Hydrogen bonds in lattice Monte Carlo simulations of surfactants", FOMMS 2003, Keystone Resort, Colorado, July 6-11, 2003.
- Hung, F., Dudziak, G., Sliwinska-Bartkowiak, M. and Gubbins, K.E., "Freezing/melting behavior within carbon nanotubes", FOMMS 2003, Keystone Resort, Colorado, July 6-11, 2003.
- Colina, C.M. and K.E. Gubbins, "The Effect of Quadrupolar Interactions within the SAFT Approach", 15th Symposium on Thermophysical Properties, Boulder, Colorado, June 22-27, 2003.
- Galindo, A., Blas, F. J., Colina, C. M. and K.E. Gubbins, "Predicting Phase Behavior of Alkanes and Perfluoroalkanes in Supercritical Carbon Dioxide Using the SAFT-VR Approach", 15th Symposium on Thermophysical Properties, Boulder, Colorado, June 22-27, 2003.
- Striolo, A., Gubbins, K.E., Burchell, T.D., Cole, D.E., Gruszkiewicz, M., Chialvo, A.A. and Cummings, P.T., "Temperature Effect on Water Adsorption in Porous Carbons", 15th Symposium on Thermophysical Properties, Boulder, Colorado, June 22-27, 2003.
- Colina, C. M., Walker, T. A., Spontak, R.J. and K. E. Gubbins, "The Influence of High-Pressure Carbon Dioxide on the Phase Behavior of PDMS/PEMS Blends: An Experimental and Theoretical Investigation", 6th International Symposium on Supercritical Fluids, Versailles, France, April 9th - 11th, 2003.
- Colina, C.M. and K.E. Gubbins, "The Effect of Quadrupolar Interactions within the SAFT Approach", 15th Symposium on Thermophysical Properties, Boulder, Colorado, June 22-27, 2003.
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- Keith E. Gubbins, "Molecular Modeling of Nano-Porous Materials and Confined Fluids", American Chemical Society Annual Meeting, New York, NY, September 11, 2003.
- F.R. Hung, E. Santiso, B. Coasne, K.E. Gubbins, G. Dudziak and M. Sliwinska-Bartkowiak, "Solid-Fluid Phase Behavior of Fluids Confined in Cylindrical Pores: Simulation and Experimental Studies", American Institute of Chemical Engineers Annual Meeting, San Francisco, Nov. 16-21, 2003.
- J.P. Pikunic, R. Pellenq, and K.E. Gubbins, "Adsorption and Diffusion in Highly Disordered Microporous Carbons: Molecular Simulation and Experiment", American Institute of Chemical Engineers Annual Meeting, San Francisco, Nov. 16-21, 2003.
- A. Striolo, K.E. Gubbins, A.A. Chialvo and P.T. Cummings, "Diffusion of Water in Activated Carbon Nanopores", American Institute of Chemical Engineers Annual Meeting, San Francisco, Nov. 16-21, 2003.
- C.M. Colina and K.E. Gubbins, "Three-Phase Equilibria for Binary Polymer Blends in a Supercritical Solvent", American Institute of Chemical Engineers Annual Meeting, San Francisco, Nov. 16-21, 2003.

- J.K. Brennan, K.E. Gubbins and B.M. Rice, "Direct Simulation of the Dynamic Properties of Reacting Mixtures using Reactive Molecular Dynamics", American Institute of Chemical Engineers Annual Meeting, San Francisco, Nov. 16-21, 2003.
- A. Striolo, K.E. Gubbins, A.A. Chialvo and P.T. Cummings, "Simulated Water Adsorption in Carbon Nanopores", American Institute of Chemical Engineers Annual Meeting, San Francisco, Nov. 16-21, 2003.
- S. Bhattacharya and K.E. Gubbins, "Modeling the Synthesis of Ordered Mesoporous Materials using Mimetic Simulation", American Institute of Chemical Engineers Annual Meeting, San Francisco, Nov. 16-21, 2003.
- L.F. Scanu, K.E. Gubbins and C.K. Hall, "Phase Separation and Micellization in Supercritical CO₂/Surfactant Systems using Lattice Monte Carlo Simulations", American Institute of Chemical Engineers Annual Meeting, San Francisco, Nov. 16-21, 2003.
- A. Striolo, C.M. Colina, K.E. Gubbins and L. Lue, "MC Simulation for the Effective Attraction between Pairs of Colloids in Non-Adsorbing Polymer Solutions", American Institute of Chemical Engineers Annual Meeting, San Francisco, Nov. 16-21, 2003.
- N. Chennamsetty and K.E. Gubbins, "Cosurfactant Effects in Supercritical CO₂", American Institute of Chemical Engineers Annual Meeting, San Francisco, Nov. 16-21, 2003.
- T.A. Walker, C.M. Colina, K.E. Gubbins and R.J. Spontak, "Thermodynamics of PDM/PEMS Blends in the Presence of High-Pressure CO₂", American Institute of Chemical Engineers Annual Meeting, San Francisco, Nov. 16-21, 2003.
- L.F. Scanu, K.E. Gubbins and C.K. Hall, "Phase Behavior of Supercritical CO₂/Surfactant/Water Systems", American Institute of Chemical Engineers Annual Meeting, San Francisco, Nov. 16-21, 2003.
- C.M. Colina, C.G. Olivera-Fuentes and K.E. Gubbins, "Predicting Thermophysical Properties with the Statistical Associating Fluid Theory", American Institute of Chemical Engineers Annual Meeting, San Francisco, Nov. 16-21, 2003.
- B. Coasne, J. Czwartos, F.R. Hung, K.E. Gubbins and M. Sliwinska-Bartkowiak, "Freezing/Melting of Binary Mixtures Confined in Nanopores", American Institute of Chemical Engineers Annual Meeting, San Francisco, Nov. 16-21, 2003.
- K.E. Gubbins and H. Bock, "Inverse Temperature Dependence of Adsorption of Surfactants from Aqueous Solution", American Institute of Chemical Engineers Annual Meeting, San Francisco, Nov. 16-21, 2003.
- Keith E. Gubbins, "Adsorption and Diffusion in Highly Disordered Microporous Carbons: Molecular Simulation vs. Experiment", Materials Research Society Annual Meeting, Boston, December 4, 2003.
- D. R. Cole, J. M. Simonson, M. S. Gruszkiewicz, A. A. Chialvo, G. D. Wignall, Y. B. Melnichenko, J. S. Lin, G. W. Lynn, B. Gu, K. L. More, T. D. Burchell, P. T. Cummings, Y. Leng, K. E. Gubbins, A. Striolo, W. T. Cooper, M. Schilling, A. Habenschuss, "Structure and dynamics of fluids in confined geometries", American Chemical Society Annual Meeting, Anaheim, CA, March 30, 2004.
- B. Coasne, K. E. Gubbins, F. Hung, E. Santiso, M. Sliwinska-Bartkowiak, "Phase transitions and chemical reactions at the nano-scale: Effects of confinement", American Chemical Society Annual Meeting, Anaheim, CA, March 30, 2004..

- C.M. Colina and K.E. Gubbins, "Phase Equilibria of *n*-Perfluoroalkane/Carbon Dioxide/*n*-Alkane Ternary Mixtures", PPEPPD 2004 (Properties and Phase Equilibria for Product and Process Design), Snowbird, Utah, May 16-22, 2004.
- E.E. Santiso, M. Kostov, K.E. Gubbins, A.M. George, M.B. Nardelli, M. Sliwinska-Bartkowiak, "Effect of Confinement on Chemical Reactions", Fundamentals of Adsorption 8 (FOA8), Sedona, Arizona, May 23-28, 2004.
- A. Striolo, K.E. Gubbins, A.A. Chialvo and P.T. Cummings, "The Effect of Pore Connectivity on Water Adsorption Isotherms in Non-Activated Graphitic Nanopores", Fundamentals of Adsorption 8 (FOA8), Sedona, Arizona, May 23-28, 2004.
- F.R. Hung, B. Coasne, K.E. Gubbins, F.R. Siperstein and K.E. Gubbins, "Effect of Confinement on Freezing in Cylindrical Pores", Fundamentals of Adsorption 8 (FOA8), Sedona, Arizona, May 23-28, 2004.
- B. Coasne, J. Czwartos, F.R. Hung, K.E. Gubbins, and M. Sliwinska-Bartkowiak, "Freezing/Melting of Binary Mixtures Confined in Nano-Pores", Fundamentals of Adsorption 8 (FOA8), Sedona, Arizona, May 23-28, 2004.
- R.J-M. Pellenq, B. Coasne and K.E. Gubbins, "A Monte Carlo Study of Capillary Condensation in Microporous Media: From a Single Regular Pore to a Disordered Porous Matrix", Fundamentals of Adsorption 8 (FOA8), Sedona, Arizona, May 23-28, 2004.
- S.K. Jain, J. Pikunic, R. Pellenq and K.E. Gubbins, "Effects of Activation on the Structure and Adsorption Properties of a Nanoporous Carbon using Molecular Simulation", Fundamentals of Adsorption 8 (FOA8), Sedona, Arizona, May 23-28, 2004.
- A. Striolo, P.T. Cummings, A.A. Chialvo and K.E. Gubbins, "Adsorption and Diffusion of Water in Activated Carbon Nanopores", Third International Conference on Computational Modeling and Simulation of Materials, Acireale, Sicily, Italy, May 30-June 4, 2004.
- E.E. Santiso, K.E. Gubbins, A.M. George, M.B. Nardelli, M. Sliwinska-Bartkowiak, "Effect of Confinement on Chemical Reactions", 5th International Symposium on Surface Heterogeneity Effects in Adsorption and Catalysis on Solids (ISSHAC-5), Gdansk, Poland, August 30, 2004.
- M. Sliwinska-Bartkowiak, G. Dudziak, M. Kempinski, R. Radhakrishnan, F.R. Hung and K.E. Gubbins, "Confinement Effects by Means of Dielectric and Electron Paramagnetic Resonance Methods", 5th International Symposium on Surface Heterogeneity Effects in Adsorption and Catalysis on Solids (ISSHAC-5), Gdansk, Poland, August 30, 2004.
- "Phase Transitions and Chemical Reactions at the Nano-Scale: Effects of Confinement", European/Japanese Molecular Liquids Group Conference on "Complex Liquids: Fundamental Properties to Industrial Applications", Sheffield, U.K., September 3-7, 2004.
- "Application of Molecular Simulation to Study Nano-Porous Materials", First International Symposium on Functional Innovation of Molecular Informatics", Fukuoka, Japan, October 13-15, 2004.
- "Application of Molecular Simulation to Study Nano-Porous Materials", K.E. Gubbins, Annual Meeting of American Institute of Chemical Engineers, Austin, Texas, November 7-12, 2004 (Plenary Lecture).
- "Solid-Liquid Phase Diagram of Mixtures Confined in Nanopores", B. Coasne, J. Czwartos, F.R. Hung, K.E. Gubbins and M. Sliwinska-Bartkowiak, Annual Meeting of American Institute of Chemical Engineers, Austin, Texas, November 7-12, 2004.

- “Solid-Fluid Phase Transitions in Confinement within Multi-Walled Carbon Nanotubes”, F.R. Hung, E.E. Santiso, B. Coasne, K.E. Gubbins, G. Dudziak and M. Sliwinska-Bartkowiak, Annual Meeting of American Institute of Chemical Engineers, Austin, Texas, November 7-12, 2004.
- “Graduate Courses in Thermodynamics, Statistical Mechanics and Multi-Scale Modeling at North Carolina State University”, K.E. Gubbins, C.M. Colina and F.R. Hung, Annual Meeting of American Institute of Chemical Engineers, Austin, Texas, November 7-12, 2004.
- “A Graduate Course in Multi-Scale Modeling of Soft Matter”, K.E. Gubbins, S. Franzen and F.R. Hung, Annual Meeting of American Institute of Chemical Engineers, Austin, Texas, November 7-12, 2004.
- “Cosurfactant Effects in Supercritical CO₂”, N. Chennamsetty, H. Bock, and K.E. Gubbins, Annual Meeting of American Institute of Chemical Engineers, Austin, Texas, November 7-12, 2004.
- “Molecular-Based Equations of State: A Parameterization Study”, F. Castro, C.M. Colina, K.E. Gubbins and C.G. Olivera-Fuentes, Annual Meeting of American Institute of Chemical Engineers, Austin, Texas, November 7-12, 2004.
- “The Impact of Temperature and Confinement on Surfactant Adsorption from Aqueous Solutions”, H. Bock and K.E. Gubbins, Annual Meeting of American Institute of Chemical Engineers, Austin, Texas, November 7-12, 2004.
- “Molecular Modeling of Polymer Systems”, C.M. Colina and K.E. Gubbins, Annual Meeting of American Institute of Chemical Engineers, Austin, Texas, November 7-12, 2004.
- “Modeling the Synthesis of Mesostuctured Cellular Foams using Mimetic Simulation”, S. Bhattacharya and K.E. Gubbins, Annual Meeting of American Institute of Chemical Engineers, Austin, Texas, November 7-12, 2004.
- “Effect of Confinement and Adsorbte-Wall Interactions on Freezing/Melting within Cylindrical Pores: Experiment and Molecular Simulation”, F.R. Hung, B. Coasne, K.E. Gubbins, G. Dudziak and M. Sliwinska-Bartkowiak, Annual Meeting of American Institute of Chemical Engineers, Austin, Texas, November 7-12, 2004.
- “Multi-Scale Modeling of Surfactant Self-Assembly”, N. Chennamsetty, H. Bock and K.E. Gubbins, Annual Meeting of American Institute of Chemical Engineers, Austin, Texas, November 7-12, 2004.
- “Simulated Water Adsorption and Diffusion in Carbon Nanotubes”, A. Striolo, P.K. Naicker, A. Chialvo and K.E. Gubbins, Annual Meeting of American Institute of Chemical Engineers, Austin, Texas, November 7-12, 2004.
- “The Coarse Graining of Water in Aqueous Surfactant Solutions”, H. Bock, S.H.L. Klapp and K.E. Gubbins, Annual Meeting of American Institute of Chemical Engineers, Austin, Texas, November 7-12, 2004.
- “Effect of Confinement on Chemical Reactions”, E.E. Santiso, K.E. Gubbins, A.M. George, M. Buongiorno Nardelli and M. Sliwinska-Bartkowiak, Annual Meeting of American Institute of Chemical Engineers, Austin, Texas, November 7-12, 2004.
- “Effects of Confinement on Phase Transitions and Chemical Reactions”, 14th Ostwald-Kolloquium on Fluids at Interfaces and in Pores: Phase Transitions and Related Phenomena, a colloquium on behalf of the 66th birthday of Gerhard Findenegg, November 22-23, 2004, Berlin, Germany (Plenary Lecture).

- “Phase Transitions and Chemical Reactions at the Nano-Scale: Effects of Confinement”, K.E. Gubbins, First Indo-US Joint Meeting in a Global Environment, organized by the Indian Institute of Chemical Engineers and the American Institute of Chemical Engineers, Mumbai, India, December 28-30, 2004 (Plenary Lecture).
- “Freezing of CCl_4 Within Carbon Nanotubes: A Combined Experimental and Simulation Approach”, F. Hung, K.E. Gubbins and M. Sliwinska-Bartkowiak, Thermodynamics 2005, Sesimbra, Portugal, April 6-8, 2005.
- “Effect of Confinement on Chemical Reactivity”, K.E. Gubbins, M. Buongiorno Nardelli, E. Santiso, A. George, M. Kostov, 93rd Statistical Mechanics Conference, Rutgers University, May 16, 2005.
- “Tight-Binding and Bond-Order Hamiltonians for Atomistic Simulations of the Stability of Porous Carbon Structures”, S.K. Jain, J. Fuhr, R.J-M. Pellenq, C. Bichara and K.E. Gubbins, Characterisation of Porous Solids VII Conference, Aix-en-Provence, France, May 26-28, 2005.
- “Confinement Effect on Freezing of Binary Mixtures”, B. Coasne, J. Czwartos, K.E. Gubbins, F.R. Hung and M. Sliwinska-Bartkowiak, Characterisation of Porous Solids VII Conference, Aix-en-Provence, France, May 26-28, 2005.
- “Modeling the Synthesis of Mesosstructured Cellular Foams using Mimetic Simulation”, S. Bhattacharya and K.E. Gubbins, Characterisation of Porous Solids VII Conference, Aix-en-Provence, France, May 26-28, 2005.
- “Freezing of Simple Fluids within Carbon and Silica Nanotubes: Experiment and Simulation”, Malgorzata Sliwinska-Bartkowiak, Monika Jazdzewska, Benoit Coasne, Francisco Hung and Keith E. Gubbins, European Materials Research Society Annual Meeting, Warsaw, Poland, September 5-9, 2005.
- “Coarse-Grained Potentials from Widom’s Particle Insertion Method”, N. Chennamsetty, H. Bock and K.E. Gubbins, Annual Meeting of the American Institute of Chemical Engineers, Cincinnati, Ohio, October 30-November 4, 2005.
- “A Simulation Study of Capillary Condensation and Freezing of Krypton within Realistic Models of MCM-41 Materials”, F.R. Hung, B. Coasne, M. Sliwinska-Bartkowiak and K.E. Gubbins, Annual Meeting of the American Institute of Chemical Engineers, Cincinnati, Ohio, October 30-November 4, 2005.
- “Water Adsorption Isotherms in Molecularly Reconstructed Models of Activated and Unactivated Carbons Obtained from Saccharose”, A. Striolo, S.K. Jain, J.P. Pikunic, R.J-M. Pellenq, A. Chialvo, K.E. Gubbins and P.T. Cummings, Annual Meeting of the American Institute of Chemical Engineers, Cincinnati, Ohio, October 30-November 4, 2005.
- “From Atomistic to Mesoscale Models: Coarse-Graining Techniques”, N. Chennamsetty, H. Bock, K.E. Gubbins, J. Silbermann, S.H.L. Klapp, M. Schoen, Annual Meeting of the American Institute of Chemical Engineers, Cincinnati, Ohio, October 30-November 4, 2005.
- “Catalytic Role of Defective Carbon Substrates in the Dissociation of Water”, M.K. Kostov, E.E. Santiso, A.M. George, M. Buongiorno Nardelli and K.E. Gubbins, Annual Meeting of the American Institute of Chemical Engineers, Cincinnati, Ohio, October 30-November 4, 2005.
- “Confinement Effects on the Isomerization Kinetics of Small Hydrocarbons”, E.E. Santiso, K.E. Gubbins, A.M. George, M. Buongiorno-Nardelli, Annual Meeting of the American Institute of Chemical Engineers, Cincinnati, Ohio, October 30-November 4, 2005.

- “Molecular Models of MCF and SBA-15 and Gas Adsorption: A Molecular Simulation Study”, S. Bhattacharya, B. Coasne, F.R. Hung and K.E. Gubbins, Annual Meeting of the American Institute of Chemical Engineers, Cincinnati, Ohio, October 30-November 4, 2005.
- “Development of Realistic Models of MCM-41 Materials for Gas Adsorption Studies”, B. Coasne, F.R. Hung and K.E. Gubbins, Annual Meeting of the American Institute of Chemical Engineers, Cincinnati, Ohio, October 30-November 4, 2005.
- “Modeling Porous Carbons by Reverse Monte Carlo and Simultaneous Energy Minimization”, S.K. Jain, J.P. Pikunic, R.J-M. Pellenq and K.E. Gubbins, Annual Meeting of the American Institute of Chemical Engineers, Cincinnati, Ohio, October 30-November 4, 2005.
- “Surfactant Self-Assembly on Nano-Structured Surfaces: Multi-Scale Computational Prediction and Design”, Nanoscale Science and Engineering Grantees Conference, National Science Foundation, Arlington, VA, December 12-15, 2005.
- “Effects of Confinement on Chemical Reactivity”, Pacificchem, International Chemical Congress of Pacific Basin Societies, Honolulu, Hawaii, December 15-20, 2005 (Keynote Lecture)
- “Freezing of Argon in a Disordered Nanoporous Structure”, B. Coasne, S.K. Jain, K.E. Gubbins, Third International Workshop on Dynamics of Confinement, Grenoble, France, March 25, 2006.
- “Realistic molecular models of porous carbons obtained from Reverse Monte Carlo simulations”, S.K. Jain, J.D. Fuhr, K.E. Gubbins and R.J-M. Pellenq, 2006 Nano Science and Technology Institute Nanotechnology Conference, Boston, May 7-11, 2006.
- “Realistic molecular models of porous carbons obtained from Reverse Monte Carlo simulations”, S. K. Jain, K. E. Gubbins and R. J-M. Pellenq, CARBON 2006, Aberdeen, Scotland, July 16-21, 2006.
- “Structural Modeling of Porous Carbons using a Hybrid Reverse Monte Carlo Method”, 4th Pacific Basin Conference on Adsorption Science & Technology, Tianjin, China, May 23, 2006.
- “Molecular Simulation of Gas Adsorption in Mesoporous Silica SBA-15”, S. Bhattacharya, K.E. Gubbins, B. Coasne and F.R. Hung, 4th Pacific Basin Conference on Adsorption Science & Technology, Tianjin, China, May 23, 2006.
- “Freezing and Melting in Ordered and Disordered Porous Carbons”, B. Coasne, S.K. Jain and K.E. Gubbins, Seventh Liblice Conference on Statistical Mechanics of Liquids, Lednice, Moravia, Czech Republic, June 11-15, 2006.
- “Capillary Condensation within MCM-41 Materials: The Role of Surface Disorder”, B. Coasne, K.E. Gubbins, F.R. Hung and R.J.M. Pellenq, Seventh Liblice Conference on Statistical Mechanics of Liquids, Lednice, Moravia, Czech Republic, June 11-15, 2006.
- “Molecular Modeling of Porous Carbons Using Hybrid Reverse Monte Carlo”, S.K. Jain, K.E. Gubbins and R.J-M. Pellenq, TRI Princeton Workshop on Characterization of Porous Solids”, Princeton, NJ, June 21, 2006.
- “Confinement Effects on Chemical Reactions – Toward an Integrated Rational Catalyst Design”, U.S. – Poland Workshop on Nanoscience and Nano-Structured Materials, Poznan, Poland, June 26-28, 2006.
- “An Apparent Critical Point in Binary Mixtures: Experimental and Simulation Study”, B. Ratajczak, M. Sliwinska-Bartkowiak, B. Coasne and K.E. Gubbins, U.S. – Poland Workshop on Nanoscience and Nano-Structured Materials, Poznan, Poland, June 26-28, 2006.

- “Freezing of Fluids Confined in Ordered and Disordered Porous Carbons”, B. Coasne, S.K. Jain and K.E. Gubbins, Sixth International Symposium on Surface Heterogeneity Effects in Adsorption and Catalysis on Solids, Zakopane, Poland, August 28-September 2, 2006.
- “Modeling Chemical Reactivity: Effects of Confinement”, K.E. Gubbins, Annual Meeting of the American Institute of Chemical Engineers, San Francisco, November 12-17, 2006 [symposium in memory of Professor Koichiro Nakanishi].
- “Effects of Confinement on Freezing and Melting”, Annual Meeting of the American Institute of Chemical Engineers, San Francisco, November 12-17, 2006 [symposium in honor of Carol Hall’s 60th birthday].
- “Dissociation of Water on Defective Carbon Substrates”, E.E. Santiso, M.K. Kostov, K.E. Gubbins, A.M. George and M. Biongiorno Nardelli, Annual Meeting of the American Institute of Chemical Engineers, San Francisco, November 12-17, 2006.
- “Effect of Confinement on Chemical Reactions”, E.E. Santiso, A.M. George, M.K. Kostov, M. Buongiorno Nardelli and K.E. Gubbins, Annual Meeting of the American Institute of Chemical Engineers, San Francisco, November 12-17, 2006.
- “Carbon Replica from Silica Template using Grand Canonical Monte Carlo Simulations”, S.K. Jain, K.E. Gubbins, R.J.-M. Pellenq, Annual Meeting of the American Institute of Chemical Engineers, San Francisco, November 12-17, 2006.
- “Coarse-Graining and Soft Matter Systems: Bridging the Atomistic-Meso Scales”, J.D. Moore, T.J. Morrow and K.E. Gubbins, Annual Meeting of the American Institute of Chemical Engineers, San Francisco, November 12-17, 2006.
- “Microstructural Analysis and Adsorption Properties of Porous Carbons using Molecular Simulation”, S.K. Jain, K.E. Gubbins, and R.J.-M. Pellenq, Annual Meeting of the American Institute of Chemical Engineers, San Francisco, November 12-17, 2006.
- “The Influence of Physical Interactions on Chemical Reactions in Confinement”, E.E. Santiso, K.E. Gubbins, A.M. George and M. Buongiorno Nardelli, Annual Meeting of the American Institute of Chemical Engineers, San Francisco, November 12-17, 2006.
- “The Properties of Asymmetric Binary Lennard-Jones Mixtures using Coarse-Grained Two-Body Effective Potentials”, T.J. Morrow and K.E. Gubbins, Annual Meeting of the American Institute of Chemical Engineers, San Francisco, November 12-17, 2006.
- “Effects of Confinement on Freezing and Melting”, International Conference on Frontier Science and Technology of Nanoporous Systems 3, Chiba University, Japan, January 27, 2007 [in honor of Professor Katsumi Kaneko’s 60th birthday]
- “Confinement Effects on Chemical Reactions – Towards an Integrated Rational Catalyst Design”, American Chemical Society Annual Meeting, Chicago, March 27, 2007.
- “Molecular Modeling of Adsorption in Porous Carbons”, International Conference on Adsorption, in honor of Ken Sing, Bristol, U.K., April 12, 2007.
- “Krypton Adsorption on Mesoporous Silica: A Combined Simulation and Experimental Approach”, F.R. Hung, B. Coasne, S. Bhattacharya, M. Thommes and K.E. Gubbins, 9th International Conference on Fundamentals of Adsorption, Giardini Naxos, Sicily, Italy, May 20-25, 2007.
- “Confinement Effect on Freezing of Mixtures: Experiment and Molecular Simulation”, J. Czwartos, M. Sliwinska-Bartkowiak, B. Coasne and K.E. Gubbins, 9th International Conference on Fundamentals of Adsorption, Giardini Naxos, Sicily, Italy, May 20-25, 2007.

- “Molecular Modeling of Porous Carbons Using Reverse Monte Carlo and Grand Canonical Monte Carlo Simulations”, S.K. Jain, K.E. Gubbins and R.-J.M. Pellenq, 9th International Conference on Fundamentals of Adsorption, Giardini Naxos, Sicily, Italy, May 20-25, 2007.
- “Effect of Confinement on the Isomerization Dynamics of Small Hydrocarbons – The Shape Catalytic Effect”, E. Santiso, M. Buongiorno Nardelli and K.E. Gubbins, 9th International Conference on Fundamentals of Adsorption, Giardini Naxos, Sicily, Italy, May 20-25, 2007.
- “Molecular Simulation of the Adsorption and Structure of Benzene Confined in Mesoporous Silicas”, B. Coasne, C. Alba-Simionesco, G. Dosseh and K.E. Gubbins, 9th International Conference on Fundamentals of Adsorption, Giardini Naxos, Sicily, Italy, May 20-25, 2007.
- “Modeling and Textural Analysis of Porous Carbons using Molecular Simulation”, S.K. Jain, R.-J.-M. Pellenq and K.E. Gubbins, Carbon 2007 Conference, Seattle, July 15-20, 2007.
- “Carbon Replica from Ordered Mesoporous Silica Template using GCMC Simulations”, S.K. Jain, R.-J.-M. Pellenq and K.E. Gubbins, Carbon 2007 Conference, Seattle, July 15-20, 2007.
- “Molecular Simulation of the Adsorption and Structure of Benzene Confined in Mesoporous Silicas”, B. Coasne, C. Alba-Simionesco, F. Audonnet, G. Dosseh and K.E. Gubbins, International Conference Thermodynamics 2007, Institut Francais du Petrole, Paris, France, September 26-28, 2007.
- “Freezing/Melting of Liquids in Carbon Nanotubes”, K.E. Gubbins, M. Sliwinska-Bartkowiak, M. Jazdzewska and F.R. Hung, International Conference Thermodynamics 2007, Institut Francais du Petrole, Paris, France, September 26-28, 2007.
- ”Surface Nanostructure and Catalysis: The Role of Confinement and Surface Chemistry”, Center for Nanophase Materials Sciences 2007 Users’ Meeting, Oak Ridge National Laboratory, October 10, 2007. (Plenary Lecture)
- “Methane Decomposition over Graphene Edges for CO- and CO₂ – Free Hydrogen Production”, L. Huang, E.E. Santiso, K.E. Gubbins and M. Buongiorno, Annual Meeting of the American Institute of Chemical Engineers, Salt Lake City, November 4-9, 2007.
- “Molecular Modeling of Carbon Replica Obtained from Silica Template using Grand Canonical Monte Carlo Simulations”, S.K. Jain, K.E. Gubbins and R. J.-M. Pellenq, Annual Meeting of the American Institute of Chemical Engineers, Salt Lake City, November 4-9, 2007.
- “A Double Exponential Effect of Confinement on Reaction Rates”, E.E. Santiso, M. Buongiorno Nardelli and K.E. Gubbins, Annual Meeting of the American Institute of Chemical Engineers, Salt Lake City, November 4-9, 2007.
- “A Monte Carlo Study of Gas Adsorption in Atomistic Models of Templated Mesoporous Silicas”, F.R. Hung, S. Bhattacharya, B. Coasne, M. Thommes and K.E. Gubbins, Annual Meeting of the American Institute of Chemical Engineers, Salt Lake City, November 4-9, 2007.
- “Multi-Scale Simulation of the Self-Assembly of Nonionic Poly(Oxyethylene) Alkyl Ether Surfactants”, J.D. Moore and K.E. Gubbins, Annual Meeting of the American Institute of Chemical Engineers, Salt Lake City, November 4-9, 2007.

- “Sequestration and Selective Oxidation of Carbon Monoxide on Graphene Edges”, S. Paul, E.E. Santiso, K.E. Gubbins and M. Buongiorno Nardelli, Annual Meeting of the American Institute of Chemical Engineers, Salt Lake City, November 4-9, 2007.
- “Confinement Effects on Chemical Reactions: Towards an Integrated Rational Catalyst Design”, Molecular Modelling 2007, Melbourne, Australia, November 27-30, 2007. (Plenary Lecture)
- J. Czwartos, M. Sliwinska-Bartkowiak, B. Coasne and K.E. Gubbins, „Confinement Effects on Freezing of Mixtures”, European Materials Research Society Annual Meeting, Strasbourg, France, May 28-June 3, 2008.
- T. Roussel, C. Bichara, R.J.-M. Pellenq and K.E. Gubbins, “Simulation Numérique de Repliques de Zeolithes en Carbone: Structures et Application au Stockage d’Hydrogene », Journée des Simulations Numérique, University of Paris, Jussieu, Paris, France, June 5, 2008.
- M.Sliwinska-Bartkowiak, M.Jazdzewska, K.E.Gubbins, Liangliang Huang, “Freezing/Melting of Liquids in Cylindrical Nanopores”, Characterization of Porous Solids 8, Edinburgh, Scotland, June 10-13, 2008.
- J.C. Palmer, S.K. Jain, K.E. Gubbins and J.E. Fischer, “Hybrid Reverse Monte Carlo Simulations of Carbide-Derived Carbons”, Characterization of Porous Solids 8, Edinburgh, Scotland, June 10-13, 2008.
- J. Czwartos, M. Sliwinska-Bartkowiak, B. Coasne and K.E. Gubbins, “Freezing of Mixtures Confined in Silica Nanopores: Experiment and Molecular Simulation”, Characterization of Porous Solids 8, Edinburgh, Scotland, June 10-13, 2008.
- B. Coasne, C. Alba-Simionesco, F. Audonnet, G. Dosseh and K.E. Gubbins, “Adsorption and Freezing of Benzene on Silica Surfaces and Nanopores”, Characterization of Porous Solids 8, Edinburgh, Scotland, June 10-13, 2008.
- R. Pellenq, T. Roussel, C. Bichara and K.E. Gubbins, « H₂ Adsorption in Pristine and Li-Doped Carbon Replicas of FAU and EMT Zeolites », Characterization of Porous Solids 8, Edinburgh, Scotland, June 10-13, 2008.
- K.E. Gubbins, “Multi-Scale Modeling of Matter: A Graduate Course”, 20th International Conference on Chemical Thermodynamics, Warsaw, Poland, August 3-8, 2008.
- M. Lisal, P. Cosoli, W.R. Smith, S.K. Jain, K.E. Gubbins and K. Aim, “Molecular Simulations of Chemical Reaction Equilibrium for Nitric Oxide Dimerization Reaction in Disordered Nanoporous Carbons”, 20th International Conference on Chemical Thermodynamics, Warsaw, Poland, August 3-8, 2008.
- K.E. Gubbins, “Molecular Simulation as a Foundation for Engineering Models: Impact and Prospects”, American Institute of Chemical Engineers Annual Meeting, Philadelphia, November 16-21, 2008.
- M. Sliwinska-Bartkowiak, M. Blazej Jazdzewska, K.E. Gubbins and L. Huang, “Freezing/Melting of Liquids in Cylindrical Nanopores”, American Institute of Chemical Engineers Annual Meeting, Philadelphia, November 16-21, 2008.
- Y-C. Liu, J.D. Moore, T.R. Roussel, Q. Chen, Q. Wang and K.E. Gubbins, “Crossover from Fickian to Single File Diffusion of Fluids Confined in Carbon Nanotubes”, American Institute of Chemical Engineers Annual Meeting, Philadelphia, November 16-21, 2008.
- J.C. Palmer, J.K. Brennan, K.E. Gubbins, M. Hurley and A. Balboa, “Hybrid Reverse Monte Carlo Simulations of Activated Carbons used as Adsorbents for Chemical and Biological

- Warfare Agents”, American Institute of Chemical Engineers Annual Meeting, Philadelphia, November 16-21, 2008.
- J.D. Moore, Q. Chen, Y-C. Liu, T.R. Roussel, Q. Wang and K.E. Gubbins, “Transition from Fickian to Single-File Diffusion for Binary Lennard-Jones Mixtures in Single Walled Carbon Nanotubes”, American Institute of Chemical Engineers Annual Meeting, Philadelphia, November 16-21, 2008.
- S.K. Jain, K.E. Gubbins and R.J-M. Pellenq, “Molecular Modeling and Adsorption Properties of Silica Templated Mesoporous Carbons”, American Institute of Chemical Engineers Annual Meeting, Philadelphia, November 16-21, 2008.
- L. Huang, E.E. Santiso, K.E. Gubbins and M. Buongiorno Nardelli, “Periodic Mesoporous Silicas (PMOs) for Hydrogen Purification and Storage”, American Institute of Chemical Engineers Annual Meeting, Philadelphia, November 16-21, 2008.
- L. Huang, D. Rocca, S. Baroni, K.E. Gubbins and M. Buongiorno Nardelli, “Molecular Design for Organic Solar Cells”, American Institute of Chemical Engineers Annual Meeting, Philadelphia, November 16-21, 2008.
- K.E. Gubbins, “Surface Nanostructure, Diffusion and Catalysis: The Role of Confinement and Surface Chemistry”, American Institute of Chemical Engineers Annual Meeting, Philadelphia, November 16-21, 2008.
- T.R. Roussel, J. Palmer, C. Bichara, R. Pellenq, and K.E. Gubbins, “A Monte Carlo Study of Molecular Selectivity of Binary Mixtures in Ordered and Disordered Microporous Carbons”, American Institute of Chemical Engineers Annual Meeting, Philadelphia, November 16-21, 2008.
- K.E. Gubbins, “Surface Nanostructure, Diffusion and Catalysis: The Role of Confinement and Surface Chemistry”, Festcollquium: SSNI Symposium “Self-Assembled Soft-Matter Nanostructures at Interfaces”, Technische Universität Berlin, Berlin, Germany, February 20, 2009.
- Joshua D. Moore, Ying-Chun Liu and Keith E. Gubbins, “Transition from Single-File to Fickian Diffusion in Carbon Nanotube Structures”, 5th Pacific Basin Conference on Adsorption Science & Technology, Singapore, May 25, 2009.
- B. Coasne, C. Alba-Simionesco, F. Audonnet, G. Dosseh and K.E. Gubbins, “Adsorption and Freezing of Benzene on Silica Surfaces and Nanopores”, 5th Pacific Basin Conference on Adsorption Science & Technology, Singapore, May 25, 2009.
- Jeremy Palmer, Sun-Hwa Yeon, Anna Llobet, Keith Gubbins, John Fischer and Yury Gogotsi, “Molecular Modeling and Simulation of Titanium Carbide Derived Carbons”, 5th Pacific Basin Conference on Adsorption Science & Technology, Singapore, May 25, 2009.
- M. Sliwinska-Bartkowiak, M. Jazdzewska, K.E. Gubbins and L. Huang, “Melting of Water in Carbon Nanopores”, 5th Pacific Basin Conference on Adsorption Science & Technology, Singapore, May 25, 2009.
- B. Coasne, J. Czwartos, M. Sliwinska-Bartkowiak and K.E. Gubbins, “Effect of Pressure on Freezing of Pure Fluids and Mixtures in Nanopores”, 5th Pacific Basin Conference on Adsorption Science & Technology, Singapore, May 25, 2009.
- B. Coasne, J. Czwartos, M. Sliwinska-Bartkowiak and K.E. Gubbins, “Effect of Pressure on Freezing of Pure Fluids and Mixtures Confined in Nanopores”, 7th International Symposium on Surface Heterogeneity Effects in Adsorption and Catalysis on Solids, Kazimierz, Poland, July 5-11, 2009.

- B. Coasne, C. Alba-Simionesco, F. Audonnet, G. Dosseh and K.E. Gubbins, "Adsorption and Freezing of Benzene on Silica Surfaces and Nanopores", 7th International Symposium on Surface Heterogeneity Effects in Adsorption and Catalysis on Solids, Kazimierz, Poland, July 5-11, 2009.
- J.C. Palmer, J.K. Brennan, M. Hurley, A. Balboa and K.E. Gubbins, « Molecular Modeling of Activated Carbons », 7th International Symposium on Surface Heterogeneity Effects in Adsorption and Catalysis on Solids, Kazimierz, Poland, July 5-11, 2009.
- M. Sliwinska-Bartkowiak, M. Jazdzewska, K.E. Gubbins and L. Huang, "Melting of Liquids in Cylindrical Nanopores", 7th International Symposium on Surface Heterogeneity Effects in Adsorption and Catalysis on Solids, Kazimierz, Poland, July 5-11, 2009.
- Y.-C. Liu, J.D. Moore, J.C. Palmer and K.E. Gubbins, "Transition from Single File to Fickian Diffusion in Ordered and Disordered Nanoporous Carbons", 7th International Symposium on Surface Heterogeneity Effects in Adsorption and Catalysis on Solids, Kazimierz, Poland, July 5-11, 2009.
- "Crossover from Single-File to Fickian Diffusion in Carbon Nanotubes and Nanotube Bundles: Pure Components and Mixtures", Diffusion Fundamentals III, Athens, Greece, August 24, 2009.
- "Bimodal Diffusion of Binary Lennard-Jones Mixtures in Atomically Detailed Single-Walled Carbon Nanotubes", Qu Chen, Joshua D. Moore, Ying-Chun Liu, Thomas J. Roussel, Qi Wang and Keith E. Gubbins, Diffusion Fundamentals III, Athens, Greece, August 24, 2009.
- "Dual-Mode Diffusion of Argon Confined in Carbon Nanotube Bundles", Ying-Chun Liu, Thomas J. Roussel, Joshua D. Moore, Qi Wang and Keith E. Gubbins, Diffusion Fundamentals III, Athens, Greece, August 24, 2009.
- "Slow and Fast (Fickian) Diffusion Modes for Argon Confined in BPL Activated Carbon", Joshua D. Moore, Jeremy C. Palmer, Ying-Chun Liu, Thomas J. Roussel, John K. Brennan and Keith E. Gubbins, Diffusion Fundamentals III, Athens, Greece, August 24, 2009.
- Jeremy Palmer, Ying-Chun Liu, Joshua D. Moore, John K. Brennan, Yury Gogotsi, John Fischer and Keith E. Gubbins, "Molecular Modeling of Disordered Micro-Porous Carbons: Atomistic Models, Adsorption and diffusion", 8th Torunian Carbon Symposium: Fabrication, Modification and Investigations of Novel Forms of Carbon, Torun, Poland, September 3-6, 2009.
- "The Theory of Non-Electrolyte Solutions: A Recent History", Keith E. Gubbins, Taylor & Francis Molecular Physics Lecturer (biannual lectureship award), Thermodynamics 2009, Imperial College London, September 25, 2009.
- "Transitions between Single-File and Fickian Self-Diffusion for Fluids Confined in Carbon Nanotubes, Bundles and Activated Carbon", Ying-Chun Liu, Joshua D. Moore, Jeremy C. Palmer, Wang Qi, Thomas Roussel and Keith E. Gubbins, 10th Symposium of Computational Chemistry in China (SCCC2009), Hangzhou, China, October 23-25, 2009.
- "Self-Diffusion of Fluids Confined in Ordered and Disordered Microporous Carbons", Joshua D. Moore, Jeremy C. Palmer, Ying-Chun Liu, Thomas J. Roussel and Keith E. Gubbins, 10th Symposium of Computational Chemistry in China (SCCC2009), Hangzhou, China, October 23-25, 2009.

- “Water Dissociation over Ti-Decorated C_{60} ”, Ying-Chun Liu, Liping Huang, Keith E. Gubbins and Marco Buongiorno Nardelli, 10th Symposium of Computational Chemistry in China (SCCC2009), Hangzhou, China, October 23-25, 2009.
- “Dissociation of Water over Ti-Decorated C_{60} ”, Ying-Chun Liu, Marco Buongiorno Nardelli and Keith E. Gubbins, Annual Meeting of the American Institute of Chemical Engineers, Nashville, TN, November 8-13, 2009.
- “Diffusion Mechanisms of Fluids Confined in Carbon Nanotubes, Carbon Nanotube Bundles and Hierarchical Carbons: Single-File, Fickian and Dual-Mode Diffusion”, Annual Meeting of the American Institute of Chemical Engineers, Nashville, TN, November 8-13, 2009.
- “Atomistic Models of Activated Carbons”, Jeremy C. Palmer, John K. Brennan, Margaret Hurley, Alex Balboa and Keith E. Gubbins, Annual Meeting of the American Institute of Chemical Engineers, Nashville, TN, November 8-13, 2009.
- “Transitions between Single-File and Fickian Diffusion for Fluids Confined in Carbon Nanotubes Bundles and Activated Carbons”, Ying-Chun Liu, Joshua D. Moore, Jeremy C. Palmer, Qu Chen, Thomas J. Roussel, Qi Wang and Keith E. Gubbins, Computational Chemistry Workshop, University of Hong Kong, Hong Kong, December 11, 2009.
- “Anomalous and Fickian Diffusion of Fluids Confined in Activated Carbon, a Carbon Replica of Zeolite and Carbon Nanotube Bundles”, Joshua D. Moore, Ying-Chun Liu, Jeremy Palmer and Keith E. Gubbins, 12th International Conference on Properties and Phase Equilibria for Product and Process Design, Suzhou, China, May 16-21, 2010.
- “Life in Confinement: The Role of Molecular Modeling”, 12th International Conference on Properties and Phase Equilibria for Product and Process Design, Suzhou, China, May 16-21, 2010.
- “Molecular Adsorption and Diffusion in Microporous Carbons”, J.C. Palmer, J.D. Moore, J.K. Brennan and K.E. Gubbins, 10th International Conference on Fundamentals of Adsorption, Awaji, Hyogo, Japan, May 23-28, 2010.
- “Freezing of Simple Fluids in Regular and Distorted Carbon Nanotubes”, B. Coasne, K.E. Gubbins and M. Sliwinski-Bartkowiak, 10th International Conference on Fundamentals of Adsorption, Awaji, Hyogo, Japan, May 23-28, 2010.
- “Water Dissociation over Ti-Decorated C_{60} ”, Y.-C. Liu, M. Buongiorno Nardelli and K.E. Gubbins, 12th International Conference on Properties and Phase Equilibria for Product and Process Design, Suzhou, China, May 16-21, 2010.
- “DFT Study of Dissociative Adsorption of H_2S on Defective Carbon Substrates”, L. Huang and K.E. Gubbins, 12th International Conference on Properties and Phase Equilibria for Product and Process Design, Suzhou, China, May 16-21, 2010.
- “Anomalous and Fickian Diffusion of Fluids Confined in Activated Carbon, a Carbon Replica of Zeolite and Carbon Nanotube Bundles”, J.D. Moore, J.C. Palmer, Y.-C. Liu, T.J. Roussel, J.K. Brennan and K.E. Gubbins, 12th International Conference on Properties and Phase Equilibria for Product and Process Design, Suzhou, China, May 16-21, 2010.
- “Modeling Adsorption and Diffusion in Microporous Carbons”, J.C. Palmer, J.D. Moore, J.K. Brennan and K.E. Gubbins, 10th International Conference on Fundamentals of Adsorption, Awaji, Hyogo, Japan, May 23-28, 2010.
- “Anomalous Diffusion in Ordered and Disordered Microporous Carbons”, J.D. Moore, J.C. Palmer, Y.-C. Liu, T.J. Roussel and K.E. Gubbins, 10th International Conference on Fundamentals of Adsorption, Awaji, Hyogo, Japan, May 23-28, 2010.

- “Freezing of Simple Fluids in Regular and Disordered Carbon Nanotubes”, B. Coasne, K.E. Gubbins and M. Sliwinska-Bartkowiak, 10th International Conference on Fundamentals of Adsorption, Awaji, Hyogo, Japan, May 23-28, 2010.
- “Melting in Cylindrical Nanopores”, M. Sliwinska-Bartkowiak, M. Jażdżewska, K.E. Gubbins and L. Huang, 10th International Conference on Fundamentals of Adsorption, Awaji, Hyogo, Japan, May 23-28, 2010.
- “Critical Behavior of n-Alkane+Nitrobenzene Systems”, K.T. Koziol, M. Sliwinska-Bartkowiak, B. Coasne and K.E. Gubbins, U.S.-Poland Workshop: Nanoscale Phenomena in Materials and Interfaces, Krakow, Poland, June 6-10, 2010.
- “Confinement Effect on Freezing of Mixtures: Experiment and Molecular Simulation”, J. Czwartos, M. Jażdżewska, M. Wałdowski, S. Rogala, W. Pawłowski, B. Coasne, K.E. Gubbins and M. Sliwinska-Bartkowiak, U.S.-Poland Workshop: Nanoscale Phenomena in Materials and Interfaces, Krakow, Poland, June 6-10, 2010.
- “Melting of Water Confined in Cylindrical Carbon Nanopores”, M. Jażdżewska, , M.M. Sliwinska-Bartkowiak, K.E. Gubbins, L. Huang and K.-Y. Chan, U.S.-Poland Workshop: Nanoscale Phenomena in Materials and Interfaces, Krakow, Poland, June 6-10, 2010.
- “An Apparent Critical Point in Binary Mixtures of m-Nitrotoluene with n-Alkanes: Experimental and Simulation Study”, B. Ratajczak, T. Koziol, M. Kokorniak, M.M. Sliwinska-Bartkowiak and K.E. Gubbins, U.S.-Poland Workshop: Nanoscale Phenomena in Materials and Interfaces, Krakow, Poland, June 6-10, 2010.
- “Under Pressure: High Pressure Effects in Nanopores”, 8th Liblice Conference on the Statistical Mechanics of Liquids, Brno, Czech Republic, June 13-17, 2010.
- “Under Pressure: High Pressure Effects in Nanopores”, IGRTG Second Annual Workshop, Berlin, Germany, July 25-27, 2010.
- “Under Pressure: Quasi-High Pressure Effects in Nano-Pores”, International Materials Research Congress, IMRC XIX, Cancún, México, August 15-20, 2010.
- “The Origin of SAFT”, SAFT 2010 Symposium: 20 Years of the SAFT Equation, Barcelona, Spain, September 19-21, 2010. (Keynote Lecture).
- “Ammonia Dissociation over Graphite Oxide, Carbon Nanotube and Fullerene”, L. Huang, K.E. Gubbins and T.J. Bandosz, American Institute of Chemical Engineers Annual Meeting, Salt Lake City, Utah, November 7-12, 2010.
- “Thermodynamics and Dynamics of Confined Nano-Phases”, K.E. Gubbins, American Institute of Chemical Engineers Annual Meeting, Salt Lake City, Utah, November 7-12, 2010.
- “Molecular Modeling of Nanoporous Carbons: Atomistic Models and Simulated Adsorption”, J.C. Palmer, J.K. Brennan and K.E. Gubbins, American Institute of Chemical Engineers Annual Meeting, Salt Lake City, Utah, November 7-12, 2010.
- “Quasi-High Pressure Effects in Nanopores”, Y. Long, J.C. Palmer, B. Coasne, M. Sliwinska-Bartkowiak and K.E. Gubbins, American Institute of Chemical Engineers Annual Meeting, Salt Lake City, Utah, November 7-12, 2010.
- “Application of the BET Method to Microporous Materials”, J.C. Palmer, J.K. Brennan, M. Thommes and K.E. Gubbins, American Institute of Chemical Engineers Annual Meeting, Salt Lake City, Utah, November 7-12, 2010.
- “Under Pressure: Quasi-High Pressure Effects in Nanopores”, Y. Long, J.C. Palmer, B. Coasne, M. Sliwinska-Bartkowiak and K.E. Gubbins, American Institute of Chemical Engineers Annual Meeting, Salt Lake City, Utah, November 7-12, 2010.

- “Thermodynamics and Dynamics of Confined Nano-Phases”, International Symposium on Recent and Emerging Advances in Chemical Engineering (REACH), Indian Institute of Technology Madras, Chennai, India, December 2-4, 2010.
- “Molecular Modeling of Nanoporous Carbons: Understanding Adsorption and Characterization”, J.C. Palmer, J.K. Brennan and K.E. Gubbins, 9th International Symposium on Characterization of Porous Solids, Dresden, Germany, June 5-8, 2011.
- “Under Pressure: Quasi-High Pressure Effects in Nano-Pores”, Y. Long, J.C. Palmer, B. Coasne, M. Śliwinska-Bartkowiak and K.E. Gubbins, 9th International Symposium on Characterization of Porous Solids, Dresden, Germany, June 5-8, 2011.
- “High Pressure Effect and Material Deformation due to Confined Nanophases”, K.E. Gubbins, Y. Long, J.C. Palmer, B. Coasne and M. Śliwinska-Bartkowiak, Compliant Solids Workshop, Chimie Paris Tech, Paris, June 9-11, 2011.
- “Novel Ice Structures in Carbon Nanopores: Pressure Enhancement Effect of Confinement”, M. Śliwinska-Bartkowiak, H. Drozdowski, M. Kempinski, Y. Long, M. Śliwinska-Bartkowiak and K.E. Gubbins, Compliant Solids Workshop, Chimie Paris Tech, Paris, June 9-11, 2011.
- “The Role of the Hydrogen Bond in Mechanism of Water Diffusion in Carbon Nanotubes”, Diffusion Fundamentals IV, Rensselaer Polytechnic Institute, Troy, NY, August 21-24, 2011.
- “Does a Hydrogen Atom/Proton Diffuse Through Graphene?”, Diffusion Fundamentals IV, Rensselaer Polytechnic Institute, Troy, NY, August 21-24, 2011.
- “High Pressure Effects in Nanopores”, Y. Long, J.C. Palmer, B. Coasne, M. Śliwinska-Bartkowiak and K.E. Gubbins, American Institute of Chemical Engineers Annual Meeting, Minneapolis, MN, October 16-21, 2011.
- “Molecular Dynamics Studies of Diffusion and Solvation of Rubidium Bromide Solutions in Nanoconfinement”, Katherine A. Phillips, Jeremy C. Palmer and Keith E. Gubbins, American Institute of Chemical Engineers Annual Meeting, Minneapolis, MN, October 16-21, 2011.
- “A Reactive Molecular Dynamics Simulation of Hydrogen Sulfide Dissociation over Graphene Oxide”, Liangliang Huang, Jeremy C. Palmer and Keith E. Gubbins, American Institute of Chemical Engineers Annual Meeting, Minneapolis, MN, October 16-21, 2011.
- “Understanding Adsorption and Diffusion in Disordered Nanoporous Carbons”, Jeremy C. Palmer and Keith E. Gubbins, American Institute of Chemical Engineers Annual Meeting, Minneapolis, MN, October 16-21, 2011.
- “Ammonia Adsorption on Cu-MOF: A Molecular Simulation Approach”, Liangliang Huang, Camille Petit, Teresa Bandoz and Keith E. Gubbins, American Institute of Chemical Engineers Annual Meeting, Minneapolis, MN, October 16-21, 2011.
- “High Pressure Effect and Material Deformation due to Adsorption in Porous Materials”, Yun Long, Jeremy C. Palmer, Benoit Coasne, Małgorzata Śliwinska-Bartkowiak and Keith E. Gubbins, 6th International Workshop on Characterization of Porous Materials: from Angstroms to Millimeters, Delray Beach, FL, April 30-May 2, 2012.
- “Melting of Liquids Confined in Nano-Pores: Novel Ice Structures”, Małgorzata Śliwinska-Bartkowiak, Monika Jazdzewska, Yun Long and Keith E. Gubbins, 6th Pacific Basin Conference on Adsorption Science & Technology, Taipei, Taiwan, May 20-23, 2012.

- “High Pressure Effect and Material Deformation due to Adsorption”, Keith E. Gubbins, Yun Long, Jeremy Palmer, Benoit Coasne and Małgorzata Śliwinska-Bartkowiak, 6th Pacific Basin Conference on Adsorption Science & Technology, Taipei, Taiwan, May 20-23, 2012.
- “Structure of Water Confined in Nanocarbons – Pressure Enhancement Effects”, M. Śliwinska-Bartkowiak, H. Drozdowski, M. Kempański, Y. Long, J. Palmer and K.E. Gubbins, Third Symposium on Future Challenges for Carbon-Based Nanoporous Materials, Shinshu University, Nagano, Japan, May 26-29, 2012.
- “Transport Properties of Methane Confined in Nanoporous Carbon”, Andrew P. Santos, Joshua D. Moore, Jeremy C. Palmer and Keith E. Gubbins, American Institute of Chemical Engineers Annual Meeting, Pittsburgh, PA, October 28-November 2, 2012.
- “Solvation Structure of Ions in Model Disordered Carbon Electrodes”, Katherine A. Phillips, Jeremy C. Palmer and Keith E. Gubbins, American Institute of Chemical Engineers Annual Meeting, Pittsburgh, PA, October 28-November 2, 2012.
- “Pressure Enhancement in Nanopores: Effect of Pore Shape”, Yun Long, Keith E. Gubbins, Erich A. Muller, George Jackson and Erik E. Santiso, American Institute of Chemical Engineers Annual Meeting, Pittsburgh, PA, October 28-November 2, 2012.
- “Exploring Solid-Fluid Phase Behavior of Adsorbed Water Nanoconfined between Mica and Graphene Surfaces”, Cody K. Addington, Yun Long and Keith E. Gubbins, American Institute of Chemical Engineers Annual Meeting, Pittsburgh, PA, October 28-November 2, 2012.
- “Surface Chemistry of TiO₂: Hydrophilic or Hydrophobic”, Liangliang Huang, Luzheng Zhang, Adri C.T. van Duin, Xiao-Hua Lu and Keith E. Gubbins, American Institute of Chemical Engineers Annual Meeting, Pittsburgh, PA, October 28-November 2, 2012.
- “Melting of Liquids Confined in Nano-Pores: Ice Structures Stabilized by Confinement”, Magdalena Cichocka, Monika Jazdzewska, Małgorzata Śliwinska-Bartkowiak, Yun Long and Keith E. Gubbins, Fundamentals of Adsorption 11, Baltimore, May 19-24, 2013.
- “Effects of Wettability on Adsorption and Pressure of Fluids in Nanopores”, Yun Long, Cody K. Addington, Małgorzata Śliwinska-Bartkowiak and Keith E. Gubbins, Fundamentals of Adsorption 11, Baltimore, May 19-24, 2013.
- “Electrochemical Properties of Model Disordered Carbon Electrodes”, Katherine Phillips and Keith E. Gubbins, Fundamentals of Adsorption 11, Baltimore, May 19-24, 2013.
- “Reactive Molecular Dynamics Simulation of Graphite Oxide and its Application in Hydrogen Sulfide Removal”, Liangliang Huang and Keith E. Gubbins, Fundamentals of Adsorption 11, Baltimore, May 19-24, 2013.
- “Diffusion of CH₄ and CH₄-CO₂ and CO₂-N₂ Mixtures Confined in Nanoporous Carbons”, Andrew Santos, Joshua D. Moore, Jeremy C. Palmer and Keith E. Gubbins, Fundamentals of Adsorption 11, Baltimore, May 19-24, 2013.
- “The Design of Titanium Oxide Surface Chemistry by Molecular Modeling”, Liangliang Huang and Keith E. Gubbins, PPEPPD 2013 (Properties and Phase Equilibria for Process and Product Design), Iguazu, Argentina, May 26-30, 2013.
- “Phase Transitions of Water in Nano-Pores: Pressure Enhancement Effect of Confinement”, M. Śliwinska-Barkowiak, A. Sterczyńska, M. Jazdzewska, M. Kempański, Y. Long, L. Huang and K.E. Gubbins, Workshop on Adsorption in Compliant Solids, Paris, France, June 5-7, 2013.

- “The Search for High Pressure Ice Phases in Nano-Confined Water via Molecular Simulation”, C.K. Addington, K.A. Phillips and K.E. Gubbins, American Institute of Chemical Engineers Annual Meeting, San Francisco, CA, November 3-8, 2013.
- “Exploring the Effect of Pore Morphology on Model Electrochemical Double-Layer Capacitor Systems”, K.A. Phillips and K.E. Gubbins, , American Institute of Chemical Engineers Annual Meeting, San Francisco, CA, November 3-8, 2013.
- “Controllable Phase Transition of CuBTC Metal-Organic Framework and its Application in CO₂ Capture and Storage”, L. Huang, S. Zhang, K.E. Gubbins and X. Lu, , American Institute of Chemical Engineers Annual Meeting, San Francisco, CA, November 3-8, 2013.
- “Molecular Simulation of the Dielectric Relaxation of Water in Graphene Pores”, K.A. Phillips, K.E. Gubbins and S.H.L. Klapp, 10th International Symposium on the Characterization of Porous Solids, Granada, Spain, May 11-14, 2014.
- “The Search for High Pressure Ice Phases in Nanoconfined Water via Molecular Simulation”, C.K. Addington, K.A. Phillips and K.E. Gubbins, 10th International Symposium on the Characterization of Porous Solids, Granada, Spain, May 11-14, 2014.
- “Molecular Dynamics Study of the Hydration & Dielectric Response of Confined Fluids”, Katherine A. Phillips, Sabine H.L. Klapp and Keith E. Gubbins, Annual Meeting of IRTG 1524 on Self-Assembled Soft-Matter Nanostructures at Interfaces, Potsdam, Germany, June 6-8, 2014.
- “Liquid/Solid Interaction-Dependent Nanofriction Coefficient at Simple Fluid/Solid Interfaces”, Rong An, Keith E. Gubbins and Liangliang Huang, Annual Meeting of IRTG 1524 on Self-Assembled Soft-Matter Nanostructures at Interfaces, Potsdam, Germany, June 6-8, 2014.
- “Confinement Effect on Chemical Reaction Yield: The Nitric Oxide Dimer Reaction”, Deepti Srivastava and Keith E. Gubbins, Annual Meeting of the American Institute of Chemical Engineers, Atlanta, GA, November 16-21, 2014.
- “Liquid-Solid Interaction-Dependent Nanofriction Coefficient at Simple Fluid-Solid Interfaces”, Rong An, Keith E. Gubbins and Liangliang Huang, Annual Meeting of the American Institute of Chemical Engineers, Atlanta, GA, November 16-21, 2014.
- “A Theoretical Understanding of Amino Acid Interaction with Graphene and its Derivatives”, Liangliang Huang, Keith E. Gubbins and Teresa Bandosz, Annual Meeting of the American Institute of Chemical Engineers, Atlanta, GA, November 16-21, 2014.
- “Computer Simulation of the Mercury-Solid Interface”, Cody K. Addington and Keith E. Gubbins, Annual Meeting of the American Institute of Chemical Engineers, Atlanta, GA, November 16-21, 2014.
- “Wetting, Pressure Effects and the Mercury-Solid Interface”, Cody K. Addington and Keith E. Gubbins, 7th International Workshop on Characterization of Porous Materials: from Angstroms to Millimeters, Delray Beach, FL, May 3-6, 2015.
- “Structure of Ice Confined in Nanopores”, M. Śliwiska-Barkowiak, K. Domin, M. Jażdżewska, Y. Long and K.E. Gubbins, 9th International Symposium on Surface Heterogeneity Effects in Adsorption and Catalysis on Solids (ISSHAC-9), Wroclaw, Poland, July 18-22, 2015.
- “Confinement Effect on Chemical Reaction Yield: The Nitric Oxide Dimer Reaction”, Deepti Srivastava, C. Heath Turner and Keith E. Gubbins, Thermodynamics 2015, Copenhagen, Denmark, September 15-18, 2015.

- “Liquids Confined in Nanopores: Novel Ice Structures – Pressure Enhancement Effects”, Kamila Domin, Kwong-Yu Chan, Małgorzata Śliwinska-Bartkowiak, Yun Long and Keith E. Gubbins, 7th Pacific Basin Conference on Adsorption Science and Technology, Xiamen, China, 24-27 September, 2015.
- “The Role of Polymer-Substrate Interaction Strength in Polymer Films on Solid Substrates: Friction Force and the Glass Transition”, Rong An, Christopher Hering, Nailiang Zhou and Keith E. Gubbins, American Institute of Chemical Engineers Annual Meeting, Salt Lake City, UT, November 8-13, 2015.

Courses Taught:

Undergraduate:

Chemical Engineering Thermodynamics (University of Florida, Cornell, NCSU) Phase and Chemical Equilibria and Applications (University of Florida, Cornell), Design (Cornell), Chemical Engineering Kinetics (University of Florida), Transport Phenomena (University of Florida), Chemical Process Design (Cornell), Separation Processes (Cornell).

Graduate:

Thermodynamics: core graduate course (University of Florida, Cornell, NCSU)
 Theory of Molecular Liquids (Cornell)
 Statistical Thermodynamics (University of California, Berkeley, Cornell, NCSU)
 Advanced Seminars in Thermodynamics and Statistical Mechanics (Cornell)
 Statistical Mechanics of Inhomogeneous Fluids (Australian National Univ.)
 Statistical Mechanics and Applications (a short course for Ph.D. students and postdoctoral workers), Chiba University, Japan, November 30-December 21, 1999
 Statistical Mechanics and Simulation of Fluids and Soft Matter (North Carolina State Univ.)
 Multi-Scale Modeling of Fluids and Soft Matter (NCSU)

North Carolina State University:

*Spring 1999

*Chemical Engineering 315, Thermodynamics I (Junior level)

*Fall 1998

*Chemical Engineering 713, Chemical Engineering Thermodynamics: core course

*Fall 1999

*Chemical Engineering 713, Chemical Engineering Thermodynamics: core course

*Spring 2000

*Chemical Engineering 315, Thermodynamics I (Junior level)

*Fall 2000

*Chemical Engineering 713, Chemical Engineering Thermodynamics: core course

*Spring 2001

*Chemical Engineering 597B, Statistical Mechanics and Simulation of Fluids and Soft Matter: new course

*Fall 2002

*Chemical Engineering 713, Chemical Engineering Thermodynamics: core course

*Spring 2003

*Chemical Engineering 315, Thermodynamics I (Junior level)

Fall 2003

Chemical Engineering 713, Chemical Engineering Thermodynamics: core course

Spring 2004

Chemical Engineering 597B, Multi-Scale Modeling of Fluids and Soft Matter

Fall 2004

Chemical Engineering 315, Thermodynamics I (Junior level)

Spring 2005

Chemical Engineering 315, Thermodynamics I (Junior level)

Fall 2005

Chemical Engineering 713, Chemical Engineering Thermodynamics: core course

Spring 2006

Chemical Engineering 596M, Multi-Scale Modeling of Matter

Fall 2006

Chemical Engineering 713, Chemical Engineering Thermodynamics: core course

Spring 2007	Chemical Engineering 315, Thermodynamics I (Junior level)
Fall 2007	Chemical Engineering 713, Chemical Engineering Thermodynamics: core course
Spring 2008	Chemical Engineering 596M, Multi-Scale Modeling of Matter
Fall 2008	Chemical Engineering 713, Chemical Engineering Thermodynamics: core course
Spring 2009	Chemical Engineering 315, Thermodynamics I (Junior level)
Fall 2009	Chemical Engineering 713, Chemical Engineering Thermodynamics
Spring 2010	Chemical Engineering 596, Multi-Scale Modeling of Matter
Fall 2010	Chemical Engineering 713, Chemical Engineering Thermodynamics
Fall 2011	Chemical Engineering 713, Chemical Engineering Thermodynamics
Spring 2012	Chemical Engineering 775, Multi-Scale Modeling of Matter
Fall 2012	Chemical Engineering 713, Chemical Engineering Thermodynamics
Spring 2013	Chemical Engineering 315, Thermodynamics I (Junior level)

Other Universities

University of California, Berkeley

Statistical Mechanics of Interfacial Properties, a short course for Ph.D. students and postdocs,
Spring 1982.

Chiba University, Chiba, Japan

Statistical Mechanics and Applications, a short course for Ph.D. students and postdoctoral workers, November 30-December 21, 1999

Zhejiang University, Hangzhou, China

Molecular Modeling of Matter using Atomistic Simulation. Molecular Dynamics and Monte Carlo Simulation. A short course for Ph.D. students, October 18-20, 2010.

Basque Centre for Applied Mathematics, Bilbao, Spain

Molecular Modeling of Matter: What We Can Do Now and in the Near Future. A short course for Ph.D. students and researchers, March 28-April 1, 2011. Attended by about 50 participants from across Spain.

Imperial College London, U.K.

Molecular Modeling of Matter at the Atomistic and Meso-Scales. A workshop for Ph.D. students, postdocs and faculty from universities in the London area, May 9-13, 2011. The workshop covered background material on statistical mechanics, the theory and application of Monte Carlo and molecular dynamics simulation, lattice Monte Carlo, and Brownian and dissipative particle dynamics. About 60 participants (graduate students, postdocs, faculty from institutions within and near London) were in attendance.

University of Hong Kong

Molecular Modeling of Matter at the Atomistic Scale. July 18-22, 2011. A short course, attended by about 60 participants (graduate students, postdocs, faculty) from the five Hong Kong universities offering science and engineering.

Professional Activities (1973 - present):

Symposia, Conferences, Workshops Chaired:

"Recent Advances in the Study of Molecular Transport Properties," AIChE Meeting, Detroit, June 4, 1973.

"Thermodynamics and Transport Properties of Interfaces and Surfactant Solutions," AIChE Meeting, Chicago, Dec. 1, 1976.

"Computer Simulation Methods for Physical Properties," AIChE Meeting, New York, Nov. 17, 1977.

"Theory of Polar Liquids," Chemical Society (London), Aberystwyth, Wales, Sept. 12-14, 1979.

"Light Scattering and Birefringence Studies of Liquids," Symposium on Structure of Molecular Liquids, Royal Society of Chemistry, University of Cambridge, England, April 6, 1981.

"Cornell Minisymposium on Liquids," Co-chairman with B. Widom, Aug. 17, 1981.

- "CCP5 Conference on Computer Simulation of Molecular Liquids," Hull, U.K., March 30, 1983.
- "Cornell Minisymposium on Liquids," Co-chairman with B. Widom, Aug. 26, 1985.
- "Theories of Interfacial Structure, Dynamics and Function," Annual Meeting of the American Chemical Society, Chicago, Sept. 9-10, 1985.
- "Critical Evaluation and Prediction of Phase Equilibria in Multicomponent Systems," Second Codata Symposium, General Section, Paris, Sept. 13, 1985.
- "Molecular Simulation," 4th International Conference on Fluid Properties and Phase Equilibria for Chemical Process Design, Helsingor, Denmark, May 12, 1986.
- "Theoretical and Simulation Studies of Solutions," 9th IUPAC Conference on Chemical Thermodynamics, Lisbon, July 15, 1986.
- "CCP5 Meeting on Industrial Applications of Molecular Simulations", Birkbeck College, London, Jan. 6-8, 1988.
- "Computer Simulations of Molecular Systems", International Symposium on Thermodynamics in Chemical Engineering and Industry, Beijing, China, May 30-June 2, 1988.
- "Cornell Minisymposium on Liquids", Co-Chairman with B. Widom, Aug. 21, 1989.
- "Cornell Minisymposium on Liquids", Co-Chairman with B. Widom, Aug. 19, 1991.
- "Fourth Liblice Conference on Statistical Mechanics of Liquids", Co-Chaired with Ivo Nezbeda, June 6-10, 1994, Lake Milovoy, Czech Republic.
- "CECAM (Centre Européen de Calcul Atomique et Moléculaire) Workshop on Adsorption, Phase Transitions and Transport in Porous Materials", Co-Chaired with Denis Evans, Alain Fuchs, David Nicholson, Nicholas Quirke and William A. Steele, Lyon, France, September 11-15, 1995.
- "Molecular Modeling of Adsorption", Annual AIChE Meeting, Los Angeles, Nov. 18, 1997.
- Fifth Liblice Conference on Statistical Mechanics of Liquids (Co-Chair), Zelezná Ruda, Czech Republic, June 7-12, 1998.
- Sixth Liblice Conference on Statistical Mechanics of Liquids (Co-Chair), Spindleruv Mlýn, Krkonoše National Park, Czech Republic, June 9-14, 2002.
- Workshop on International Graduate Program between Berlin and the U.S., Co-Chair, Berlin, Germany, June 11-13, 2003.
- CECAM (Centre Européen de Calcul Atomique et Moléculaire) Workshop on Multiscale Modeling of Chemical Reactions", Lyon, France, September 1-5, 2003.
- Workshop on International Graduate Program between Berlin and the U.S., Chair, Raleigh, NC, September 15-17, 2003.
- Seventh Liblice Conference on Statistical Mechanics of Liquids (Co-Chair), Plzeň, Czech Republic, June, 2006.
- U.S. – Poland Workshop on Nanoscience and Nano-Structured Materials, Poznań, Poland, June 26-28, 2006. Co-Chair. [First National Science Foundation sponsored workshop]
- U.S.-Poland Workshop on Interfacial Phenomena and Advanced Materials, Gdańsk, Poland, June 4-6, 2008. Chair. [Second National Science Foundation sponsored workshop]

U.S.-Germany Workshop on Self-Assembled Nanostructures, Raleigh, NC, April 7-8, 2009.

2nd U.S.-Germany Workshop on Self-Assembled Nanostructures, Berlin, Germany, July, 2010.

3rd U.S.-Germany Workshop on Self-Assembled Nanostructures, New Bern, NC, October 3-5, 2011.

4th U.S.-Germany Workshop on Self-Assembled Nanostructures, Berlin, Germany, July, 2012.

5th U.S.-Germany Workshop on Self-Assembled Nanostructures, New Bern, NC, Sept. 29 - October 3, 2013.

Memberships in Professional Societies:

American Association for the Advancement of Science

American Chemical Society

American Institute of Chemical Engineers

American Institute of Physics

Chemical Society (London)

National Academy of Engineering

International Activities: Committees, Boards

International Program Committee and Co-Chair, Liblice III Conference on Statistical Mechanics of Liquids, Bechyne, Czechoslovakia, May 28-June 1, 1990.

International Program Committee and Co-Chair, Liblice IV Conference on Statistical Mechanics of Liquids, June 6-10, 1994, Lake Milovoy, Czech Republic.

International Organizing Committee and Co-Chair, CECAM (Centre Européen de Calcul Atomique et Moléculaire) Workshop on Adsorption, Phase Transitions and Transport in Porous Materials", Lyon, France, September 11-15, 1995.

International Program Committee and Co-Chair, Liblice V Conference on Statistical Mechanics of Liquids, Zelezna Ruda, Czech Republic, June 7-12, 1998

Scientific Committee for the Third International Symposium on Effects of Surface Heterogeneity in Adsorption and Catalysis, August 9-16, 1998 in Turin, Poland

Scientific Advisory Committee, 2nd Pacific Basin Conference on Adsorption Science and Technology, Brisbane, Australia, May 14-18, 2000

International Organizing Committee, 9th International Conference on Properties and Phase Equilibria for Product and Process Design, Kurashiki/Kyoto, Japan, May 20-25, 2001

Scientific Committee for the Fourth International Symposium on Effects of Surface Heterogeneity in Adsorption and Catalysis on Solids, August 27-31, 2001 in Krakow, Poland

International Program Committee and Co-Chair, Liblice VI Conference on Statistical Mechanics of Liquids, Spindleruv Mlyn, Czech Republic, June 9-14, 2002.

International Advisory Board, XIV International Conference on Chemical Thermodynamics, St. Petersburg, Russia, July 1-5, 2002.

Scientific Advisory Board, Yangtze Conference of Fluids and Interfaces, Nanjing-Three Gorges-Chongqing, China, October 12-18, 2002.

International Advisory Committee, 3rd Pacific Basin Conference on Adsorption Science and Technology, Kyongju, Korea, May 25-29, 2003.

Chair of International Organizing Committee, CECAM (Centre Européen de Calcul Atomique et Moléculaire) Workshop on “Multiscale Modeling of Chemical Reactions”, Lyon, France, September 1-5, 2003.

International Scientific Committee, Symposium: “SAFT 03: 15 Years of SAFT”, Barcelona, Spain, December 12, 2003.

International Advisory Committee, European Molecular Liquids Group Annual Meeting: Complex Liquids – Fundamental Properties to Industrial Applications”, Sheffield, U.K., September 3-7, 2004.

Scientific Advisory Committee, 8th International Conference on Fundamentals of Adsorption, Sedona, Arizona, May 2004.

International Organizing Committee, 10th International Conference on Properties and Phase Equilibria for Product and Process Design, Snowbird, Utah, May 16-21, 2004.

Scientific Committee for the Fifth International Symposium on Effects of Surface Heterogeneity in Adsorption and Catalysis on Solids, August 28 – September 3, 2004 in Gdansk, Poland

International Advisory Committee, 3rd International Conference on Computational Modeling and Simulation of Materials: Modeling and Simulating Materials Nanoworld”, Acireale, Sicily, Italy, May 30-June 4, 2004.

International Advisory Committee, European Molecular Liquids Group Conference, “Complex Liquids – Fundamental Properties to Industrial Applications”, Sheffield, U.K., September 3-7, 2004.

International Advisory Committee, 1st Pacific Rim Conference in Nano-Sciences, Broome, Western Australia, September 6-12, 2004.

International Advisory Committee, 4th International Workshop on Characterization of Porous Materials: from Angströms to Millimeters, Princeton, June 21-23, 2006.

International Program Committee and Co-Chair, Liblice VII Conference on Statistical Mechanics of Liquids, Lednice, Czech Republic, June 11-16, 2006.

Scientific Committee for the Sixth International Symposium on Effects of Surface Heterogeneity in Adsorption and Catalysis on Solids, August 28 – September 2, 2006 in Zakopane, Poland

International Committee for the Second Pacific Basin Nanoscience Conference, Hanoi, Vietnam, February 2007.

Scientific Committee for the 9th Fundamentals of Adsorption Conference, Giardini Naxos, Sicily, Italy, May 20-25, 2007.

International Advisory Board, Eleventh International Conference on Properties and Phase Equilibria for Product and Process Design, PPEPPD2007, Hersonissos, Crete, Greece, May 20-25, 2007.

International Advisory Committee, 5th Pacific Basin Adsorption Science & Technology Conference, Singapore, May 25-27, 2009.

Scientific Committee for the Seventh International Symposium on Effects of Surface Heterogeneity in Adsorption and Catalysis on Solids, July 5-11, 2009 in Kazimierz, Poland

International Advisory Committee, 5th International Workshop on Characterization of Porous Materials: from Angströms to Millimeters, Rutgers University, June 24-26, 2009.

International Advisory Committee, 3rd U.S.-Poland Workshop, Krakow, Poland, June 7-10, 2010.

International Program Committee and Co-Chair, Liblice VIII Conference on Statistical Mechanics of Liquids, Brno, Czech Republic, June 13-18, 2010.

Scientific Committee for the 10th Fundamentals of Adsorption Conference, Kyoto, Japan, May , 2010.

International Advisory Committee, 24th Statistical Physics Conference (STATPHYS24), Cairns, Australia, July 19-23, 2010.

International Advisory Board, Twelfth International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD), Suzhou, China, May 16-21, 2010.

International Advisory Committee, 6th International Workshop on Characterization of Porous Materials: from Angströms to Millimeters, West Palm Beach, April 30-May2, 2012.

International Advisory Board for the 13th International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD), held in Iguazu, Argentina, in May 2013.

Scientific Advisory Board, International Fundamentals of Adsorption Conference, Baltimore, MD, May19-24, 2013.

International Advisory Committee, STATPHYS25. Seoul, Korea, July 22-26, 2013.

International Advisory Board, 13th International Ceramics Congress, Porous Ceramics for Environmental Protection, Energy-Related Technologies and Advanced Industrial Cycles, June 8-20, 2014.

International Advisory Committee, 7th International Workshop “Characterization of Porous Materials: from Ångströms to Millimeters”, Delray Beach, FL, May 3-6, 2015.

International Advisory Committee, 7th Pacific Basin Conference on Adsorption Science and Technology (PBAST-7), Xiamen, China, September 24 – 27, 2015.

International Advisory Board for the 14th International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD), to be held in Porto, Portugal, in May 2016.

International Advisory Committee, 26th Statistical Physics Conference (STATPHYS26), Lyon, France, July 18-22, 2016.

International Advisory Board, International Conference on Molecular Simulation 2016 (ICMS 2016), Shanghai, China, October 2016.

External Examiner for Ph.D. Thesis Candidates

Berend Smit, University of Utrecht, Amsterdam, Netherlands, 1992

Amparo Galindo, University of Sheffield, Sheffield, U.K., 1995

Felipe Jimenez Blas, University of Tarragona, Tarragona, Spain, 1996

Fabienne Porcheron, University of Paris XI, Orsay, France, 2001

Josep Pamiès, University of Tarragona, Spain, December 11, 2003.

Nguyen Than, University of Queensland, Australia, July, 2006.

Shenghua Mao, University of North Carolina at Chapel Hill, April 2007

Alekandros Lymperiadis, Imperial College, London, U.K., 2007
 Jianhui Li, Swinburne University of Technology, Melbourne, Australia, March 2008
 Wei Li, Nanjing University of Technology, Nanjing, China, December 19, 2008
 Qing Shao, Nanjing University of Technology, Nanjing, China, December 19, 2008
 Sergej Naumov (Dr. rer. nat.), University of Leipzig, Leipzig, Germany, June 2009.
 Omar M. Zaki, Cairo University, Egypt, December 2011.
 Wei Mingjie, Nanjing University of Technology, Nanjing, China, December 15, 2011.
 Manuel Greschek, Technical University of Berlin, Berlin, Germany, January 25, 2012.

External Examiner for Habilitation Thesis Candidates

Sabine Klapp, Technical University of Berlin, 2005
 Adham Ramadan, American University of Cairo, November 2007

National Committees, Panels:

Program Committee (Thermodynamics and Mass Transfer), AIChE (1974-1981).
 National Academy of Sciences Committee to study formation of NRCC (National Resource Center for Computing in Chemistry), 1976-1977.
 National Research Council Assessment Board to review NIST Programs, 1988-1991.
 Review Board, Separation and Related Sciences, Exxon Research & Engineering Co., June 4-6, 1990.
 Peer Review Committee, National Academy of Engineering, 1994-97.
 Review Committee for Chemical Technology Division, Oak Ridge National Laboratory, 1996-
 Board on Chemical Sciences and Technology, National Research Council, 1997-2000.
 NSF Panel, CTS Interfacial and Transport Section, December 16, 2004.
 NSF Panel, CTS Interfacial and Transport Section, March 17, 2005.
 Scientific Committee, First NCSU Workshop on Nanotechnology for Energy and Environment, October 26, 2005.
 Selection Committee, Joel Henry Hildebrand Award in the Theoretical and Experimental Study of Liquids, American Chemical Society, 2009.

University Committees: Cornell

Curriculum Committee
 CADIF (Computer Aided Design Instructional Facility) Policy Board
 Advisory Committee, History and Philosophy of Science Program
 Debye Lecture Committee
 Program Committee for History & Philosophy of Science Program
 Program Committee for Center for Applied Mathematics
 Search Committee, Dean of Engineering
 Search Committee, Director of Theory Center
 Program Committee for Biotechnology Center

Chairman, Program for Center for Applied Mathematics
 A.D.White Professor-at-Large Committee
 University Governance Committee 1994-95
 Faculty Council of Representatives, 1994-95
 Executive Committee, Theory Center, 1996-
 Program Committee, Center of Applied Mathematics, 1996-
 Academies Nomination Committee, 1995-

University Committees, Councils, Task Forces, etc.: NCSU

Council of University Professors
 Department Head Search Committee, 1999
 Co-Chair (with J. Bernholc), Strategic Computing Task Force and author of final report to the
 VC for Research and Provost, 2004-2005
 Co-Chair (with J. Bernholc) of task force to prepare White Paper on Computational Science and
 Engineering for Chancellor, January 2006.
 University Faculty Scholar Award Selection Committee, College o Engineering, 2012.
 Department Head Search Committee, 2012.

College Committees: NCSU

Promotion and Tenure Committee, 1999-
 Nomination Committee for Prof. C.K. Hall, 2005.

Department Committees: Florida and Cornell

Graduate Committee (Florida, Cornell)
 Faculty Search Committee (Florida, Cornell)
 Computer Use Committee (Florida, Cornell: Chairman)
 Graduate Field Representative (Cornell) 1977-83
 Policy Committee (Cornell) 1983-
 Building Renovation Committee (Cornell) 1983-1990
 Faculty Search Committee (Cornell; Chair) 1995-
 Awards Committee (Cornell; Chair) 1995-

Department Committees: NCSU

Faculty Search Committee
 New Building Committee
 Comprehensive Review of Tenured Faculty Committee
 Search Committee for Head of Department, Chemical Engineering

Consulting (1979-):

Regular Consultant:

Exxon Research and Engineering Co., Clinton, NJ, Oct. 25, 1985-1995
 Molecular Simulations, Cambridge, U.K., 1992-99
 Quantachrome Instruments, Boynton Beach, FL, 2005-

Occasional Consultant:

Mobil Oil, 1979, 1980
 Union Carbide Corp., 1981
 Process Simulation International, 1982
 Exxon Engineering, 1980, 1981
 National Bureau of Standards, May 1983
 BP Research, U.K., April 1985
 Unilever Research, Port Sunlight, U.K., Dec. 11, 1985
 Linde Division, Union Carbide, Nov 23, 1988
 Shell Development Corp., Westhollow Lab., Houston, TX, April 21, 1989.
 BP Research, U.K., Dec. 15, 1989
 Shell Research, Amsterdam, Dec. 11, 1990.
 Mobil Research, Princeton, June 10, 1991.
 Exxon Chemical Co., Baton Rouge, LA, October 14, 1991; Feb. 27, 1997.
 BHP Research Lab., Melbourne, Australia, October 5, 1993.
 Johnson Matthey Technology Centre, Sonning Common, U.K., June 22, 1994.
 Chevron Research & Technology, Richmond, CA, May 12, 1995.
 Exxon Chemical Co., Baton Rouge, LA, February 26-27, 1997.
 Westvaco Charleston Technical Center, Charleston, SC, October 27, 2000.
 Gaz de France, Research and Development Division, St. Denis, France, January 10, 2002.
 Dow Chemical Co., Midland, MI, April 22-23, 2002.
 MeadWestvaco, Charleston Technical Center, Charleston, SC, August 12, 2003.
 Quantachrome Instruments, Boynton Beach, FL, March 7, 2005.
 Textiles Research Institute, Princeton, NJ, May 17, 2005.
 Quantachrome Instruments, Boynton Beach, FL, March 7, 2006.
 Quantachrome Instruments, Boynton Beach, FL, April 2-4, 2008.
 Quantachrome Instruments, Boynton Beach, FL, April 19-21, 2010.
 Babcock & Wilcox Co., Akron, Ohio, November 12, 2012.
 Quantachrome Instruments, Boynton Beach, FL, March 26-27, 2013.

Undergraduate Research Assistants Advised [1983-]:

<i>Student</i>		<i>Present Location</i>
Sonbol Sepahban	1983	Northrup Grumman (VP Engng.)
Maryam Golnaraghi	1984	Harvard (Ph.D. program)

David Berry	1991-92	Univ. Massachusetts (PhD program)
Peter Gordon	1991-92	Univ. Pennsylvania (PhD program)
Wilbelto Adorno	1995	Univ. Puerto Rico (was at Cornell in REU program)
Carlos Rinaldi Ramos	1995	Univ. Puerto Rico (was at Cornell in REU program)
Scott Kostojohn	1995-96	Cornell
Eugene Yoo	1995-96	Cornell
Lisa Chang	1997-98	Cornell
Elaine Tam	1997-98	Cornell
Aaron Fabas	1997-98	Cornell
Brandon Hindmarsh	1999	NCSU
Gabriel Hudson	2005	NCSU
Qu ('Frank') Chen	2007	Zhejiang University
Siwei Luo	2008	Tsinghua University
David Crawford	2010-11	NCSU
Andrew Santos	2011-13	Princeton University
William Harris	2014-	NCSU
Christopher Hering	2014-	NCSU

Graduate Students Advised:

Master of Science

<i>Student</i>		<i>Present Location</i>
Ed Bing	1965	Unknown
K.K. Bhatia	1965	Unknown
Ram N. Bhatia	1967	Exxon Chemical, Baton Rouge
Jatindar Jolly	1968	Unknown
Min Kwan Tham	1968	U. S. Bureau of Mines
Miretta Stephanopoulos	1975	Tufts Univ.
Sohail Murad	1976	Univ. of Illinois Chicago
James Downs	1977	Kodak
Jean J. Nicolas	1978	Paris
José R. S. Machado	1979	Air Products
Mark Wojcik	1981	Unknown
C. D. Naik	1983	Singer Link
George Charos	1984	Georgia Tech
Walter R. Cooney	1987	Dow Chemical
Wojciech Gozdz	1993	Inst. Phys. Chem., Warsaw, Poland
Christine L. McCallum	1997	Intel, Phoenix
Sandra Gavalda	2000	Akzo Nobel Catalysts
Yun Long	2009	NCSU
Liangliang Huang	2010	NCSU

M. Eng. (Project)

Zahra Maher	1984	Lazard-Freres, NYC
R. Norat	1996	Unknown
D. Zeid	1996	Unknown

(3)

Ph.D.

	<u>Graduated</u>	
Jean Brunet	1968	Univ. Quebec
Satyendra K. Shoor	1968	Shell Development
Min Jack Tham	1968	Shell Development
Min Kwan Tham	1970	U.S. Bureau of Mines
Erich W. Tiepel	1971	Westinghouse
M. S. Ananth	1972	IIT Madras
James M. Haile	1976	Clemson University
Chorng H. Twu	1976	Aspen Technology Inc.
Lynn E. Groome	1977	Unknown
Sohail Murad	1979	Univ. Illinois, Chicago
Katherine Shing	1982	Univ. Southern Calif.
Venkat Venkatasubramanian	1983	Columbia Univ.
Mark Wojcik	1984	unknown
Der Jiun Lee	1985	?
John Eggebrecht	1986	Iowa State University
Kwong-Yu Chan	1987	Hong Kong University (Chem.)
John H. Thurtell	1987	Mobil Research, Princeton
Walter G. Chapman	1987	Rice University
Brian K. Peterson	1987	Exxon-Mobil Research, Annendale
Grant S. Heffelfinger	1988	Sandia National Laboratories
Manoj Chalam	1990	Mobil Research, Paulsboro
Ziming Tan	1991	British Oxygen, NJ
Karl Johnson	1992	University of Pittsburgh
Christian Lastoskie	1994	University of Michigan
Charles Rhykerd	1996	Sandia National Laboratories
Shaoyi Jiang	1993	University of Washington
Joanne Button		unknown
Erich Müller	1995	Imperial College, London
Susanne Sowers	1997	Westvaco
Kenji Kiyohara	1997	Osaka National Research Institute
Ravi Radhakrishnan	2000	University of Pennsylvania
C. Heath Turner	2002	University of Alabama
Jorge Pikunic	2003	McKinsey Consulting Co., London, UK
Coray Colina	2004	Penn State University
Francisco Hung	2005	Louisiana State University

Supriyo Bhattacharya	2006	City of Hope Med. Ctr., CA
Naresh Chennamsetty	2006	Bristol-Myers Squibb, NJ
Erik Santiso	2007	North Carolina State University
Surendra Kumar Jain	2007	Indian Institute of Science, Bangalore
Joshua D. Moore	2010	Army Research Laboratory
Jeremy Palmer	2011	University of Houston
Liangliang Huang	2012	University of Oklahoma
Yun Long	2012	National University of Singapore
Katherine Phillips	2014	EPA Laboratory, Durham, NC
Cody Addington		NCSU
Deepti Srivistava		NCSU
James M. Mansell		NCSU
Kaihang ('Kevin') Shi		NCSU

(46) (22 academia)

Postdoctoral Associates:

		From	Present location
1969-70	Min Kwan Tham	Univ. Florida	U.S. Bur. of Mines
1970-71	Anthony Barker	?	Australian CSIRO
1972-74	Kingtse C. Mo	Univ. Maryland	NMC/NOAA
1976-77	Denis J. Evans	Australian Natl. U.	Austr. Nat. Univ.
1977-80	Steve M. Thompson	Oxford Univ.	Cornell University
1978-80	Paulette Clancy	Oxford Univ.	Cornell University
1978	Dominic J. Tildesley	Oxford Univ.	Unilever Research
1978-79	J. Lyklema	T. U. Delft	Unknown
1979-80	Ulrich Dieters	Ruhr Univ., Bochum	Univ Cologne
1979-81	Joe J. Salacuse	SUNY (Stony Brook)	General Motors
1980-82	Gary P. Morriss	Univ. of Melbourne	Univ. New South Wales
1981-82	Peter A. Monson	Univ. of London	Univ. of Mass.
1982-84	Eduardo Enciso	Complutense U., Madrid	Complutense Univ., Madrid
1982-85	Margarida Telo da Gama	Univ. of Bristol	Univ. de Lisboa
1983-84	Nick Quirke	BP Research	Imperial College, London
1984-85	Jeremy P.R.B. Walton	Univ. of Oxford	BP Research
1986-88	Frank van Swol	Univ. of Amsterdam	Un. New Mex., Sandia Labs.
1987-88	George Jackson	Oxford Univ.	Imperial College, London
1988	Umberto Marini Bettolo Marconi	Univ. Rome	Univ. Rome
1989-90	Mitsuhiro Matsumoto	Kyoto Univ.	Kyoto University
1989-91	John Walsh	John Hopkins Univ.	Shell Research, Houston
1990-92	Roger Cracknell	Imperial College	Shell Res., Thornton, UK
1991-92	Anne-Marie Williamson	Sheffield Univ.	ICI, Runcorn, U.K.

1991-93	Carolyn Koh	Brunel Univ.	Colorado School of Mines
1991-92	Hideki Tanaka	Kyoto Univ.	Okayama Univ.
1991-93	Dima Ulberg	Inst. Th. Phys., Kiev	Emory University
1992-95	Lourdes Vega	Univ. Seville	Univ. Barcelona, Spain
1992-94	Taka Suzuki	Chiba University	Chiba University
1992-94	Osamu Kitao	Kyoto University	Inst. Chem. Matls., Tsukuba
1993-95	Thomas Kraska	Ruhr Univ., Bochum	Univ. Cologne
1993- 96	Michael Maddox	Oxford University	HS Teacher, Davis, CA
1995-96	Minoru Miyahara	Kyoto University	Kyoto University
1996-99	Lev D. Gelb	Cambridge University	University of Texas, Dallas
1997-99	Karl P. Travis	Austalian National Univ.	Sheffield University
1997-99	Simon C. McGrother	University of Sheffield	Acelarys, San Diego, CA
1999-2000	Kendal Thomson	University of Minnesota	Purdue University
1999-2001	John Brennan	Wayne State University	Army Research Lab
2000-02	Flor Siperstein	University of Pennsylvania	Univ. of Manchester, UK
2000-01	Martin Lisal	Czech Academy of Science	Czech Academy of Science
2001-03	Lauriane Fillous Scanu	Univ. Montpellier II	Kraft Co., Chicago
2002-05	Henry Bock	Technical Univ. Berlin	Heriot-Watt University
2002-03	Alberto Striolo	Padua Univ. & UC Berkeley	University College London
2003-05	Benoit Coasne	Univ. Paris VI	Univ. Montpellier II
2004-06	Milen Kostov	Pennsylvania State Univ.	Florida State Univ.
2005-07	Tim Morrow	Notre Dame University	Louisiana Tech. University
2006-08	Liping Huang	Univ. Michigan	Rensselaer Polytechnic Univ
2007-08	Thomas Roussel	Univ. Marseille	Univ. of Barcelona
2007-09	Ying-Chun ('Lucy') Liu	Zhejiang University	Zhejiang University
2012-14	Liangliang ('Paul') Huang	Nanjing Univ. Tech.	University of Oklahoma
2013-	Rong ('Ruby') An	Nanjing Univ. Tech.	Nanjing Univ. Sci. & Tech.
2014-15	Katherine Phillips	University of Alabama	US EPA, Res. Triangle Park

(51) (34 academia)

Visiting Professors and Scholars (1978-):

- 1978/79:** Prof. J. M. Haile (Clemson Univ.)
 Prof. K. Lucas (Univ. of Duisburg, W. Germany)
 Prof. J. Dufty (Univ. of Florida)
 Prof. C. G. Gray (Univ. of Guelph, Ontario)
 Prof. J. G. Powles (Univ. of Kent, U.K.)
- 1979/80:** Dr. U. Dieters (Univ. of Bochum, W. Germany)
- 1980/81:** Prof. K. Lucas (Univ. of Duisburg, W. Germany)
 Prof. S. Murad (Univ. of Illinois)
 Prof. J. C. G. Calado (Univ. of Lisbon)
 Prof. J. Zollweg (Univ. of Maine)

Prof. D. A. Jonah (Univ. of Sierra Leone)
 Prof. F. del Rio (Metropolitana University, Mexico)
 Dr. M. Rigby (Univ. of London)

1981/82: Prof. J. G. Powles (Univ. of Kent, U.K.)
 Prof. J. S. Rowlinson (Oxford Univ., U.K.)
 Dr. N. Quirke (Univ. of London, U.K.)
 Dr. R. Evans (Univ. of Bristol, U.K.)
 Dr. T. Krolkowski-Buck (Union Carbide, Charleston)
 Prof. J. C. G. Calado (Univ. of Lisbon)

1982/83: Prof. J. M. Haile (Clemson Univ.)
 Dr. E. Enciso (Univ. of Madrid)
 Dr. W-C. Kok (National Univ. of Singapore)
 Prof. J. G. Powles (Univ. of Kent, U.K.)
 Dr. R. Basu (Allied Chemical)
 Prof. J. C. G. Calado (Univ. of Lisbon)
 Prof. K. Lucas (Univ. Duisburg, W. Germany)

1983/84: Prof. K. R. Jolls (Iowa State Univ.)
 Dr. E. Enciso (Univ. of Madrid)

1984/85: Dr. Margarida Telo da Gama (Bristol University, U.K.)
 Dr. Nicholas Quirke (BP Research, U.K.)

1985/86: Dr. Asok Sen (Ohio State University)
 Prof. D. Sullivan (University of Guelph)
 Dr. F. van Swol (Oxford University)
 Prof. Ziming Tan (East China Institute of Chem. Tech.)
 Dr. George Jackson (Oxford University, U.K.)

1986/87 Dr. F. van Swol (Oxford University)
 Dr. G. Jackson (Oxford University)

1987/88 Prof. J.S. Rowlinson (Oxford University), M.B. Upson Visiting Prof.
 Dr. G. Jackson (Oxford University)
 Dr. F. van Swol (Oxford University)

1988/89 Prof. L. Rull (Universidad de Sevilla, Sevilla, Spain)
 Dr. Margarida Telo da Gama (Lisbon University, Portugal)
 Prof. Javier Nuñez Delgado (Universidad Complutense, Madrid, Spain)
 Dr. F. van Swol (Oxford University)
 Dr. G. Jackson (Oxford University)

1989/1990 Dr. L. Pozhar (Inst. Low Temp. Phys. & Engng, Ukr Acad. Sci., Kharkov, USSR)

Prof. E.U. Franck (Univ. Karlsruhe, FRG), M.B. Upson Visiting Prof.
Dr. N. Quirke (BP Research, Sunbury-on Thames, U.K.)

- 1990/1991** Prof. Perla Balbuena (Univ. Littoral, Argentina)
Dr. L.A. Pozhar (Institute of Low Temperature Physics & Engineering, Academy of Sciences Ukr, Kharkov, USSR).
- 1991/1992** Prof. Perla Balbuena (Univ. Littoral, Argentina)
Dr. L.A. Pozhar (Institute of Low Temperature Physics & Engineering, Academy of Sciences Ukr, Kahrkov, USSR).
- 1992/93** Dr. L.A. Pozhar (Institute of Low Temperature Physics & Engineering, Academy of Sciences Ukr, Kahrkov, USSR).
Dr. E. Akhmatskaya (Institute of Low Temperature Physics & Engineering, Academy of Sciences Ukr, Kahrkov, Ukraine).
Dr. T. Suzuki (Chemistry Dept., Chiba University, Japan).
Dr. O. Kitao (Industrial Chemistry Dept., Kyoto Univ., Japan).
- 1993/94** Dr. E. Akhmatskaya (Institute of Low Temperature Physics & Engineering, Academy of Sciences Ukr., Ukraine)
Dr. T. Suzuki (Chemistry Dept., Chiba Univ., Japan)
Dr. O. Kitao (Industrial Chem. Dept., Kyoto Univ., Japan)
- 1994/95** Dr. E. Akhmatskaya (Institute of Low Temperature Physics & Engineering, Academy of Sciences Ukr., Ukraine)
Mr. I. Wold, Trondheim University, Norway
- 1995/96** Dr. Minoru Miyahara (Kyoto University, Chemical Engineering Dept.)
Dr. David Nicholson (Imperial College of Science & Technology, London)
Professor J.S. Rowlinson (Oxford University)
Dr. C.A. Koh (King's College London)
Professor Jan Stecki (Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw)
Dr. Liudmila Pozhar, Institute for Low Temperature Physics and Engineering, Kharkov, Ukraine
- 1996/97** Professor Jan Stecki (Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw)
Dr. Liudmila Pozhar, Institute for Low Temperature Physics and Engineering, Kharkov, Ukraine
Professor Antonio Estévez, University of Puerto Rico, Chemical Engineering Dept.
Dr. Nigel Seaton, Chemical Engineering Dept., Cambridge Univ., U.K.
- 1998/99** Professor M. Sliwinska-Bartkowiak, University of Poznan, Poland

Professor E. A. Müller, Simon Bolivar University, Venezuela

- 1999/2000** Dr. Mark Biggs, University of Surrey, U.K.
 Professor Erich Müller, Simon Bolivar University, Venezuela
 Professor Gerhard Schneider, Ruhr University, Germany
 Professor N. Quirke, Imperial College London, U.K.
 Dr. Jorge Hernandez, Mexico
 Professor M. Sliwinska-Bartkowiak, Adam Mickiewicz Univ., Poznan, Poland
 Dr. Liudmila Pozhar, University of Surrey, U.K.
 Professor T. Hilczer, Adam Mickiewicz University, Poznan, Poland
 Professor S. Jurga, Adam Mickiewicz University, Poznan, Poland
- 2000/2001** Dr. Philip Llewellyn, CNRS Marseille, France
 Prof. Erich Müller, Simon Bolivar University, Venezuela
 Prof. Lourdes Vega, University of Rovira i Virgili, Tarragona, Spain
 Professor M. Sliwinska-Bartkowiak, Adam Mickiewicz Univ., Poznan, Poland
 Professor N. Quirke, Imperial College London, U.K.
 Professor G. Schneider, Ruhr University, Bochum, Germany.
 Dr. Lauriane Fillous, Universidad de los Andes, Merida, Venezuela
- 2002/2003** Prof. Gerhard Findenegg, Technical University, Berlin, Germany
 Prof. Malgorzata Sliwinska-Bartkowiak, Adam Mickiewicz Univ., Poznan, Poland
 Prof. Alain Fuchs, Université Paris-Sud, Orsay, France
 Prof. Martin Schoen, Technical University, Berlin, Germany
 Dr. Roland Pellenq, CNRS, Orléans, France
 Dr. Ganapathy Ayappa, Indian Institute of Science, Bangalore, India
 Dr. Jorge Hernandez, U.N.A.M. Cuernavaca, Mexico
 Professor Santiago Lago, Universidad Pablo de Olavide, Seville, Spain
- 2003/2004** Professor Martin Schoen, Technical University of Berlin, September 13-22
 Professor Reinhard Schomäcker, Technical University of Berlin, September 13-18
 Dr. Sabine Klapp, Technical University of Berlin, September 13-19
 Professor Peter T. Cummings, Vanderbilt University & ORNL, October 5-8
 Professor Ruth Lynden-Bell, Princeton University and Cambridge University, U.K.,
 November 23-25, 2003.
 Professor Margaret Sliwinska-Bartkowiak, Adam Mickiewicz University, Poznan,
 Poland, November 22 – December 2, 2003.
 Professor Christiane Alba-Simionesco, Laboratoire Chimie Physique, Université
 Paris-Sud, France, December 4-6, 2003.
 Professor Carolyn A. Koh, Colorado School of Mines, May 3-7, 2004.
 Dr. Roland Pellenq, CNRS Marseille, France, May 28-June 3, 2004.
 Professor Claudio Olivera-Fuente, Simon Bolivar University, Caracas, Venezuela,
 May 29 to June 4, 2004.
- 2004/2005** Professor Martin Schoen, Technical University of Berlin, August 23-20 November,
 2004
 Dr. Sabine Klapp, Technical University of Berlin, October 5-14

Dr. Tomonori Ohba, Chiba University, Japan, September-October, 2004
 Mr. Than Nguyen, University of Queensland, Brisbane, Australia
 Mr. Blazej Ratajczak, Institute of Physics, Adam Mickiewicz University, Poznan, Poland, October 18-December 17, 2004
 Ms. Joanna Czwartos, Institute of Physics, Adam Mickiewicz University, Poznan, Poland, October 18-December 17, 2004
 Professor Nick Quirke, Chemistry Department, Imperial College London, November 3-7, 2004.
 Professor Malgorzata Sliwinska-Bartkowiak, Institute of Physics, Adam Mickiewicz University, Poznan, Poland, October 18-December 17, 2004
 Dr. Jorge Pikunic, Department of Biochemistry, Oxford University, U.K., March 10-21, 2005.
 Dr. Jorge Hernandez, U.N.A.M. Cuernavaca, Mexico, March 10-19, 2005.
 Ms. Anna Andrzejewska, Department of Theoretical Chemistry, Marie Curie-Sklodowska University, Lublin, Poland, March 22-April 5, 2005.
 Dr. Jorge Hernandez, U.N.A.M. Cuernavaca, Mexico, April 19-23, 2005.
2005/2006 Professor Perla Balbuena, Chemical Engineering Department, Texas A&M University, August 25-26, 2005
 Professor Sharon Glotzer, Chemical Engineering Department, University of Michigan, September 20-21, 2005
 Mr. Mark Horsch, Chemical Engineering Department, University of Michigan, September 20-21, 2005
 Ms. Chetana Singh, Chemical Engineering Department, University of Michigan, September 20-21, 2005
 Professor Gerhard H. Findenegg, Stranski Institute of Physical Chemistry, Technical University of Berlin, Germany, November 3-29, 2005
 Professor Malgorzata Sliwinska-Bartkowiak, Professor of Physics and Head, Dielectric Physics Program, Adam Mickiewicz University, Poznan, Poland, November 4-19, 2005.
 Professor Martin Schoen, Stranski Institute of Physical Chemistry, Technical University of Berlin, Germany, November 22-28, 2005.
 Dr. Henry Bock, School of Engineering and Physical Sciences, Heriot-Watt University, Edinburgh, Scotland, November 29-December 11, 2005.
 Dr. Liping Huang, Department of Materials Science & Engineering, University of Michigan, February 12-14, 2006.
 Dr. Yunfeng Shi, Department of Materials Science & Engineering, University of Michigan, February 12-14, 2006.
 Professor Garegin Papoian, Chemistry Department, University of North Carolina at Chapel Hill, March 29, 2006.
 Professor Hans Fraaije, University of Leiden, Netherlands, April 1 – 9, 2006.
 Professor Branislav Vlahovic, Physics Department, North Carolina Central University, Durham, NC, April 5, 2006.
 Professor Stefano Curtarolo, Department of Mechanical Engineering and Materials Science, Duke University, April 19, 2006.

- Professor Katsumi Kaneko, Department of Chemistry, Chiba University, Japan, June 18-20, 2006.
- 2006/2007** Professor K.Y. Chan, Department of Chemistry, Hong Kong University, Hong Kong, August 10-15, 2006.
- *Professor Teresa J. Bandosz, Department of Chemistry, City College of New York, October 9-November 7, 2006.
- *Professor Gerhard H. Findenegg, Stranski Institute of Physical Chemistry, Technical University of Berlin, Berlin, Germany, October 19-November 11, 2006.
- Dr. Gernot Rother, Center for Neutron Scattering, Oak Ridge National Laboratory, October 24-26, 2006.
- *Professor Malgorzata Sliwinska-Bartkowiak, Professor of Physics and Head, Dielectric Physics Program, Adam Mickiewicz University, Poznan, Poland, November 5-December 2, 2006.
- Professor Xiaohua Lu, Department of Chemical Engineering, Nanjing University of Technology, Nanjing, China, November 20-26, 2006.
- Professor Xin Feng, Department of Chemical Engineering, Nanjing University of Technology, Nanjing, China, November 20-26, 2006.
- Professor Stefano Curtarolo, Department of Mechanical Engineering & Materials Science, Duke University, Durham, NC, December 4, 2006.
- Professor Frerich Keil, Chemical Reaction Engineering and Process Optimization Department, Technical University of Hamburg-Harburg, Hamburg, Germany, March 10-14, 2007.
- Dr. Matthias Thommes, Director of Research, Quantachrome Inc., Boynton Beach, FL, April 15-17, 2007.
- 2007/2008** Mr. Qu Chen, Zhejiang University, China, July 13 – August 20, 2007.
- Professor Simcha Srebnik, Chemical Engineering Department, Technion – Israel Institute of Technology, Haifa, Israel.
- Professor Xiaohua Lu, Department of Chemical Engineering, Nanjing University of Technology, Nanjing, China, October 4-10, 2007.
- Professor Xin Feng, Department of Chemical Engineering, Nanjing University of Technology, Nanjing, China, October 4-10, 2007.
- Professor Gerhard H. Findenegg, Stranski Institute of Physical Chemistry, Technical University of Berlin, Berlin, Germany, November 9-16, 2007.
- Professor Malgorzata Sliwinska-Bartkowiak, Professor of Physics and Head, Dielectric Physics Program, Adam Mickiewicz University, Poznan, Poland, November 10-25, 2007.
- Professor Martin Schoen, Stranski Institute of Physical Chemistry, Technical University of Berlin, Germany, November 9-15, 2007.
- Professor Jehane Ragai, Chemistry Department, American University in Cairo, Cairo, Egypt, April 6-11, 2008.
- Professor Martin Schoen, Stranski Institute of Physical Chemistry, Technical University of Berlin, Germany, April 3-14, 2008.

Dr. Erik Santiso, Department of Chemical Engineering, M.I.T., Cambridge, MA, April 11-20, 2008.

- 2008/2009** Professor K.Y. Chan, Department of Chemistry, Hong Kong University, Hong Kong, July 10-18, 2008.
- Professor Phillip Westmoreland, Department of Chemical Engineering, University of Massachusetts, Amherst, MA
- Professor Malgorzata Sliwinska-Bartkowiak, Professor of Physics and Head, Dielectric Physics Program, Adam Mickiewicz University, Poznan, Poland, November 10-25, 2007.
- Dr. Benoit Coasne, Laboratoire de Physicochimie de la Matiere Condensee, CNRS & Université de Montpellier II, Montpellier, France, December 3-7, 2008.
- Professor Martin Schoen, Department of Chemistry, Technical University of Berlin, March 2-April 9, 2009.
- Dr. Marco Mozza, Department of Physics, Boston University, March 18, 2009.
- Dr. Erik Santiso, Department of Chemical Engineering, M.I.T., March 28-April 5, 2009.
- Participants in US-Berlin Workshop, April 6-8, 2009:
- Professor Peter K. Kilpatrick, Department of Chemical Engineering, Notre Dame University, April 6-8, 2009.
- Professor Max Berkowitz, Department of Chemistry, University of North Carolina at Chapel Hill, April 6-8, 2009.
- Professor Nancy L. Thompson, Department of Chemistry, University of North Carolina at Chapel Hill, April 6-8, 2009.
- Professor Dennis Discher, Department of Chemical and Biomolecular Engineering, University of Pennsylvania, April 6-8, 2009.
- Professor Martin Schoen, Stranski Institute of Physical Chemistry, Technical University of Berlin, Berlin, Germany, November 11-25, 2010.
- Dr. Daniela Fliegner, Stranski Institute for Physical Chemistry, Technical University of Berlin, April 6-8, 2009.
- Professor Michael Gradzielski, Stranski Institute for Physical Chemistry, Technical University of Berlin, April 6-8, 2009.
- Professor Sabine Klapp, Stranski Institute for Physical Chemistry, Technical University of Berlin, April 6-8, 2009.
- Dr. Holger Stark, Stranski Institute for Physical Chemistry, Technical University of Berlin, April 6-8, 2009.
- Professor Regine von Klitzing, Stranski Institute for Physical Chemistry, Technical University of Berlin, April 6-8, 2009.
- Professor Jurgen Rabe, Department of Physics, Humboldt University, Berlin, April 6-8, 2009.
- Dr. Volker Knecht, Max Planck Institute for Colloid and Interface Science, Golm, Potsdam, April 6-8, 2009.
- Dr. Hans Riegler, Max Planck Institute for Colloid and Interface Science, Golm, Potsdam, April 6-8, 2009.

Dr. Thomas Weigl, Max Planck Institute for Colloid and Interface Science, Golm, Potsdam, April 6-8, 2009.

Professor Kwong-Yu Chan, Department of Chemistry, Hong Kong University, Hong Kong, June 4-8, 2009.

- 2009/2010** Dr. Luis Ricardez-Sandoval, Department of Chemical Engineering, University of Waterloo, Ontario, Canada, August 17-19, 2009.
 Professor Xiaohua Lu, Department of Chemical Engineering, Nanjing University of Technology, Nanjing, China, November 15-18, 2009.
 Professor Xin Feng, Department of Chemical Engineering, Nanjing University of Technology, Nanjing, China, November 15-18, 2009.
 Professor Martin Schoen, Stranski Institute of Physical Chemistry, Technical University of Berlin, Berlin, Germany, November 14-25, 2009.
 Professor Malgorzata Sliwinska-Bartkowiak, Professor of Physics and Head, Dielectric Physics Program, Adam Mickiewicz University, Poznan, Poland, November 12-26, 2009.
 Professor Slawomir Bartkowiak, Institute of Plant Genetics, Polish Academy of Sciences, Poznan, Poland, November 12-26, 2009.
 Dr. Roland Pellenq, University of Marseille and M.I.T., April 11-13, 2010.
 Professor Luis Ricardez, Department of Chemical Engineering, University of Waterloo, Canada, April 26-28, 2010.
- 2010-2011** Dr. Luis Ricardez-Sandoval, Department of Chemical Engineering, University of Waterloo, Ontario, Canada, July 1-31, 2010.
 Professor Katsumi Kaneko, Shinshu University, Japan, July 8-10, 2010.
 Dr. Erik Santiso, M.I.T., August 3-10, 2010
 Mr. Gerald Rosenthal, Technical University of Berlin, Germany, October-December, 2010
 Mr. Philipp Kahlitz, Technical University of Berlin, Germany, November, 2010 – April, 2011
 Professor Lourdes Vega, Universidad Autónoma de Barcelona and Director, MATGAS Institute, Barcelona, November 12 – 16, 2010
 Professor Malgorzata Sliwinska-Bartkowiak, Professor of Physics and Head, Dielectric Physics Program, Adam Mickiewicz University, Poznan, Poland, November 11-26, 2010.
 Professor Martin Schoen, Stranski Institute of Physical Chemistry, Technical University of Berlin, Berlin, Germany, November 11-25, 2010.
 Professor Sabine Klapp, Technical University of Berlin, Berlin, Germany, January 2011.
 Professor Luis Ricardez Sandoval, University of Waterloo, March 21-25, 2011
 Professor K.-Y. Chan, University of Hong Kong, April 19-22, 2011
- 2011-2012** Professor Ying-Chun ('Lucy') Liu, Zhejiang University, Hangzhou, China, August 7-20, 2011

Mr. Manuel Greschek, Technical University of Berlin, September 20-December 19, 2011

Professor Sabine Klapp, Stranski Institute for Physical Chemistry, Technical University of Berlin, October, 2011.

Professor Martin Schoen, Stranski Institute of Physical Chemistry, Technical University of Berlin, Berlin, Germany, October-November, 2011.

Professor Gerhard Findenegg, Stranski Institute of Physical Chemistry, Technical University of Berlin, Berlin, Germany, October, 2011.

Professor Jurgen Rabe, Department of Physics, Humboldt University, Berlin, October 2011.

Dr. Holger Stark, Stranski Institute for Physical Chemistry, Technical University of Berlin, October, 2011.

Professor Regine von Klitzing, Stranski Institute for Physical Chemistry, Technical University of Berlin, October, 2011.

Professor Xiaohua Lu, Nanjing University of Technology, October 21-28, 2011

Professor Xin Feng, Nanjing University of Technology, October 21-28, 2011

Professor Malgorzata Sliwinska-Bartkowiak, Adam Mickiewicz University, Poznan, Poland, October 20-November 30, 2013

Dr. Erik Santiso, Imperial College London, February 11-March 4, 2012.

Dr. Luzheng Zhang, University of Illinois at Urbana-Champaign, February 21-24, 2012.

Professor M.S. Ananth, Indian Institute of Science, Bangalore, India, April 11, 2012.

2012-2013

Dr Ruby Zhang, Babcock & Wilcox Company, July 29 to August 1, 2012

Professor Martin Schoen, Technical University of Berlin, October 30-November 9, 2012

Professor Malgorzata Sliwinska-Bartkowiak, Adam Mickiewicz University, Poznan, Poland, October 31 to November 17, 2012

Professor Xiaohua Lu, Nanjing University of Technology, April 3-6, 2013

Professor Jun Li, Nanjing University of Technology, April 3-6, 2013

Professor Giovanni Ciccotti, University of Rome, La Sapienza, April 18-25, 2013

2013-2014

Professor Sabine Klapp, Technical University of Berlin, Berlin, Germany, September 26-October 4, 2013

Professor Martin Schoen, Technical University of Berlin, Berlin, Germany, September 26-October 10, 2013

Professor Gerhard Findenegg, Technical University of Berlin, Berlin, Germany, September 26-October 4, 2013

Professor Malgorzata Sliwinska-Bartkowiak, Adam Mickiewicz University, Poznan, Poland, November 9-23, 2013

Dr. Henry Bock, Heriot-Watt University, Edinburgh, Scotland, November 17-22, 2013

Professor Xiaohua Lu, Department of Chemical Engineering, Nanjing University of Technology, Nanjing, China, November 15-18, 2013.

Professor Xin Feng, Department of Chemical Engineering, Nanjing University of Technology, Nanjing, China, November 15-18, 2013.

Professor Malgorzata Sliwinska-Bartkowiak, Adam Mickiewicz University, Poznan, Poland, April 16-18, 2014.

Dr. Yun Long, National University of Singapore, May 25-30, 2014.

2014-2015

Dr. Daphne Klotsa, University of Michigan, July 16-18, 2014.

Professor Martin Schoen, Technical University of Berlin, September 30 – October 6, 2014.

Professor Gerhard Findenegg, Technical University of Berlin, November 8-16, 2014.

Professor Yudan Zhu, Nanjing Technical University, Nanjing, China, November 11-16, 2014.

Professor Fernando Luis Barroso da Silva, University of Sao Paulo, Ribeirao Preto, Sao Paulo, Brazil, March 22-24, 2015.

Professor Gerhard Findenegg, Technical University of Berlin, April 29 – May 1, 2015.

Professor Liangliang ('Paul') Huang, University of Oklahoma, Norman, OK, May 6-9, 2015.

Professor Katsumi Kaneko, Shinshu University, Nagano, Japan, May 7-9, 2015.

2015-2016

Professor Martin Schoen, Technical University of Berlin, October 1 – October 8, 2015.

Publications:

A. Books:

1. Reed, T.M. and Gubbins, K.E., "Applied Statistical Mechanics," McGraw-Hill (1973). (A graduate-level text.). Republished by Butterworth-Heinemann Reprint Series in Chemical Engineering, Butterworth-Heinemann, Boston (1991).
2. Gray, C.G. and Gubbins, K.E., "Theory of Molecular Fluids. I. Fundamentals," Oxford University Press, International Series of Monographs on Chemistry, 1984 (reprinted 2011).
3. Gubbins, K.E. and Quirke, N., editors, "Molecular Simulation and Industrial Applications: Methods, Applications and Prospects", Gordon & Breach, London, (1996).
4. Gray, C.G., Gubbins, K.E. and Joslin, C.G., "Theory of Molecular Fluids. II. Applications," Oxford University Press, International Series of Monographs on Chemistry (2011).
5. Gubbins, K.E. and Santiso, E., "Multi-Scale Modeling of Matter", in preparation.

B. Journal Articles:

1. Morris, D.R., Gubbins, K.E. and Watkins, S.B., "Solid Mixing Studies in Fluidized Beds," *Trans. of the Institution of Chemical Engineers* (London), **42**, 323 (1964).
2. Gubbins, K.E. and Walker, R.D., "The Solubility and Diffusivity of Oxygen in Fuel Cell Electrolytes", *Journal of the Electrochemical Society*, **111**, C178 (1964).
3. Gubbins, K.E. and Walker, R.D., "Solubility of Oxygen and Hydrocarbons in Phosphoric Acid", *Journal of the Electrochemical Society*, **112**, C175 (1965).
4. Gubbins, K.E., Carden, S.N. and Walker, R.D., "Determination of Gas Solubilities in Electrolyte Solutions," *Journal of Gas Chromatography*, **3**, 98 (1965).
5. Gubbins, K.E. and Walker, R.D., "The Solubility and Diffusivity of Oxygen in Electrolytic Solutions," *Journal of the Electrochemical Society*, **112**, 469 (1965).

6. Gubbins, K.E., Carden, S.N. and Walker, R.D., "Determination of Gas Solubilities in Liquids", *Journal of Gas Chromatography*, **3**, 330 (1965).
7. Gubbins, K.E., Bhatia, K.K. and Walker, R.D., "Diffusion of Gases in Electrolytic Solutions," *American Institute of Chemical Engineers Journal*, **12**, 548 (1966).
8. Tham, M.K., Gubbins, K.E. and Walker, R.D., "Densities of Potassium Hydroxide Solutions," *Journal of Chemical and Engineering Data*, **12**, 525 (1967).
9. Tham, M.J., Bhatia, K.K. and Gubbins, K.E., "Steady-State Method for Studying Diffusion of Gases in Liquids," *Chemical Engineering Science*, **22**, 309 (1967).
10. Gubbins, K.E., "Temperature Dependence of the Rigid-Sphere Diameter in the Enskog Equations," *Journal of Chemical Physics*, **48**, 1404-1405 (1968).
11. Bhatia, R.N., Gubbins, K.E. and Walker, R.D., "Mutual Diffusion in Concentrated Aqueous Potassium Hydroxide Solutions," *Transactions of the Faraday Society*, **64**, 2091 (1968).
12. Brunet, J. and Gubbins, K.E., "General Theory of the Long-Range Pair-Correlation Function," *Journal of Chemical Physics*, **49**, 5265 (1968).
13. Brunet, J. and Gubbins, K.E., "Viscosity of Binary Liquid Mixtures Near the Critical Mixing Point," *Transactions of the Faraday Society*, **65**, 1255 (1969).
14. Shoor, S.K., Walker, R.D. and Gubbins, K.E., "Salting Out of Nonpolar Gases in Aqueous Potassium Hydroxide Solutions," *Journal of Physical Chemistry*, **73**, 312 (1969).
15. Shoor, S.K. and Gubbins, K.E., "Solubility of Nonpolar Gases in Concentrated Electrolyte Solutions," *Journal of Physical Chemistry*, **73**, 498 (1969).
16. Gubbins, K.E. and Tham, M.J., "Free Volume Theory for Viscosity of Simple Nonpolar Liquids. Part I. Pure Components" *American Institute of Chemical Engineers Journal*, **15**, 264 (1969).
17. Gubbins, K.E. and Tham, M.J., "Free Volume Theory for Viscosity of Simple Nonpolar Liquids. Part II. Mixtures," *American Institute of Chemical Engineers Journal*, **15**, 269 (1969).
18. Tham, M.J. and Gubbins, K.E., "Free Volume Theory for Self-Diffusivity of Simple Nonpolar Liquids," *American Institute of Chemical Engineers Journal*, **15**, 306 (1969).
19. Tham, M.J. and Gubbins, K.E., "The Correspondence Principle for Transport Properties of Dense Fluids. I. Pure Monatomic Fluids," *Industrial Engineering Chemistry Fundamentals*, **8**, 791 (1969).
20. Tham, M.J. and Gubbins, K.E., "The Correspondence Principle for Transport Properties of Dense Fluids. II. Nonpolar Polyatomic Fluids," *Industrial Engineering Chemistry Fundamentals*, **9**, 63 (1970).

21. Tham, M.K., Walker, R.D. and Gubbins, K.E., "Diffusion of Oxygen and Hydrogen in Aqueous Potassium Hydroxide Solutions," *Journal of Physical Chemistry*, **74**, 1747 (1970).
22. Tham, M.K. and Gubbins, K.E., "Kinetic Theory of Multicomponent Dense Fluid Mixtures of Rigid Spheres," *Journal of Chemical Physics*, **55**, 268 (1971).
23. Eglestaff, P.A., Gray, C.G. and Gubbins, K.E., "Density Hierarchy for the Time-Dependent Correlation Functions," *Physics Letters*, **37A**, 321 (1971).
24. Gubbins, K.E., Smith, W.R., Tham, M.K. and Tiepel, E.W., "Perturbation Theory for the Radial Distribution Function," *Molecular Physics*, **22**, 1089 (1971).
25. Jalan, V.M., Tham, M.K. and Gubbins, K.E., "Theory of Diffusion of Gases in Protein Solutions," *Canadian Journal of Chemical Engineering*, **50**, 85 (1972).
26. Gubbins, K.E. and Gray, C.G., "Perturbation Theory for the Angular Pair Correlation Function in Molecular Fluids," *Molecular Physics*, **23**, 187 (1972).
27. Tham, M.K. and Gubbins, K.E., "Effect of Salts on the Diffusion of Dissolved Non-Electrolytes," *Journal of the Chemical Society, Faraday Transactions I*, **68**, 1339 (1972).
28. Tiepel, E.W. and Gubbins, K.E., "Theory of Gas Solubility in Mixed Solvent Systems," *Canadian Journal of Chemical Engineering*, **50**, 361 (1972).
29. Gubbins, K.E., "Thermal Transport Coefficients for Simple Dense Fluids," *Specialist Periodical Report on Statistical Mechanics*, Volume 1, Chapter 4, Chemical Society of London (1973).
30. Tiepel, E.W. and Gubbins, K.E., "Partial Molal Volumes of Gases Dissolved in Electrolyte Solutions," *Journal of Physical Chemistry*, **76**, 2044 (1972).
31. Tiepel, E.W. and Gubbins, K.E., "Thermodynamic Properties of Gases Dissolved in Electrolyte Solutions," *Industrial Engineering Chemistry Fundamentals*, **12**, 18 (1973).
32. Wang, S.S., Egelstaff, P.A. and Gubbins, K.E., "Monte Carlo Study of Perturbation Theory for the Radial Distribution Function," *Molecular Physics*, **25**, 461 (1973).
33. O'Connell, J.P., Gubbins, K.E. and Prausnitz, J.M., "Application of Molecular Concepts of Predicting Properties Needed for Design," *Chemical Engineering Education*, **7**, 203 (1973).
34. Gubbins, K.E., Gray, C.G., Egelstaff, P.A. and Ananth, M.S., "Angular Correlation Effects in Neutron Diffraction from Molecular Fluids," *Molecular Physics*, **25**, 1353 (1973).
35. Gubbins, K.E., "Perturbation Methods for Calculating Properties of Liquid Mixtures," *American Institute of Chemical Engineers Journal*, **19**, 684=698 (1973).

36. Wang, S.S., Gray, C.G., Egelstaff, P.A. and Gubbins, K.E., "Monte Carlo Study of the Pair Correlation Function for a Liquid with Non-Central Forces," *Chemical Physics Letters*, **21**, 123 (1973).
37. Wang, S.S., Egelstaff, P.A., Gray, C.G. and Gubbins, K.E., "Monte Carlo Study of the Angular Pair Correlation Function in a Liquid with Quadrupolar Forces," *Chemical Physics Letters*, **24**, 453 (1974).
38. Ananth, M.S., Gubbins, K.E., Gray, C.G., "Perturbation Theory for Equilibrium Properties of Molecular Fluids," *Molecular Physics*, **28**, 1005-30 (1974).
39. Mo, K.C., Gubbins, K.E., Jacucci, G. and McDonald, I.R., "The Radial Distribution Function in Fluid Mixtures: Conformal Solution Theory and Molecular Dynamics Results," *Molecular Physics*, **27**, 1173-83 (1974).
40. Twu, C.H., Gray, C.G. and Gubbins, K.E., "The Mean Squared Torque in Pure and Mixed Dense Fluids," *Molecular Physics*, **27**, 1601 (1974).
41. Mo, K.C. and Gubbins, K.E., "Molecular Principle of Corresponding States for Viscosity and Thermal Conductivity of Fluid Mixtures," *Chemical Engineering Communications*, **1**, 281 (1974).
42. Gray, C.G., Wang, S.S. and Gubbins, K.E., "Monte Carlo Calculations of the Mean Squared Force in Molecular Liquids," *Chemical Physics Letters*, **26**, 610 (1974).
43. Gubbins, K.E. and O'Connell, J.P., "Isothermal Compressibility and Partial Molal Volume for Polyatomic Liquids," *Journal of Chemical Physics*, **60**, 3449-53 (1974).
44. Mo, K.C. and Gubbins, K.E., "Perturbation Theory for Molecular Fluids Using a Nonspherical Reference Potential," *Chemical Physics Letters*, **27**, 144-48 (1974).
45. Egelstaff, P.A., Gray, C.G. and Gubbins, K.E., "Equilibrium Properties of Molecular Fluids," in "Molecular Structure and Properties," International Review of Science. *Physical Chemistry, Series 2*, Volume 2, ed. A. D. Buckingham, Butterworths, London (1975).
46. Twu, C.H., Gubbins, K.E. and Gray, C.G., "Excess Thermodynamic Properties for Liquid Mixtures of Non-Spherical Molecules," *Molecular Physics*, **29**, 713-29 (1975).
47. Mo, K.C. and Gubbins, K.E., "A New Perturbation Expansion for Fluids of Nonspherical Molecules," *Journal of Chemical Physics*, **63**, 1490-98 (1975).
48. Gray, C.G. and Gubbins, K.E., "Theory of Surface Tension for Molecular Liquids," *Molecular Physics*, **30**, 179-92 (1975).

49. Tiepel, E.W. and Gubbins, K.E., "Thermodynamic Properties of Gases Dissolved in Electrolyte Solutions," *Industrial Engineering Chemistry Fundamentals*, **14**, 143-44 (1975).
50. Gray, C.G. and Gubbins, K.E., "Calculation of the Dielectric and Kerr Constant angular Correlation Parameters," *Molecular Physics*, **30**, 1481-87, (1975).
51. Egelstaff, P.A., Gray, C.G., Gubbins, K.E. and Mo, K.C., "Theory of Inelastic Neutron Scattering from Molecular Fluids," *Journal of Statistical Physics*, **13**, 315-30 (1975).
52. Flytzani-Stephanopoulos, M., Gubbins, K.E. and Gray, C.G., "Thermodynamics of Mixtures of Non-Spherical Molecules. II. Strong Polar, Quadrupolar, and Overlap Forces," *Molecular Physics*, **30**, 1649-76 (1975).
53. Twu, C.H., Gubbins, K.E., and Gray, C.G., "Mean Squared Torque in Dense Fluids: Strong Polar and Quadrupolar Forces," *Molecular Physics*, **30**, 1607-10 (1975).
54. Mo, K.C. and Gubbins, K.E., "Conformal Solution Theory for Viscosity and Thermal Conductivity of Mixtures," *Molecular Physics*, **31**, 825-847 (1976).
55. Haile, J.M., Mo, K.C. and Gubbins, K.E., "Viscosity of Cryogenic Liquid Mixtures, Including LNG," *Advances in Cryogenic Engineering*, **21**, 501 (1976).
56. Groome, L.J., Gubbins, K.E. and Dufty, J.W., "Time-Dependent Triplet Correlation Functions and Pressure Derivative of the Dynamic Structure Factor," *Physical Review*, **A13**, 437 (1976).
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