

# Henry Frederick Schaefer III

BORN

June 8, 1944 - Grand Rapids, Michigan

## *Educational Background*

Massachusetts Institute of Technology      September 1962 - June 1966      S.B. Chemical Physics

Stanford University      September 1966 - April 1969      Ph.D. Chemical Physics

National Defense Education Act Fellow 1966-1969.

## *Professional Experience*

Assistant Professor of Chemistry, University of California, Berkeley, 1969-1974.

Associate Professor of Chemistry, University of California, Berkeley, 1974-1978.

Professor of Chemistry, University of California, Berkeley, 1978-1987.

Faculty Senior Scientist, Lawrence Berkeley Laboratory, 1977-1987.

Wilfred T. Doherty Professor of Chemistry, University of Texas, Austin, 1979-1980.

Director, Institute for Theoretical Chemistry, University of Texas, Austin, 1979-1980.

Graham Perdue Professor of Chemistry, University of Georgia, 1987-present.

Director, Center for Computational Quantum Chemistry, University of Georgia, 1987-present.

Visiting Fellow, Research School of Chemistry, Australian National University, Canberra, 1975, 1977, 1980, 1982, 1985, 1989, 1991, 1993, 1995, 1997, 1999, 2003 and 2014.

Professeur d'Echange, Orsay Campus, University of Paris, 1977.

Visiting Professor, University of Buenos Aires, Argentina, 1994.

Gastprofessur, Eidgenössische Technische Hochschule (ETH), Swiss Federal Institute of Technology, Zurich, June/July, 1994; June/July 1995; June/July, 1997; June/July, 2000; June/July 2002; June/July 2004; June/July 2006; May-July 2008; June-July 2010.

Visiting Professor, Swiss Center for Scientific Computing, Lugano, Switzerland, July/August, 1998.

Visiting Professor, Ludwig – Maximilians University, 2012, 2013, 2014.

Advisory Committee, The Institute for Amorphous Studies, Bloomfield Hills, Michigan, 1983-1987.

Science Advisor, Quantum Chemistry College, Oxford Molecular Ltd., Oxford, England, 1994-1996.

Joint Review of the Institute of Advanced Studies, Australian National University, April 9-14, 1995.

Chairman, Subdivision of Theoretical Chemistry, Division of Physical Chemistry, American Chemical Society, 1982.

Executive Committee, Division of Physical Chemistry, American Chemical Society, 1984-1987.

Vice-Chairman, Division of Physical Chemistry, American Chemical Society, 1990.

Chairman Elect, Division of Physical Chemistry, American Chemical Society, 1991.

Chairman, Division of Physical Chemistry, American Chemical Society, 1992.

National Science Foundation Advisory Committee for Chemistry, 1989-1992.

President, World Association of Theoretical and Computational Chemists (WATOC), 1996-2005.

Professor of Chemistry, Emeritus, University of California, Berkeley, 2004-.

Chair, Northeast Georgia Section, American Chemical Society, 2011.

Chemist of the Year for Distinguished Service to the Section, Northeast Georgia Section, American Chemical Society, 2012.

### ***Editorial Responsibilities***

Editor, *Molecular Physics*, 1991-1994

Editor-in-Chief, *Molecular Physics*, 1995-2005.

Editorial Board, *Nouveau Journal de Chimie*, 1977-1989.

Editorial Board, *International Journal of Quantum Chemistry*, 1978-1986.

Associate Editor, *Journal of Chemical Physics*, 1979-1981.

Editorial Board, *Journal of Molecular Structure*, 1981-1988; 1994-2010.

Editorial Board, *Chemical Physics Letters*, 1979-present.

Associate Editor, *Theoretica Chimica Acta*, 1985-1996.

Editorial Board, *Advances in Quantum Chemistry*, 1987-present.

Editorial Board, *John Wiley & Sons Programme in Theoretical Chemistry*, 1994-1998.

Editor, *Encyclopedia of Computational Chemistry*, John Wiley & Sons, 1995-2006.

Editorial Board, *Theoretical Chemistry Accounts*, 1997- 2000.

Editorial Review Board, *American Institute of Chemists*, 2003 - .

Editorial Advisory Board, *Journal of Chemical Theory and Computation*, 2004 - present.

Associate Editor, Book Series in Theoretical and Computational Chemistry, World Scientific Publishing, 2004 - .

Advisory Board, *Molecular Physics*, 2005-.

Co-Editor, *Journal of Atomic and Molecular Sciences*, 2009-present.

Editorial Board, *Computational and Theoretical Chemistry*, 2011- present.

Editorial Board, *Organic Chemistry: Current Research*, 2012.

### ***Honors and Awards***

Alfred P. Sloan Research Fellow, 1972-74.

John Simon Guggenheim Fellow, 1976-77.

Fellow, American Physical Society 1976.

Fellow, Japan Society for the Promotion of Science, 1976.

American Chemical Society Award in Pure Chemistry, 1979.

Leo Hendrik Baekeland Award, American Chemical Society, 1983.

International Academy of Quantum Molecular Sciences, 1984.

Special Creativity Award, National Science Foundation, 1986-1988.

Fellow, American Institute of Chemists, 1988.

Schrödinger Medal, World Association of Theoretical and Computational Chemists, 1990.

Centenary Medal, Royal Society of Chemistry (London), 1992.

Lamar Dodd Award, University of Georgia, 1995.

The Gold Medal of the Comenius University, Bratislava, Slovakia, May, 2000.

Fellow, American Association for the Advancement of Science, 2002

American Chemical Society Award in Theoretical Chemistry, sponsored by the IBM Corporation, 2003.

Ira Remsen Award, American Chemical Society, 2003.

Fellow, American Academy of Arts and Sciences, April 2004.

Joseph O. Hirschfelder Prize for 2005 – 2006, University of Wisconsin, Madison, Wisconsin.

Fellow, Royal Society of Chemistry (London), 2005.

Biennial Grand Award for Research of Sofia University, Bulgaria, November 2008.

Fellow, American Chemical Society, Inaugural Class, 2009.

The Ide P. and Luella H. Trotter Prize and Endowed Lecture Series, College of Science, Texas A&M University, College Station, Texas, April 2011.

Alexander von Humboldt Foundation Award, 2012.

SURA Distinguished Scientist Award, March 29, 2012. Given to the outstanding scientist (all fields) in the 17 Southeastern states of the USA, from Missouri to Texas to Florida to Virginia.

American Institute of Chemists (AIC) Chemical Pioneer Award, April 5, 2013.

Fellow, International Union of Pure and Applied Chemistry, 2013.

American Chemical Society Peter Debye Award in Physical Chemistry, March 18, 2014

### ***Honorary Degrees***

1. Professor Honoris Causa, St. Petersburg State University, St. Petersburg, Russia. Honorary degree conferred September 24, 1996.
2. Professor Honoris Causa, Beijing Normal University, Beijing, China. Conferred September 21, 1999.
3. Doctor Honoris Causa, University of Plovdiv, Bulgaria. Conferred May 14, 1998.
4. Doctor Honoris Causa, University of Sofia, Bulgaria. Conferred May 12, 1999.
5. Doctor Honoris Causa, Beijing Institute of Technology, Beijing, China. Conferred September 22, 1999.
6. Professor Honoris Causa, Fudan University, Shanghai, China. Conferred November 13, 2001.
7. Professor Honoris Causa, Institutes of Biological Sciences, Chinese Academy of Sciences, Shanghai, China. Conferred November 16, 2001.
8. Doctor Honoris Causa, Huntington University, Indiana. Conferred May 18, 2002.
9. Professor Honoris Causa, Yunnan University, Kunming, China. Conferred October 10, 2002.
10. Professor Honoris Causa, Guangxi Normal University, Guilin, China. Conferred September 25, 2003.
11. Professor Honoris Causa, Chengdu University, Chengdu, China. Conferred September 29, 2003.
12. Professor Honoris Causa, Xinjiang University, Urumqi, China. Conferred September 8, 2004.
13. Professor Honoris Causa, Sichuan University, Chengdu, China. Conferred September 21, 2005.
14. Professor Honoris Causa, Lanzhou University, Lanzhou, China. Conferred September 26, 2006.
15. Doctor Honoris Causa, North-Eastern Hill University, Shillong, India. Conferred October 24, 2008.

16. Professor Honoris Causa, South China Normal University, Guangzhou (formerly Canton), China. Conferred November 5, 2007.
17. Professor Honoris Causa, Southern Yangtze University, Wuxi, China. Conferred November 9, 2007.
18. Doctor Honoris Causa, Babes-Bolyai University, Cluj-Napoca, Romania. Conferred May 12, 2009.
19. Professor Honoris Causa, Sichuan University of Science and Technology (XiHua University) Chengdu, China. Conferred December 2, 2009.
20. Professor Honoris Causa, Southwest Jiaotong University, Chengdu, China. Conferred December 3, 2009.
21. Professor Honoris Causa, Shaanxi Normal University, Xian, China. Conferred September 2010.
22. Professor Honoris Causa, Jinan University, Guangzhou, China. Conferred December 3, 2010.
23. Professor Honoris Causa, Shanghai University of Traditional Chinese Medicine, Shanghai, China. Conferred April 5, 2012.
24. Professor Honoris Causa, Changzhou University, Changzhou, China. Conferred April 5, 2012.
25. Professor Honoris Causa, East China Normal University, Shanghai, China. Conferred October 25, 2012.
26. Professor Honoris Causa, Minzu University, Beijing, China. Conferred April 15, 2013.
27. Professor Honoris Causa, Beijing University of Technology, Beijing, China, Conferred October 11, 2013.
28. Professor Honoris Causa, Sichuan Normal University, Chengdu, China. Conferred September 15, 2014.
29. Professor Honoris Causa, Soochow University, Suzhou, China, Conferred September 18, 2014.

### ***Named/Endowed Lectures***

1. Albert Einstein Centennial Lecturer, National University of Mexico, February 1979.

2. Lester P. Kuhn Lecturer, Johns Hopkins University, May 1982.
3. John Howard Appleton Lecturer, Brown University, April 1985.
4. The J. A. Erskine Lectures, University of Canterbury, Christchurch, New Zealand, February 1986.
5. Edward Curtis Franklin Lecturer, University of Kansas, April 1986.
6. John Lee Pratt Lecturer, University of Virginia, January 1988.
7. Louis Jacob Bircher Lecturer, Vanderbilt University, February 1988.
8. Harry Emmett Gunning Lectures, University of Alberta, May 1990.
9. Thomas F. Staley Lectures, Huntington College, Indiana, November 1990.
10. The Guelph-Waterloo Distinguished Lecturer for 1991, University of Guelph and University of Waterloo, Ontario, May 1991.
11. John M. Templeton Lecturer, Case Western Reserve University, April 1992.
12. Inaugural Lecture, A Celebration of the New Science Complex, Indiana University Purdue University at Indianapolis, March, 1993.
13. Herbert H. King Lecturer, Kansas State University, April, 1993.
14. The President's Lecture, University of Georgia, November, 1994.
15. Francis A. Schaeffer Lectures, Covenant Seminary, St. Louis, Missouri, March 1995; lectures delivered at Washington University, St. Louis.
16. Forty-Sixth Annual Convocation Lecture, Covenant College, Lookout Mountain, Georgia, August, 1995.
17. The Forester Lectures, Huntington College, Indiana, October, 1995 and September, 1999.
18. Thomas F. Staley Lectures, Union University, Jackson, Tennessee, November 1995.
19. Twentieth Mary E. Kapp Lecture, Virginia Commonwealth University, Richmond, Virginia, April, 1996.
20. Fifteenth Annual C. S. Lewis Lecture, University of Tennessee, Chattanooga, Tennessee, April, 1997.

21. The Bowen Liu Memorial Lecture, University of California, Lawrence Berkeley Laboratory, April, 1997.
22. The George A. Abbott Lectures, University of North Dakota, Grand Forks, North Dakota, April, 1997.
23. Richard M. Smoot Memorial Lecture, Atlanta Medical Society, October, 1997.
24. Joseph Frank Gregory Lecture, Colgate University, Hamilton, New York, October, 1997.
25. 1997 Distinguished Lecturer in Computational Chemistry, Indiana University, Bloomington, Indiana, December, 1997.
26. Kenneth S. Pitzer Lecture, University of California, Berkeley, October, 1998.
27. John M. Templeton Lecture, Montana State University, Bozeman, Montana, March, 1999.
28. The John Albert Southern Lecture, Furman University, Greenville, South Carolina, March, 1999.
29. Ninth Rudolf Brdicka Lecture, J. Heyrovsky Institute of Physical Chemistry, Prague, Czech Republic, June, 1999.
30. The David P. Craig Lectures, Australian National University, Canberra, Australia, December, 1999.
31. The Ede Kapuy Lecture, Eötvös Loránd University, Budapest, Hungary, May, 2000.
32. The Donald Frederick and Mildred Topp Othmer Lectures in Chemistry, Tokyo, Japan, September, 2000.
33. The Gary Boggess Distinguished Lecture in Chemistry, Murray State University, Murray, Kentucky, September, 2000.
34. The Fall 2000 Distinguished Visiting Professor in Chemistry, University of Florida, Gainesville, October 2000.
35. The Coochbehar Professorship Lecture, Indian Association for the Cultivation of Science, Calcutta, India, January, 2001.
36. The Distinguished Israel Pollak Lectures, Technion-Israel Institute of Technology, Haifa, Israel, March, 2001.



37. Lise Meitner Lecture, the Hebrew University, Jerusalem, Israel, March 2001.
38. The President's Lecture, University of Texas at Arlington, October 2001.
39. The Lawrence J. Schaad Lecture, Vanderbilt University, Nashville, Tennessee, September 2002.
40. Oakley R. Vail Lecture, Wake Forest University, Winston-Salem, North Carolina, October 2002.
41. The Annual Lecturer of the Croatian Chemical Society, Zagreb, Croatia, November 2002.
42. Fifth Distinguished Theory Lecturer, Chemische Gesellschaft Muelheim, Max Planck Institute, Muelheim, Germany, April 2003.
43. The 2003 - 2004 Brenzier and Wilhelmina Price Lectures, Wingate College, Wingate, North Carolina, October 2003.
44. John Marks Templeton Lecture, Princeton University, Princeton, New Jersey, February, 2004.
45. John Marks Templeton Lecture, Carnegie Mellon University, Pittsburgh, Pennsylvania, March 2004.
46. The Sigma Zeta Science Lectures, Asbury College, Wilmore, Kentucky, April 2004.
47. The Pew Foundation Lectures, Union University, Jackson, Tennessee, October 2004.
48. Metanexus Lecture, Valley Forge College, Pennsylvania, October 2004.
49. The 2004 New College Lectures, University of New South Wales, Sydney, Australia, October 2004.
50. Nanqiang Lecture, Amoy University, Xiamen, China, September 2005.
51. Metanexus Lecture, Southeastern University, Lakeland, Florida, February 2006.
52. Distinguished Lecture Series, Indian Institute of Technology Bombay, Mumbai, India, February 2006.
53. Goa Distinguished Lecture Series, Goa University, India, February 2006.
54. Paisii Hilendarski Lecture, University of Plovdiv, Plovdiv, Bulgaria, May 2006.
55. C. V. Raman Memorial Lecture, Indian Association for the Cultivation of Science, Kolkata (Calcutta), India, January 2007.

56. Per-Olov Löwdin Lectures, University of Uppsala, Sweden, October 2007.
57. Hartman Hotz Trust Lecture, University of Arkansas, Fayetteville, Arkansas, March 2008.
58. Kazuo Nakamoto Lecture, Marquette University, Milwaukee, Wisconsin, April 2008.
59. The Inaugural Steven Adelman Lectures in Theoretical Chemistry, Purdue University, West Lafayette, Indiana, September 2009.
60. Distinguished Science Lectures, Trinity University, San Antonio, Texas, October 2009.
61. Russell M. Pitzer Lecture, Ohio State University, Columbus, Ohio, November 2009.
62. Paul V. Beck Lectures, Southwestern College, Winfield, Kansas, April 2010.
63. College of Sciences Distinguished Lecturer, University of Central Florida, Orlando, Florida, January 2011.
64. Distinguished Lecture Series, *Frontiers in Chemical Research*, Texas A&M University, October 2011.
65. Sigma Zeta Lecture Series, Bethel University, St. Paul, Minnesota, March 2012.
66. William E. Palke Lectures, University of California, Santa Barbara, January 2013.
67. The Dalton Lecture Series, George Fox University, Newberg, Oregon, February 2013.
68. President's Distinguished Scholar Lecture, Palm Beach Atlantic University, West Palm Beach, Florida, October 2013.
69. The Gerald D. Smith Lecture Series, Huntingdon University, October 2013.
70. Science at the Edge Lecture Series, Michigan State University, East Lansing, Michigan, May 2013.
71. Jan Almlöf – Odd Gropen Lectures, University of Tromsø and University of Oslo, Norway, September 2013.
72. Annual Lecturer, Australian Association of Theoretical and Computational Chemists, Australian National University and University of Sydney, January 2014.

73. James William McBain Lecture, National Chemical Laboratory, Pune, India, February 2014

74. The Institute Lecture, Indian Institute of Technology Bombay, Mumbai, India, February 2014.

### ***Other Recognition***

Continuously included in Who's Who in America, Beginning 42nd Edition, 1982-1983.

Continuously included in Who's Who in the World, Beginning 7th Edition, 1984-1985.

One of the 100 Outstanding Young Scientists in America (Age 40 and under), *Science Digest*, December 1984.

One of the 1000 most highly cited scientists in the world for the period 1965-1978; *Current Contents*, October 12, 1981; *Chemical and Engineering News*, October 19, 1981. No. 62 among all chemists.

One of the 500 most highly cited scientists in the world for the period 1973-1984; *The Scientist*, August 20, 1990. No. 339 among all scientists, No. 19 among all chemists.

One of the 50 most highly cited chemists in the world for the period 1984-1991; *Science Watch*, May, 1992. Actual ranking was No. 3.

Sixth most highly cited chemist in the world for the period 1981-1997; Institute of Scientific Information, Philadelphia. Reported in *Chemistry*, Autumn, 2000, pages 31-33.

Honorary President, Institute for Chemical Physics (ICP), Beijing, China.

Director, Center for Computational Quantum Chemistry, South China Normal University, Guangzhou, China, 2007 - 2014.

Director, Center for Advanced Numerical Computation and Simulation, XiHua University, Chengdu, China, 2009 -

A six-day conference in honor of Dr. Schaefer was held in Gyeongju, Korea in February 2004. The title of the conference was "Theory and Applications of Computational Chemistry: A Celebration of 1000 Papers of Professor Henry F. Schaefer III". A total of 300 scientists attended from 35 countries.

At the 228<sup>th</sup> National Meeting of the American Chemical Society (Philadelphia, August 2004) the Division of Computers in Chemistry and the Division of Physical Chemistry cosponsored a four-day symposium in honor of Professor Schaefer.

The *Journal of Physical Chemistry* published a 431 page special issue in honor of Professor Schaefer on April 15, 2004.

The book *Theory and Applications of Computational Chemistry: The First Forty Years*, Editors C. E. Dykstra, G. Frenking, K. S. Kim, and G. E. Scuseria (1308 pages, Elsevier, 2005) was published in honor of Professor Schaefer.

Subject of feature article "Leading the Computational Chemistry Field", pages 9-11 of the September 2006 issue of *Scientific Computing World*.

The journal *Molecular Physics* published a 590 page special issue in honor of Professor Schaefer in June 2009.

In Professor Schaefer's honor, the University of California at Berkeley hosted the international conference "Molecular Quantum Mechanics: From Methylene to DNA and Beyond", May 23-29, 2010. Simultaneously, the conference published the book *Selected Papers of Henry Schaefer III*, Editors R. J. Bartlett, T. D. Crawford, M. Head-Gordon, and C. D. Sherrill (316 pages, Brandon, 2010).

The journal *Molecular Physics* published a 376 page special issue in honor of Professor Schaefer in October 2010.

In Professor Schaefer's honor, the Peking University Graduate School hosted an international conference May 4 -7, 2014 in Shenzhen, China.

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### ***Conference Organization***

1. Co-Chair, West Coast Theoretical Chemistry Conference, IBM San Jose, May 1979.
2. Chair, International Meeting on State Specific Photodissociation, Berkeley, California, November 11-13, 1981.
3. Chair, American Chemical Society Symposium on "Electron Correlation in Molecules", Las Vegas, Nevada, March 29-April 1, 1982.
4. Chair, Fifth American Conference on Theoretical Chemistry, Grand Teton National Park, Jackson, Wyoming, June 15-20, 1984.
5. Co-Chair, American Chemical Society "Nobel Laureate Symposium on Applied Quantum Chemistry", Pacific Basin Chemical Conference, Honolulu, Hawaii, December 16-21, 1984.

6. Chair, "International Conference on the Theory of the Structure of Non-Crystalline Solids", Institute for Amorphous Studies, Bloomfield Hills, Michigan, June 3-6, 1985.
7. Co-Chair, "Forty Years of Quantum Chemistry - An International Conference in Honor of Professor John A. Pople", Center for Computational Quantum Chemistry, University of Georgia, Athens, Georgia, October 16-19, 1989.
8. Co-Chair, "Molecular Quantum Mechanics: Methods and Applications - An International Conference in Memory of Samuel Francis Boys and in Honor of Isaiah Shavitt", Department of Theoretical Chemistry, University of Cambridge, Cambridge, England, September 3 - 7, 1995.
9. Co-Chair, "Computational Quantum Chemistry: A Viable Partner to Experiment in Chemical Research," International Chemical Congress of Pacific Basin Societies, Honolulu, Hawaii, December 17-22, 1995.
10. Co-Chair, "Structural and Mechanistic Organic Chemistry: A Tribute to Professor Norman L. Allinger", University of Georgia, Athens, Georgia, June 4-7, 1997.
11. Chair, "Electronic Structure Theory: From Methods to Molecules and Materials", American Physical Society 100th Annual Meeting, Atlanta, Georgia, March 21-26, 1999.
12. Co-Chair, "Computational Quantum Chemistry: Theoretical and Experimental Perspectives", International Chemical Congress of Pacific Basin Societies, Honolulu, Hawaii, December 14-19, 2000.
13. Co-Chair, "Molecular Quantum Mechanics: The Right Answer for the Right Reason. An International Conference in Honor of Professor Ernest R. Davidson", University of Washington, Seattle, Washington, July 21-26, 2001.
14. Co-Chair, "Molecular Quantum Mechanics: The No Nonsense Approach to Progress. An International Conference in Honor of Professor Nicholas C. Handy", St. John's College, Cambridge, England, July 24-29, 2004.
15. Co-Chair, "Computational Quantum Chemistry: Methodology and Applications", International Chemical Congress of Pacific Basin Societies, Honolulu, Hawaii, December 15 - 20, 2005.
16. Co-Chair, "Molecular Quantum Mechanics - Analytic Gradients and Beyond: An International Conference in Honor of Professor Peter Pulay", Margaret Island, Budapest, Hungary, May 29 - June 3, 2007.
17. Co-Chair, "Fourth Workshop on Computational Chemistry and its Applications (CCA)", Louisiana State University, Baton Rouge, Louisiana, May 25-29, 2009.

18. Co-Chair, "Fifth Workshop on Computational Chemistry and Its Applications", University of Amsterdam, The Netherlands, May 31 – June 2, 2010.
19. Co-Chair, "Computational Quantum Chemistry: Theory and Interactions with Experiment", International Chemical Congress of Pacific Basin Societies, Honolulu, Hawaii, December 15-20, 2010.
20. Co-Chair, "Sixth Workshop on Computational Chemistry and its Applications", University of Tsukuba, Japan, June 1-3, 2011.
21. Co-Chair, "Molecular Quantum Mechanics. Electron Correlation: The Many Body Problem at the Heart of Chemistry", Lugano, Switzerland, June 2-7, 2013.
22. Co-Chair, "Synergistic Relationships between Computational Chemistry and Experiment", International Chemical Congress of Pacific Basin Societies, Honolulu, Hawaii, December 15-20, 2015.
23. Co-Chair, "Eighth Molecular Quantum Mechanics: Celebration of the Swedish School", University of Uppsala, Sweden, June 26 – July 1, 2016.

### ***Research Support***

1. U.S. Department of Energy, "Molecular Electronic Structure Theory", 1969-1987. Note that the present U. S. Department of Energy incorporates research programs supported earlier by the U. S. Atomic Energy Commission (1969-1974) and the U. S. Energy Research and Development Administration (1975-1977).
2. American Chemical Society Petroleum Research Fund, "The Electronic Structure of Small Organic and Inorganic Molecules", 1969-1971.
3. Research Corporation Frederick Gardner Cottrell Grant, "Quantum Mechanical Calculations of the Electronic Structure of Atoms and Diatomic Molecules", 1970-1971.
4. National Science Foundation, "Electron Correlation in Molecules", 1972-1973.
5. National Science Foundation, "Large Scale Scientific Computation via Minicomputer", 1973.
6. National Science Foundation, "Theory of Simple Chemical Reactions", 1974-1979.
7. American Chemical Society Petroleum Research Fund, "Chemical Applications of a Theory of Self-Consistent Electron Pairs", 1976-1978.

8. North Atlantic Treaty Organization, "A Theory of Self-Consistent Electron Pairs: Development and Applications", 1977-1978.
9. American Chemical Society Petroleum Research Fund, "Effect of Electron Correlation on Potential Energy Surfaces. The Diels-Alder Reaction", 1978-1980.
10. U. S. - Australia Cooperative Science Program, "Theoretical Studies of Aromaticity", 1978-1980.
11. Robert A. Welch Foundation, "Studies in Theoretical Chemistry", 1979-1980.
12. National Science Foundation, "Electronic Theory of Simple Chemical Reactions", 1980-1995.
13. Fonds der Chemischen Industrie, Frankfurt, West Germany, "Theoretical Studies of Phosphonium Cyclopropylide", 1982.
14. Energy Conservation Devices, Inc., Troy, Michigan, "Theoretical Studies of Gas Phase Silicon Chemistry, 1983-1985
15. National Science Foundation, "Theoretical Chemistry via Minicomputer", 1984.
16. U. S. Army Research Office, "The Coupled Cluster Method and the Properties of Energetic Materials", 1986-1988.
17. American Chemical Society Petroleum Research Fund, "[n]Paracyclophanes: Important Examples of Strain and Aromaticity in Hydrocarbon Compounds", 1986-1987.
18. U. S. Air Force Office of Scientific Research, "Fundamental Studies of Carbon, NH, and Oxygen Rings and Other High Energy Density Molecular Systems", 1987-1994.
19. U. S. Department of Energy, "Potential Energy Surfaces for Chemical Reactions", 1987-1990.
20. U. S. Department of Energy, "Theoretical Studies of Hydrocarbon Combustion Chemistry", 1991-1994.
21. U. S. Air Force Office of Scientific Research, "Environmental Effects on High Energy Density Materials", 1993-1996.
22. U. S. Air Force Office of Scientific Research, "Fundamental Studies of Ions and Ionic Processes", 1994-1997.
23. North Atlantic Treaty Organization, "Definitive Characterization of Molecular Species of Environmental Interest", 1999-2001; renewed 2003 – 2004.

24. Department of Energy, "Explicitly Correlated Coupled Cluster and Brueckner Methods for Computations of Properties of Chemical Accuracy for Open Shell Systems", 2001-2004.
25. U.S. National Science Foundation, "Next Generation Aromatics", 2002-2007.
26. U.S. National Science Foundation, "U.S.-Hungary Research on the Definitive Structural Characterization of Building Units of Biomolecules", 2003-2006.
27. Department of Energy, "Next Generation, Explicitly Correlated Electronic Structure Methods", 2004-2007.
28. U. S. Department of Energy, "Theoretical Studies of Elementary Hydrocarbon Species and Their Reactions", 1994-2016.
29. U. S. National Science Foundation, "Molecular Electronic Structure Theory: Methods and Applications", 1995-2017.

### ***Invited Lecturer at Scientific Conferences***

1. "Gordon Research Conference on Theoretical Chemistry", Tilton School, Tilton, New Hampshire, June 22-26, 1970.
2. "Summer Research Conference on Theoretical Chemistry", Boulder, Colorado, June 22-30, 1972.
3. "Dynamics of Molecular Collisions", Gordon Conference, Plymouth, New Hampshire, July 24-28, 1972.
4. "Computation of Reaction Paths and Reaction Mechanisms", Centre Européen De Calcul Atomique Et Moléculaire, Paris, France, September 11-14, 1972.
5. "Fuglsang Meeting on Molecular Electronic Structure", Danish Ministry of Education, Fuglsang, Denmark, September 25-29, 1972.
6. "Spring Meeting of American Chemical Society", Peter Debye Award Symposium, in Honor of W. N. Lipscomb, Dallas, Texas, April 9-13, 1973.
7. "Symposium on Molecular Structure and Spectroscopy", Ohio State University, Columbus, Ohio, June 11-15, 1973.
8. "Critical Evaluation of Chemical and Physical Structural Information", National Academy of Sciences, Dartmouth College, Hanover, New Hampshire, June 24-29, 1973.



9. "Symposium on Potential Energy Surfaces for Chemical Reactions", American Physical Society, Philadelphia, Pennsylvania, March 25-28, 1974.
10. "Quantum Chemistry--The State of the Art", British Scientific Research Council, Oxford University, England, April 8-10, 1974.
11. "Fifth Canadian Symposium on Theoretical Chemistry", Ottawa, Canada, June 23-29, 1974.
12. "Atomic and Molecular Interactions", Gordon Conference, Wolfeboro, New Hampshire, August 12-16, 1974.
13. "Symposium on National Academy of Sciences Study of a National Center for Computation in Chemistry", American Chemical Society, Atlantic City, New Jersey, September 9-13, 1974.
14. "Eleventh Annual IEEE Computer Society Conference", Washington, D.C., September 9-11, 1975.
15. "Relation Between Science and Technology in Heterogeneous Catalysis", a symposium in honor of Professor W. F. Libby, University of California, Los Angeles, California, March 18-19, 1976.
16. "Potential Energy Surfaces" General Discussion No. 62 of the Faraday Division of the Chemical Society, University of Sussex, Brighton, England, September 8-10, 1976.
17. "Third Oji International Seminar", Japan Society for the Promotion of Science, Tomakomai, Hokkaido, Japan, September 14-17, 1976.
18. "Symposium on Minicomputers and Large Scale Computations", Chemical Institute of Canada/American Chemical Society, Montreal, Quebec, May 29-June 2, 1977.
19. "The Reliability of Quantum Chemical Predictions", American Chemical Society, Chicago, Illinois, August 28-September 2, 1977.
20. "Linus Pauling Award Symposium", in Honor of J. A. Pople, Northwest Section, American Chemical Society, University of Oregon, Eugene, Oregon, November 4-5, 1977.
21. "Seventh Symposium on Gas Phase Molecular Structure", University of Texas, Austin, Texas, February 27-March 1, 1978.
22. "International Symposium on Atomic, Molecular, and Solid State Theory", University of Florida, Palm Coast, Florida, March 13-18, 1978.

23. "Conference on the Spin States of Organic Molecules", Joint Institute for Laboratory Astrophysics, Boulder, Colorado, June 21-24, 1978.
24. "American Conference on Theoretical Chemistry", University of Colorado, Boulder, Colorado, June 26-30, 1978.
25. "Symposium on Methylene Chemistry", American Chemical Society, Miami Beach, Florida, September 11-15, 1978.
26. "The Sudden Polarization Effect", Universite de Paris-Sud, Orsay, France, January 8-9, 1979.
27. "ACS Pure Chemistry Award Symposium", American Chemical Society, Honolulu, Hawaii, April 1-6, 1979.
28. "International Symposium on Atomic, Molecular, and Solid State Theory, Collisional Phenomena, Quantum Statistics, and Computational Quantum Chemistry", University of Florida, Palm Coast, Florida, March 12-17, 1979.
29. "Nobel Symposium on Many Body Theory of Atomic Systems", Aspenäsgården, Lerum, Sweden, June 11-16, 1979.
30. "The Relationship Between Cluster Compounds, Metal Surfaces, and Catalysis", U. S. National Science Foundation, Pacific Grove, California, November 18-21, 1979.
31. "Discussion Meeting on Polyatomic Photodissociation", Eindhoven University of Technology, Eindhoven, Holland, December 3-4, 1979.
32. "Australian Conference on Molecular Physics and Quantum Chemistry", The Science Centre, Sydney, Australia, February 17-20, 1980.
33. "Seventh Canadian Symposium on Theoretical Chemistry", Banff, Alberta, Canada, June 15-21, 1980.
34. "Theoretical Approaches to Chemical Dynamics", Institute for Theoretical Chemistry, University of Texas, Austin, Texas, March 1-4, 1981.
35. "Sanibel Symposium on Atomic, Molecular, and Solid State Theory, Collision Phenomena, and Computational Quantum Chemistry", University of Florida, Palm Coast, Florida, March 8-14, 1981.
36. "Physical Organic Chemistry", Gordon Conference, Wolfeboro, New Hampshire, June 8-12, 1981.
37. "Vibrational Intensities", Gordon Conference, Plymouth, New Hampshire, June 8-12, 1981.

38. "Fourth American Conference on Theoretical Chemistry", University of Colorado, Boulder, Colorado, June 22-26, 1981.
39. "Dynamics of Chemical Reactions", Gordon Conference, Holderness, New Hampshire, July 27-31, 1981.
40. "Symposium für Theoretische Chemie", Walberberg, West Germany, October 11-15, 1981.
41. "Symposium on Theoretical Organic Chemistry/Computational Quantum Chemistry", Australian National University, Canberra, Australia, February 11-12, 1982.
42. "High Temperature Chemistry", Gordon Research Conference, Tilton, New Hampshire, July 26-30, 1982.
43. "Symposium on Transition States in Physical, Chemical, and Biological Processes", American Chemical Society, Kansas City, Missouri, September 13-17, 1982.
44. "Coupled-Cluster and Many Body Methods", International Symposium on the Quantum Theory of Matter, University of Florida, Palm Coast, Florida, March 7-12, 1983.
45. "Molecular Properties", Science and Engineering Research Council, St. Catharine's College, Cambridge University, England, March 25-27, 1983.
46. "XVII Organosilicon Symposium", North Dakota State University, Fargo, North Dakota, June 2-4, 1983.
47. "29th International Congress of Pure and Applied Chemistry", Cologne, West Germany, June 4-12, 1983.
48. "Vectorization of Advanced Methods for Molecular Electronic Structure", NATO, Colorado Springs, Colorado, September 25-29, 1983.
49. "Baekeland Award Symposium", American Chemical Society, Kean College, Union, New Jersey, October 24, 1983.
50. "Mardi Gras Symposium in Theoretical Chemistry", Tulane University, New Orleans, Louisiana, March 1-2, 1984.
51. "Spectroscopy, Structures, and Dynamics of Molecular Ions", American Chemical Society, St. Louis, Missouri, April 10, 1984.

52. "Comparison of *Ab Initio* Quantum Chemistry with Experiment for Small Molecules: State-of-the-Art", American Chemical Society, Philadelphia, Pennsylvania, August 26-30, 1984.
53. "Seventh International Conference on Lasers and Applications", Society for Optical and Quantum Electronics, San Francisco, California, November 26-30, 1984.
54. "Molecular Electronic Structure Calculations - Methods and Applications", Faraday Division of the Royal Society of Chemistry, University of Cambridge, Cambridge, England, December 11-13, 1984.
55. "David P. Craig Symposium: The Interface Between Theory and Experiment", Australian National University, Canberra, Australia, February 5-8, 1985.
56. "The Role of Theoretical Chemistry in Chemical Education and Research", American Chemical Society, Miami Beach, Florida, April 29, 1985.
57. "Symposium on Gas Phase Ions - Chemistry and Structure", American Chemical Society, Miami Beach, Florida, April 30-May 2, 1985.
58. "International Conference on Chemical Kinetics", National Bureau of Standards, Gaithersburg, Maryland, June 17-19, 1985.
59. "Geometrical Derivatives of Energy Surfaces and Molecular Properties", NATO Advanced Research Workshop, Sandbjerg, Denmark, August 1-4, 1985. Lecture presented by Dr. Mark Hoffmann.
60. "Electronic Theory of Chemical Reaction Systems", Japan - U.S. Joint Symposium, Indiana University, Bloomington, Indiana, August 13-16, 1985.
61. "Theoretical and Experimental Studies of Transient Species", American Chemical Society, Chicago, Illinois, September 8-12, 1985. Lecture presented by Mr. Andrew Scheiner.
62. "God and Modern Science: Who Shapes Whom," American Scientific Affiliation, Stanford University, Stanford, California, April 12, 1986.
63. "Symposium on Structure, Spectroscopy, and Dynamics of Atomic, Molecular, and Ionic Clusters", American Chemical Society, New York, New York, April 13-18, 1986.
64. "Eighth Combustion Research Meeting", U. S. Department of Energy, Airlie, Virginia, May 28-30, 1986.
65. "Electronic Structure of Transition States", American Chemical Society, Anaheim, California, September 8-10, 1986.

66. "Symposium on the History of Computers in Chemistry", Divisions of History of Chemistry and Computers in Chemistry, American Chemical Society, Anaheim, California, September 8-10, 1986.
67. "Theory and Simulation in Chemistry: The Impact of Minisupercomputers and Supercomputers", American Chemical Society, Denver, Colorado, April 5-10, 1987.
68. "Scientific and Technical Computing Symposium", IBM National Engineering and Scientific Support Center, Dallas, Texas, July 14-16, 1987.
69. "Sixth American Conference on Theoretical Chemistry", Gull Lake, Minnesota, July 26-31, 1987.
70. "Conference for University Research Executives", IBM Research Laboratory, Yorktown Heights, New York, October 13-16, 1987.
71. "International Symposia on Atomic, Molecular, and Condensed Matter, Computational Methods, and the Application of Fundamental Theory to Problems in Biology and Pharmacology", Whitney Laboratory, University of Florida, Marineland, Florida, March 12-19, 1988.
72. "Computational Atomic and Nuclear Physics at One Gigaflop," Oak Ridge National Laboratory, Oak Ridge, Tennessee, April 14-16, 1988.
73. "Seventeenth Southeast Theoretical Chemistry Association Conference", Emory University, Atlanta, Georgia, May 19-21, 1988.
74. "Sixth International Congress on Quantum Chemistry", Jerusalem, Israel, August 22-26, 1988.
75. "Frontiers in Molecular Vibrations: Theory and Experiment", American Chemical Society, Los Angeles, California, September 25-30, 1988.
76. "Tenth Canadian Symposium on Theoretical Chemistry," Banff, Alberta, Canada, August 24-30, 1989.
77. "Forty Years of Quantum Chemistry - An International Conference in Honor of Professor John A. Pople", University of Georgia, Athens, Georgia, October 16-19, 1989.
78. "Recent Advances in Bonding at Main Group Element Centers: Structure and Theory", International Chemical Congress of Pacific Basin Societies, Honolulu, Hawaii, December 17-22, 1989.

79. "Advances in Computational Chemistry", International Chemical Congress of Pacific Basin Societies, Honolulu, Hawaii, December 17-22, 1989.
80. "Symposium on Cluster Chemistry", American Association for the Advancement of Science, New Orleans, Louisiana, February 15-20, 1990.
81. "International Symposia of Atomic, Molecular and Condensed Matter, Computational Methods, and the Application of Fundamental Theory to Problems in Biology and Pharmacology", St. Augustine, Florida, March 17-24, 1990.
82. "Nineteenth Southeast Theoretical Chemistry Association Conference", Florida State University, Tallahassee, Florida, May 17-19, 1990.
83. "Twelfth Combustion Research Meeting", U.S. Department of Energy, Granlibakken Conference Center, Tahoe City, California, May 30-June 1, 1990.
84. "National Science Foundation Workshop on Computational Chemistry by Microcomputer", Calvin College, Grand Rapids, Michigan, June 4-8, 1990.
85. "Second WATOC World Congress", World Association of Theoretical Organic Chemists, University of Toronto, Ontario, Canada, July 8-14, 1990.
86. "Seventh American Conference on Theoretical Chemistry," San Diego, California, July 30-August 3, 1990.
87. "Fifty-Seventh Meeting of the Southeastern Section," American Physical Society, Atlanta, Georgia, November 15-17, 1990.
88. "Reactions, Spectroscopy, and Structure of Molecular Ions," American Chemical Society, Atlanta, Georgia, April 14-19, 1991. Lecture presented by Dr. Tracy Hamilton.
89. "Silicon Hydride Chemistry And Silicon Chemical Vapor Deposition Mechanisms," American Chemical Society, Atlanta Georgia, April 14-19, 1991. Lecture presented by Dr. Brenda Colegrove.
90. "*Ab Initio* Methods: An International Symposium in Honor of Professor Klaus Ruedenberg," Iowa State University, Ames, Iowa, May 9-11, 1991.
91. "Twentieth Southeast Theoretical Chemistry Association Conference," Clemson University, Clemson, South Carolina, May 16-18, 1991.
92. "Comparison of *Ab Initio* Quantum Chemistry with Experiment: State-of-the-Art", American Chemical Society, New York, New York, August 25-30, 1991.
93. "Twenty-First Southeast Theoretical Chemistry Association Conference," University of Alabama, Huntsville, Alabama, May 28-20, 1992.

94. "Structures and Conformations of Non-Rigid Molecules," NATO Advanced Research Workshop, University of Ulm, Germany, September 6-10, 1992.
95. "Current Trends in Computational Chemistry," Army Research Office, Department of Energy and the Upjohn Company, Jackson State University, Jackson, Mississippi, November 6-7, 1992.
96. "Centenary Medal Award Symposium", Royal Society of Chemistry (London), University of Cambridge, England, December, 1992.
97. "XXVI Organosilicon Symposium," Indianapolis, Indiana, March 26-27, 1993.
98. "Fifteenth Combustion Research Meeting", U. S. Department of Energy, Split Rock Resort and Conference Center, Lake Harmony, Pennsylvania, June 2-4, 1993.
99. "Eighth American Conference on Theoretical Chemistry", University of Rochester, Rochester, New York, June 28 - July 3, 1993.
100. "Ninth Strasbourg Seminar on Computational Methods in Quantum Chemistry", University of Girona, Girona, Spain, July 12-14, 1993.
101. "Third WATOC World Congress", World Association of Theoretical Organic Chemists, Toyohashi, Japan, July 18-24, 1993.
102. "Connecting Molecular Level Computational Tools with Experiment," American Chemical Society, Chicago, Illinois, August 22-27, 1993.
103. "Michael J. S. Dewar Award Symposium", American Chemical Society, San Diego, California, March 13-18, 1994.
104. "From Methylene to Proteins and Beyond: A Quarter Century of Scientific Computation," Atlanta Marriott Perimeter Center, Georgia, June 3-5, 1994.
105. "25th Reaction Mechanisms Conference", University of Notre Dame, South Bend, Indiana, June 10-15, 1994.
106. "High Performance Computing Conference '94", National Supercomputing Research Centre, National University of Singapore, Hyatt Regency Singapore, September 29-30, 1994.
107. "Chemical Dynamics of Transient Species", Robert A. Welch Foundation, Houston, Texas, October 24-25, 1994.
108. "Australian Conference on Chemical Physics, Incorporating the Sixth Australian Conference on Chemical Reaction Dynamics," Royal Australian Chemical Institute, Canberra, Australia, February 12-16, 1995.

109. "Thirty-Fifth Sanibel Symposium", University of Florida, St. Augustine, Florida, February 24-March 4, 1995.
110. "Experimental and Computational Chemistry: The Fruitful Interplay", an International Symposium in Honor of Professor Paul von Rague Schleyer", Erlangen, Germany, April 27-28, 1995.
111. "Gordon Research Conference on the Chemistry and Physics of Matrix Isolated Species", Plymouth State College, Plymouth, New Hampshire, July 30-August 4, 1995.
112. "Molecular Quantum Mechanics: Methods and Applications", University of Cambridge, England, September 3-7, 1995.
113. Keynote Lecture, "International Conference on Parallel and Distributed Processing Techniques and Applications", University of Georgia, Athens, November 2-4, 1995.
114. "Computational Quantum Chemistry: A Viable Partner to Experiment in Chemical Research", International Chemical Congress of Pacific Basin Societies, Honolulu, Hawaii, December 17-22, 1995.
115. "Eighteenth Combustion Research Meeting", U. S. Department of Energy, Tahoe City, California, May 28-31, 1996.
116. "Molecular Dynamics", University of Colorado, Boulder, Colorado, June 2-5, 1996.
117. "Fourteenth International Conference on Radical Ions", University of Uppsala, Uppsala, Sweden, July 1-5, 1996.
118. "Fourth World Congress of Theoretically Oriented Chemists", Jerusalem, Israel, July 7-12, 1996.
119. "Computational Advances in Inorganic Chemistry", American Chemical Society 212th National Meeting, Orlando, Florida, August 25-29, 1996.
120. "Elucidation of Organic Reaction Mechanisms by *Ab Initio* Methods", American Chemical Society 212th National Meeting, Orlando, Florida, August 25-29, 1996.
121. "Swedish-American Symposium on the Foundations of Quantum Theory in Chemistry, Molecular Physics, and Biology: A Symposium in Honor of Per-Olov Löwdin", Sanibel Island, Florida, October 26-30, 1996.
122. "Eighteenth Annual West Coast Theoretical Chemistry Conference", University of California, Berkeley, April 9 -11, 1997.



123. "Frontiers of Electronic Structure Theory", American Chemical Society 213th National Meeting, San Francisco, California, April 13-17, 1997.
124. "Canadian Conference on Computational Chemistry", University of Alberta, Edmonton, Alberta, July 19-23, 1997.
125. "36th Congress of the International Union of Pure and Applied Chemistry", (IUPAC), Geneva, Switzerland, August 18-22, 1997.
126. "XII International Conference on Computers in Chemical Research and Education", University of Pune, Pune, India, January 5-9, 1998.
127. "The Frank E. Harris Symposium", University of Utah, Salt Lake City, Utah, February 20-21, 1998.
128. "The William A. Goddard III Symposium", California Institute of Technology, Pasadena, March 20-21, 1998.
129. "Twenty-Seventh Southeast Theoretical Chemistry Association Conference", Florida State University, Tallahassee, May 28-30, 1998.
130. "Faraday Discussion 111. Chemical Reaction Theory", Royal Society of Chemistry, St. Andrews, Scotland, July 1-3, 1998.
131. "European Summer School on Computational Quantum Chemistry", Centro Svizzero di Calcolo Scientifico, Lugano, Switzerland, July 27-31, 1998.
132. "A Celebration of 20 Years of the Subdivision of Theoretical Chemistry", American Chemical Society 216th National Meeting, Boston, Massachusetts, August 23-27, 1998.
133. "Modeling Chemical Shifts", American Chemical Society 216th National Meeting, Boston, Massachusetts, August 23-27, 1998.
134. "Symposium in Honor of Professor Rudolf Zahradnik", Villa Lanna, Prague, Czech Republic, September 6-7, 1998.
135. "Quantum Chemistry Symposium in Honor of Robert G. Parr", Research Triangle Park, North Carolina, November 6-7, 1998.
136. "Electron Correlation Effects in Spectroscopy and Dynamics", University of Kaiserslautern, Germany, December 9-12, 1998.
137. "Forty Years in the Frontiers of Quantum Chemistry", Emory University, Atlanta, Georgia, May 20-22, 1999.

138. "Twenty-First Combustion Research Meeting", U. S. Department of Energy, Tahoe City, California, June 9 - 12, 1999.
139. "Tenth American Conference on Theoretical Chemistry", University of Colorado, Boulder, Colorado, June 27-July 2, 1999.
140. "Gordon Conference on the Chemistry and Physics of Matrix Isolated Species", Plymouth, New Hampshire, July 11-16, 1999.
141. "Fifth World Congress of Theoretically Oriented Chemists", London, England, August 1-6, 1999.
142. "Nobel Laureate Symposium in Honor of John A. Pople", American Chemical Society 218<sup>th</sup> National Meeting, New Orleans, Louisiana, August 22-26, 1999.
143. "The Sixteenth Colloquium on High Resolution Molecular Spectroscopy", University de Bourgogne, Dijon, France, September 6-10, 1999.
144. "Annual Meeting of the Argentine Physical Society", Tucuman City, Argentina, September 13-17, 1999. Participation cancelled.
145. "Kenneth S. Pitzer Memorial Symposium on Theoretical Chemistry", University of California, Berkeley, January 11 - 15, 2000.
146. "Workshop on Computational Chemistry", Hong Kong University of Science and Technology, Hong Kong, China, February 21-23, 2000.
147. "The Nature of Nature: An Interdisciplinary Conference on the Role of Naturalism in Science", Michael Polanyi Center, Baylor University, Waco Texas, April 12-15, 2000.
148. "Ninth Conference on Current Trends in Computational Chemistry", Vicksburg, Mississippi, November 2-4, 2000.
149. "Symposium on the Frontiers of Theoretical Chemistry", University of Tokyo, Japan, March 12-14, 2001.
150. "Chemical Dynamics Symposium in Honor of William H. Miller", University of California, Berkeley, California, March 28-31, 2001.
151. "Quantum Chemistry: A Conference in Honour of Professor Nicholas C. Handy", Cambridge University, England, June 13-14, 2001.
152. "World Chemical Congress of the International Union of Pure and Applied Chemistry", Brisbane, Australia, July 1-6, 2001.

153. "Molecular Quantum Mechanics: The Right Answer for the Right Reason: An International Conference in Honor of Professor Ernest R. Davidson", University of Washington, Seattle, Washington, July 21-26, 2001.
154. "Eighth European Symposium on Organic Reactivity", Dubrovnik, Croatia, September 1-6, 2001.
155. "Fifty-Third Annual Meeting of the Southeastern Region of the American Chemical Society", Savannah, Georgia, September 23-26, 2001.
156. "Tenth Conference on Current Trends in Computational Chemistry" Jackson State University, Vicksburg, Mississippi, November 1-3, 2001.
157. "Fourth National Symposium in Chemistry", Chemical Research Society of India, National Chemical Laboratory and Poona University, Pune, India, February 1 – 3, 2002.
158. "Symposium in Memory of Professor Peter Kollman", American Chemical Society 223<sup>rd</sup> National Meeting, Orlando, Florida, April 7-11, 2002.
159. "Recent Advances in Electron Correlation Methodology", American Chemical Society 223<sup>rd</sup> National Meeting, Orlando, Florida, April 7-11, 2002.
160. "Thirtieth Peter Leermakers Symposium", Wesleyan University, Middletown, Connecticut, May 8-9, 2002.
161. "Thirty-First Southeast Theoretical Chemistry Association (SETCA) Conference", Georgia Institute of Technology, Atlanta, Georgia, May 23-25, 2002.
162. "Twenty-Fourth Combustion Research Meeting", U.S. Department of Energy, Airlie Conference Center, Warrenton, Virginia, May 28-31, 2002.
163. "Exploring Modern Computational Chemistry", University of Nottingham, England, July 31 - August 2, 2002. Participation cancelled due to daughter's hospitalization.
164. "Symposium on Chemical Studies Important to Astrobiology", American Chemical Society 224th National Meeting, Boston, Massachusetts, August 18-22, 2002.
165. "Quantum Systems in Chemistry and Physics VII", Bratislava, Slovakia, September 10-15, 2002.
166. "Second Annual Computational Chemistry Conference", University of Kentucky, Lexington, Kentucky, October 7-8, 2002. Lecture presented by Dr. Wesley D. Allen.

167. "Advances in Quantum Chemistry", Robert A. Welch Foundation, Houston, Texas, October 27-29, 2002.
168. "Fifty-Fourth Annual Meeting of the Southeastern Region of the American Chemical Society", Charleston, South Carolina, November 13 - 16, 2002. Lecture given by Dr. Nancy Richardson.
169. "Trends in Theoretical Chemistry: The Ninth Biennial Conference of Indian Theoretical Chemists", Indian Association for the Cultivation of Science, Calcutta, India, January 17 -19, 2003.
170. "Awards Symposium", Division of Physical Chemistry, American Chemical Society 225th National Meeting, New Orleans, Louisiana, March 23 -27, 2003.
171. "Integrating Diverse Computational Approaches to Complex Problem Solving", Division of Computational Chemistry, American Chemical Society 225th National Meeting, New Orleans, Louisiana, March 23-27, 2003.
172. "Symposium in Honor of Professor Rudolf A. Marcus", University of Southern California, Los Angeles April 8 - 10, 2003.
173. "Symposium on Computational Chemistry", Emory University, Atlanta, Georgia, April 11-12, 2003.
174. "Quantum Inorganic Chemistry", Faraday Discussion 124, University of York, England, April 14-16, 2003.
175. "Thirty-Second Southeast Theoretical Chemistry Association (SETCA) Conference", Clemson University, Clemson, South Carolina, May 22 - 24, 2003. Participation cancelled due to bypass surgery.
176. "Conference in Honor of Professor Vic Saunders", Daresbury Laboratory, Warrington, Cheshire, England, June 8-10, 2003. Participation cancelled due to bypass surgery.
177. "Eighth Conference on Quantum Systems in Chemistry and Physics", Spetses, Greece, August 30 - September 4, 2003. Participation cancelled due to bypass surgery.
178. "Fifty-Fifth Annual Meeting of the Southeastern Region of the American Chemical Society", Atlanta, Georgia, November 16 - 19, 2003.
179. "Theory and Applications of Computational Chemistry", Gyeongju, Korea, February 15 - 19, 2004.

180. "Graham Richards Award Symposium", Division of Computers in Chemistry, 226th National Meeting, American Chemical Society, Anaheim, California, March 28-30, 2004.
181. "Symposium in Honor of Professor Jean-Marie André", Georgia Institute of Technology, Atlanta, Georgia, April 5, 2004.
182. "Science, Information and Complexity Symposium", Biola University, La Mirada, California, April 22 -24, 2004.
183. "The Systematic Treatment of Electron Correlation. A Celebration of the Science of Rodney J. Bartlett", St. Simons Island, Georgia, April 23 – 25, 2004.
184. "Thirty-Third Southeast Theoretical Chemistry Association (SETCA) Conference", University of Mississippi, Oxford, Mississippi, May 20-22, 2004.
185. "Symposium of the Division of Computers in Chemistry", 227th National Meeting, American Chemical Society, Philadelphia, Pennsylvania, August 22-26, 2004.
186. "Electronic Structure: Principles and Applications", ESPA 2004 Conference, Valladolid, Spain, September 15-18, 2004.
187. "Molecular Quantum Mechanics: The No Nonsense Path to Progress. An International Conference in Honour of Professor Nicholas C. Handy", University of Cambridge, England, July 24-29, 2004.
188. "Symposium in Honor of Henry F. Schaefer's 60<sup>th</sup> Birthday", Co-sponsored by the Division of Computers in Chemistry and the Division of Physical Chemistry, 227<sup>th</sup> National Meeting, American Chemical Society, Philadelphia, Pennsylvania, August 22 – 26, 2004.
189. "Electronic Structure: Principles and Applications", ESPA 2004 Conference, Valladolid, Spain, September 15 – 18, 2004. Participation cancelled.
190. "WATOC 05, the Eighth Congress of the World Association of Theoretically Oriented Chemists", Cape Town, South Africa, January 16-21, 2005.
191. "CHEMFEST – 2005", University of Hyderabad, India, February 18 – 19, 2005.
192. "Advances in Spectroscopy", Indian Institute of Science, Bangalore, India, February 21-24, 2005.
193. "John A. Pople Symposium", 228<sup>th</sup> National Meeting, American Chemical Society, San Diego, California, March 12 –16, 2005.

194. "Computational Chemistry Symposium", National Center for Supercomputer Applications, University of Illinois, Urbana, Illinois, April 17-19, 2005.
195. "Science-Ethics-Faith", Polish Professors' Forum, Wisla, Poland, April 29 – May 3, 2005.
196. "Symposium in Honor of Professor Noel Hush", University of Sydney, Sydney, Australia, June 30 – July 2, 2005.
197. "Twelfth National Convention of Royal Australian Chemical Institute", Sydney Australia, July 3 – 7, 2005.
198. "Twenty-Eighth International Symposium on Free Radicals", Leysin, Switzerland, September 4 – 9, 2005.
199. "Theoretical Determination of Energy Landscapes: Methodology and Applications", 229<sup>th</sup> National Meeting, American Chemical Society, Washington, D. C., August 28 – September 1, 2005.
200. "Astrochemistry – From Laboratory Studies to Astronomical Observations", International Chemical Congress of Pacific Basin Societies, Honolulu, Hawaii, December 15 – 20, 2005.
201. "Computational Quantum Chemistry: Methodology and Applications", International Chemical Congress of Pacific Basin Societies, Honolulu, Hawaii, December 15-20, 2005.
202. "Eighth Chemical Research Society of India (CRSI) National Symposium", Indian Institute of Technology Bombay, Mumbai, India. February 2-5, 2006.
203. "Quantitative Quantum Chemistry", Santa Fe, New Mexico, March 17-20, 2006.
204. "Frontier Applications and Developments of Density Functional Theory: A Symposium in Honor of Robert G. Parr", 231<sup>st</sup> National Meeting, American Chemical Society, Atlanta, Georgia, March 26-30, 2006.
205. "Symposium in Honor of Professor Gernot Frenking", Universities of Giessen and Marburg, Germany, April 11-13, 2006.
206. "International Conference of Computational Methods in Science and Engineering (ICCMSE)", Chania, Crete, Greece, October 27-November 1, 2006.
207. "Fifteenth Conference on Current Trends in Computational Chemistry", Jackson State University, Jackson, Mississippi, November 2 – 4, 2006.
208. "Trends in Chemical Dynamics: From Small Molecules to Biomolecules: In Celebration of Yuan T. Lee's 70<sup>th</sup> Birthday", Chiao-Hsi, Yi-La County, Taiwan, December 10-15, 2006.

209. “Forty-Seventh Sanibel Symposium”, King and Prince Hotel, St. Simons Island, Florida, February 22-27, 2007.
210. “William A. Lester Symposium”, University of California, Berkeley, California, March 28-31, 2007.
211. “Thirty-Sixth Southeast Theoretical Chemistry Association (SETCA) Conference”, Virginia Tech University, Blacksburg, Virginia, May 17-19, 2007.
212. “William A. Goddard III Symposium”, 234<sup>th</sup> National Meeting, American Chemical Society, Boston, Massachusetts, August 19-23, 2007.
213. “Dennis Marynick Symposium”, University of Texas, Arlington, Texas, August 30 – September 1, 2007.
214. “International Conference on Computational Methods in Science and Engineering”, Corfu, Greece, September 25-30, 2007.
215. “TECHFEST, An International Science and Technology Congress”, Indian Institute of Technology, Bombay, Mumbai, India, January 25-27, 2008.
216. 215. “22<sup>nd</sup> Austin Symposium on Molecular Structure”, University of Texas, Austin, March 1-4, 2008.
217. “Computational Spectroscopy”, 235<sup>th</sup> National Meeting, American Chemical Society, New Orleans, Louisiana, April 6-10, 2008.
218. “European Scientific Network”, Budapest, Hungary, May 24-29, 2008.
219. “Ernest R. Davidson Symposium”, Sixth Congress of the International Society of Theoretical Chemical Physics, University of British Columbia, Vancouver, British Columbia, July 19-24, 2008.
220. “Twentieth International Conference on Chemical Education”, Pointe Aux Piments, Mauritius, August 3-8, 2008.
221. “The Latsis Symposium: Intramolecular Dynamics, Symmetry, and Spectroscopy”, ETH Zurich, September 6-10, 2008.
222. “Eighth Triennial Congress of the World Association of Theoretical and Computational Chemists”, Sydney, Australia, September 14-19, 2008.
223. “Sason Shaik Symposium”, Lise Meitner-Minerva Center for Computational Quantum Chemistry, Hebrew University, Jerusalem, Israel, November 12-13, 2008.

224. "Gas Phase Ion Spectroscopy: State of the Art and Perspectives", Kloster Eberbach, Germany December 14-16, 2008.
225. "Eleventh National Symposium of the Chemical Research Society of India", National Chemical Laboratory, Pune, India, February 6-8, 2009.
226. "Compute. Discover. Innovate. International Conference on Computational Science", Louisiana State University, Baton Rouge, Louisiana, May 25-27, 2009.
227. "International Conference on Computational Methods in Science and Engineering (ICCMSE)", Rhodes, Greece, September 29 – October 4, 2009.
228. "International Symposium on Molecular Theory for Real Systems", University of Kyoto, Kyoto, Japan, January 7-9, 2010.
229. "Summer Lectures in Santiago: Recent Developments in Quantum Chemistry", Pontificia Universidad Catolica de Chile, Santiago, Chile, January 2010.
230. 228. "Symposium on Recent Trends in Biophysics", Indian Biophysical Society and Banaras Hindu University, Varanasi, India, February 13-15, 2010.
231. "Theoretical and Computational Chemistry", Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany, February 28 – March 2, 2010.
232. "Molecular Quantum Mechanics: From Methylene to DNA and Beyond", University of California, Berkeley, California, May 24-29, 2010.
233. "Electrons in Biomolecules", 240<sup>th</sup> National Meeting, American Chemical Society, Boston, Massachusetts, August 22-26, 2010.
234. "Theory and Experiment: Synergy or Competition?", Friedrich-Alexander-Universität, Erlangen-Nurnberg, Germany, August 26-28, 2010.
235. "Fifteenth International Workshop on Quantum Systems in Chemistry and Physics", Magdalene College, University of Cambridge, England, August 31 – September 5, 2010.
236. "Computational Quantum Chemistry: Theory and Interactions with Experiment", PACIFICHEM, The International Chemical Congress of Pacific Basin Societies, Honolulu, Hawaii, December 15-20, 2010.
237. "Pioneers of Quantum Chemistry", 241<sup>st</sup> National Meeting, American Chemical Society, Anaheim, California, March 27-31, 2011.
238. "Ninth Triennial Congress of the World Association of Theoretical and Computational Chemists", Santiago de Compostela, Spain, July 17-22, 2011.



239. "Forty-Third World Chemistry Congress of the International Union of Pure and Applied Chemistry (IUPAC)", San Juan, Puerto Rico, July 30 – August 7, 2011.
240. "Reduced Density Matrices in Quantum Chemistry and Physics", 242<sup>nd</sup> National Meeting, American Chemical Society, Denver, Colorado, August 28-September 1, 2011.
241. "Twentieth Conference on Current Trends in Computational Chemistry", Jackson State University, Jackson, Mississippi, October 27-29, 2011.
242. "Applied Theory on Molecular Systems-ATOMS 2011", Indian Institute of Chemical Technology, Tarnaka, Hyderabad, India, November 2-5, 2011.
243. "Quantum Molecular Dynamics", University of California, Berkeley, California, January 9-12, 2012.
244. "Symposium on Molecular Structure and Dynamics", Southern Methodist University, Dallas, Texas, March 3-6, 2012.
245. "Fleming Crim Symposium", University of Wisconsin, Madison Wisconsin, May 24-26, 2012.
246. "Accurate Methods for Accurate Properties: An International Conference in Honor of Peter R. Taylor", University of Zürich, Zürich, Switzerland, June 4-6, 2012.
247. "Exploring Potential Energy Surfaces in Quantum Chemistry", 244<sup>th</sup> National Meeting, American Chemical Society, Philadelphia, Pennsylvania, August 19-23, 2012.
248. "Frontiers in Scientific Computing", University of Cape Town, South Africa, September 31 – October 2, 2012.
249. "National Seminar on Quantum Mechanics in Chemistry", University of Calicut, Thrissur, India, December 3-4, 2012.
250. "Symposium in Honor of Professor Joel Bowman", Emory University, Atlanta, Georgia, February 8-9, 2013.
251. "International Conference on New Emerging Trends in Chemistry", IIS University, Jaipur, Rajasthan, India, March 2 – 4, 2013.
252. "Chemical Theory for Complex Systems", University of Strasbourg, France, March 6 – 8, 2013.
253. "Award Symposium: F. Albert Cotton Award in Synthetic Inorganic Chemistry", 245<sup>th</sup> National Meeting, American Chemical Society, New Orleans, Louisiana, April 7 – 11, 2013.

254. “Molecular Quantum Mechanics. Electron Correlation: The Many-Body Problem at the Heart of Chemistry”, Palazzo dei Congressi, Lugano, Switzerland, June 2-7, 2013.
255. “17<sup>th</sup> Brazilian Symposium on Theoretical Chemistry”, Angra dos Reis, Brazil, November 24-28, 2013.
256. “Fifty-Fourth Sanibel Symposium on Quantum Chemistry, Solid State Physics, and Quantum Biology”, St. Simons Island, Georgia, February 16-21, 2014.
257. “Twenty-Fifth Austin Symposium on Molecular Structure and Dynamics”, Southern Methodist University, Dallas, Texas, March 1-4, 2014.
258. “Peter Debye Award Symposium”, 247<sup>th</sup> National Meeting, American Chemical Society, Dallas, Texas, March 16-20, 2014.
259. “International Symposium on Frontiers of Theoretical and Computational Chemistry—A Celebration in Honor of Henry Schaefer and Leo Radom”, Peking University, The Graduate School, Shenzhen, China, May 4-6, 2014.
260. Southeast Theoretical Chemistry Association (SETCA), Emory University, Atlanta, Georgia, May 15-17, 2014.
261. “Biological and Inorganic Charge Transfer Dynamics,” Ludwig – Maximilians University, Munich, Germany, July 16-18, 2014.
262. “Symposium in Memory of Professor Nicholas C. Handy”, 248<sup>th</sup> National Meeting, American Chemical Society, San Francisco, California, August 10-14, 2014.
263. “Symposium on Physical Chemistry in the Twenty-First Century”, 248<sup>th</sup> National Meeting, American Chemical Society, San Francisco, California, August 10-14, 2014.
264. “Tenth International Congress of the World Association of Theoretical and Computational Chemists”, Santiago, Chile, October 5-10, 2014
265. “Third International Seminar in Chemistry”, University of Padjadjaran, Bandung, Indonesia, November 19-21, 2014.
266. “Concepts from Mathematical Physics to Chemistry”, Quintana Roo, Mexico, December 10-13, 2014.
267. “International Symposium on Recent Advances in Chemistry,” North-Eastern Hill University, Shillong, India, March 3-5, 2015.