

Keith E. Gubbins
Biographical Information

Title: W.H. Clark Distinguished University Professor
Address: Department of Chemical & Biomolecular Engineering, North Carolina State University, Box 7905, Raleigh, NC 27695-7905
Telephone: (919) 513 2262, Fax: (919) 515 3465
E-mail: keg@ncsu.edu Web: <http://gubbins.ncsu.edu>

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 (main events):

W.H. Clark Distinguished University Professor of Engineering, North Carolina State University, 1998-
Endowed Chair (T.R. Briggs Professorship) in Engineering, Cornell University, September 1976 -1997; Director, School of Chemical Engineering, July 1983-1990.
T.R. Briggs Professor Emeritus, Cornell University, 1998-present.
Postdoctoral Fellow, 1962-64; Assistant Professor, 1964-68; Associate Professor, 1968-72; Professor, 1972-76, University of Florida.
Co-Director, Center for High Performance Simulation, North Carolina State University, July 1, 2004-2017
Founding Director, Institute for Computational Science and Engineering, North Carolina State University, November, 2008-2012

Visiting Professorships: Imperial College, London 1971-1972; University of Guelph, Canada, July-December 1971; University of Kent, Canterbury, England, June-July 1975; University of Oxford, England, 1979-1980; also 1986-1987; University of California, Berkeley, April-August, 1982; University of Wisconsin, Madison, January-June 1993; Australian National University, Canberra, Aug. 1993-Jan. 1994; Imperial College, London, Jan. -Aug. 1994; Chiba University, Nov.-Dec. 1999; Université Paris-Sud, Orsay, June 2001-January 2002; Imperial College London, February-July 2002.
Royal Society Visiting Professor, University of Hong Kong, Hong Kong, June-July 2007.
Royal Academy of Engineering 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; Imperial College London, January-June 2011.

Recent Named Lectureships: McCabe Lecturer, North Carolina State University, 1986; Lindsay Lecturer, Texas A & M University, 1989; Dodge Lecturer, Yale University, 1989; Katz Lecturer, University of Michigan, 1991; Wohl Lecturer, University of Delaware, 1991; Merck Distinguished Lecturer, Rutgers Univ., 1992; Merck Lecturer, Univ. of Puerto Rico, 1995; Miles Lecturer, Univ. of Pittsburgh, 1995; Robb Lecturer, Pennsylvania State Univ., 1997; James Fair Lecturer, Univ. of Oklahoma, 1997; Frontier Science Lecture, Chiba Univ., Japan, November 1999; T.W. Leland Lecture, Rice Univ., March 2001;

Frontiers in Science Lecture, Chiba University, Japan, October 2006; Computational Physics and Numerical Methods Lecture, University of Hong Kong, June 2006. 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 Lecture, University of Manchester, September 4, 2013; Academic Poznań Public Lecture, City of Poznań, Poland, May 24, 2017.

Major Research Awards (1986-date):

Guggenheim Fellow 1986-87 (Oxford University, U.K.).
Senior Visiting Fellow (Science & Engineering Research Council Award), Oxford University, U.K., 1986-87.
American Institute of Chemical Engineers Awards: Alpha Chi Sigma Research Award, 1986; William H. Walker Award, 2000; Elected Fellow, 2003.
National Academy of Engineering, elected 1989.
Olaf Hougen Visiting Professor, University of Wisconsin, Madison, January-June 1993.
Fulbright Senior Scholar, Australian National University, Canberra, Aug. 1993-Jan. 1994.
Science and Engineering Research Council Visiting Fellow, Imperial College London, 1994.
Chercheur de Haute Niveau, French Ministry of Education, June 2001-February 2002.
Fellow, American Institute of Chemical Engineers, elected 2003.
Alumni Outstanding Research Award, North Carolina State University, 2004.
Joel Henry Hildebrand Award in the Theoretical and Experimental Study of Liquids, American Chemical Society, 2007.
Royal Society (London) Visiting Professor, University of Hong Kong, 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.
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.
Rossini Lecture 2012 Award, International Association for Chemical Thermodynamics, IUPAC, 2010
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")
Royal Society (London) Visiting Scientist, Imperial College London, January-March 2011.
Honorary Director, International Cooperation Center, Nanjing University of Technology, Nanjing, China, October, 2013.
Lennard-Jones Prize and Lectureship, Royal Society of Chemistry, London, 2013. Presented at the Thermodynamics 2013 conference, Manchester, U.K., September 4, 2013

Honorary Professor, Chinese Academy of Sciences, Institute of Process Engineering, Beijing,
2017-

Teaching Awards

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

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.

Editorships, Editorial Boards

Delegate to the Press, Oxford University Press, 1991-2008

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

Founding Editor of book series, *Topics in Chemical Engineering*, Oxford University Press, 1991-2008

Editorial Board, Journal of Chemical Physics, 1996-99

Editorial Board, Adsorption, 1994-2013

Guest Editor, Special Issue of *Engineering* on the topic of *Green Industrial Processes*, published by Chinese Academy of Engineering (to appear 2018).

Research Interests

Application of statistical mechanics, atomistic simulation, and *ab initio* methods to problems of interest in physical chemistry and chemical engineering, particularly in the areas of surface phenomena, phase equilibria, microporous materials, chemical reactivity in nano-structured materials, self-assembled nanostructures.

Recent Invited Lectures

“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.
- Academic Poznań Public Lecture, City of Poznań, Poland, May 24, 2017: “Molecular Modeling of Matter at the Nanoscale: Impact and Prospects”. Annual lecture by distinguished world scientist & engineers, organized by the Mayor of Poznań in conjunction with Adam Mickiewicz University.

Doctoral Students and Postdocs Advised

Ph.D.

	<u>Graduated</u>	<u>Present Location</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 Bangalore
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	Purdue Univ.
Mark Wojcik	1984	unknown
Der Jiun Lee	1985	National Taiwan Univ.
John Eggebrecht	1986	Iowa State University
Kwong-Yu Chan	1987	Hong Kong University (Chem.)
John H. Thurtell	1987	Mobil Research
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		Cornell University
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	Princeton University
Liangliang Huang	2012	University of Oklahoma
Yun Long	2012	National Univ. of Singapore
Katherine Phillips	2014	Environmental Protection Agency
Cody Addington	2017	Environmental Protection Agency
Deepti Srivastava		NCSU
Kaihang Shi		NCSU
James Mansell		NCSU

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. National Univ.
1977-80	Steve M. Thompson	Oxford Univ.	Cornell University
1978-80	Paulette Clancy	Oxford Univ.	Cornell University
1978-80	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 Massachusetts
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	Univ. New Mexico
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, U.K.
1991-92	Anne-Marie Williamson	Sheffield Univ.	ICI, Runcorn, UK
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. Materials, Tsukuba, Japan
1993-95	Thomas Kraska	Ruhr Univ., Bochum	Univ. Cologne
1993- 96	Michael Maddox	Oxford University	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	Australian National Univ.	Sheffield University
1997-99	Simon C. McGrother	University of Sheffield	Acelerys, 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, U.K.
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	M.I.T.
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 Poly. University

2007-08	Thomas Roussel	Univ. Marseille	Univ. of Barcelona
2007-09	Ying-Chun ('Lucy') Liu	Zhejiang University	Zhejiang University, China
2012-	Liangliang ('Paul') Huang	Nanjing Univ. Tech.	Univ. of Oklahoma
2013-15	Rong ('Ruby') An	Nanjing Univ. Tech.	Nanjing Univ. Sci. & Tech.