Curriculum Vitae

WILLIAM HUGHES MILLER

Personal:

Born: 16 March 1941, Kosciusko, Mississippi, USA

Married: Margaret Ann Westbrook, (two daughters, Alison b. 1970, Emily b. 1972)

Education and Positions:

1956-59	Provine High School, Jackson, MS, Valedictorian
1959-63	Georgia Institute of Technology, General Motors National Scholarship, B.S. 1963 (Chemistry), Phi Kappa Phi Cup (Valedictorian)
1963-67	Harvard University, National Science Foundation Fellow, A.M. 1964 (Chemistry) Ph.D. 1967 (Chemical Physics), E. Bright Wilson, Jr., Research Director
1967-68	NATO Postdoctoral Fellow, University of Freiburg, Germany
1967-69	Junior Fellow, Society of Fellows, Harvard University
1969-72	Assistant Professor, Department of Chemistry, University of California, Berkeley
1969-present	Staff Senior Scientist, Chemical Sciences Division, Lawrence Berkeley National Laboratory
1972-74	Associate Professor, Department of Chemistry, University of California, Berkeley
1974-2010	Professor, Department of Chemistry, University of California, Berkeley
1984-88	Vice-Chairman, Department of Chemistry, University of California, Berkeley
1989-93	Chairman, Department of Chemistry, University of California, Berkeley
1998-2001	Chancellor's Research Professor, University of California, Berkeley
1999-2012	Kenneth S. Pitzer Distinguished Professor of Chemistry, University of California, Berkeley
2012-present	Kenneth S. Pitzer Distinguished Professor Emeritus, and Professor of the Graduate School, University of California, Berkeley

Honors:
Alfred P. Sloan Research Fellow, 1970-1972
Camille and Henry Dreyfus Teacher-Scholar, 1973-1979
Annual Prize of the International Academy of Quantum Molecular Science, 1974
John Simon Guggenheim Memorial Fellow, 1975-76
Overseas Fellow, Churchill College, University of Cambridge, 1975-1976
Miller Research Professor, University of California, 1978-1979
Alexander von Humboldt Senior Scientist Award, 1981-1982
Member, International Academy of Quantum Molecular Science, elected 1985
Ernest Orlando Lawrence Memorial Award, 1985
Member, National Academy of Sciences, elected 1987
American Chemical Society Irving Langmuir Award in Chemical Physics, 1990
Fellow, American Academy of Arts and Sciences, elected 1993
Christensen Visiting Fellowship, St. Catherine's College, Oxford, 1993
American Chemical Society Award in Theoretical Chemistry, 1994
Honorary Professor, Shandong University, Jinan, PRC, 1994
J. O. Hirschfelder Prize in Theoretical Chemistry, University of Wisconsin, 1996
Ira Remsen Award, Chesapeake Bay Section of the American Chemical Society, 1997
College of Sciences Alumni Achievement Award, Georgia Institute of Technology, 1997
Spiers Medal, Faraday Division of the Royal Society of Chemistry (London), 1998
Miller Research Professor, University of California, 1998-1999
Cherry L. Emerson Distinguished Visiting Professor, Emory University, 2000
American Chemical Society Peter Debye Award in Physical Chemistry, 2003
Welch Award in Chemistry, 2007
Herschbach Award in Molecular Dynamics, 2007
Ahmed Zewail Prize in Molecular Sciences, 2011
Member, Leopoldina (German National Academy of Sciences) elected 2011

Societies:
Member, American Chemical Society, 1980-present
Fellow, American Association for the Advancement of Science, 1983-present
Fellow, American Physical Society, 1984-present

Editorial Boards:
Member, Advisory Editorial Board of *Chemical Physics*, 1973-1996
Associate Editor, *The Journal of Chemical Physics*, 1976-1979
Member, Editorial Board of *Nouveau Journal de Chimie*, 1977-1987
Member, Advisory Editorial Board of the *International Journal of Quantum Chemistry*, 1979-1989
Member, Advisory Editorial Board of *Chemical Physics Letters*, 1982-present
Member, Advisory Editorial Board of *The Journal of Physical Chemistry*, 1983-1989
Cooperating Editor, *Theoretica Chimica Acta*, 1985-1997
Member, Advisory Editorial Board of *Advances in Quantum Chemistry*, 1987-present
Divisional Associate Editor, *Physical Review Letters*, 1993-99
Member, International Advisory Editorial Board of *Faraday Transactions*, 1996-1999
Member, International Advisory Board of the *Encyclopedia of Computational Chemistry*, 1996
Member, Editorial Board of *Theoretical Chemistry Accounts*, 1997-present
Member, International Advisory Board of Physical Chemistry Chemical Physics, 1999-2006
Member, Advisory Editorial Board of *Theoretical and Computational Chemistry*, 2001-present
Member, Editorial Board of the *Central European Journal of Chemistry*, 2002-present
Member, Editorial Board of the *Journal of Chemical Theory and Computation*, 2002-present
Member, International Honorary Board of *Physical Chemistry Chemical Physics*, 2006-present

Academic and Government Committee Service:

Member, Theoretical Chemistry Review Committee for Los Alamos National Scientific Laboratory, September 12-13, 1977.
Member, Policy Board of the National Resource for Computation in Chemistry (NRCC), 1977-1980.
Member, ad hoc Visiting Committee for the Chemistry Department of Texas A&M University, January 25-27, 1979.
Consultant, Molecular Physics Department of SRI International, 1972-1979.
Member of the Scholarship Committee for the Winston Churchill Foundation of the United States, 1985-86.
Member, External Review Panel for the Department of Chemistry of the University of California, Santa Barbara, November 21-22, 1986.
Member, Steering Committee of the American Physical Society Topical Group on Few Body Systems and Multiparticle Dynamics, 1987-1989.
Member, Chemistry Panel of the National Research Council Associateships Program, 1987-1989.
Member, Committee on Recommendations for U.S. Army Basic Scientific Research, 1987-90.
Member, External Review Committee for the Ames Laboratory for Physical Research and Technology, Ames, Iowa, May 10-11, 1988.
Member, Committee on Atomic, Molecular, and Optical Sciences of the National Research Council, 1988-1991.
Member of the Fellowship Committee of the American Physical Society, 1988-1990.
Honorary Board Member of the World Congress of Theoretical Organic Chemists, 1989-present.
Chairman, 1989 Conference on the Dynamics of Molecular Collisions, Asilomar, CA, 16-21 July 1989.
Chairman, Chemistry Panel of the National Research Council Associateships Program, 1990-1991.
Chairman of the Associateships and Fellowships Program Advisory Committee (AFPAC) of the National Research Council (NRC), 1991-92.
Member, Advisory Board of the Office of Scientific and Engineering Personnel (OSEP) of the National Research Council (NRC), 1991-1999.
Member, Board of Visitors, Office of Naval Research, 1992-1994.
Chairman, Associateships Program Advisory Committee (APAC) of the Office of Scientific and Engineering Personnel (OSEP) of the National Research Council (NRC), 1992-1999.
Member, Program Committee for the Alfred P. Sloan Research Fellowships in Chemistry, 1995-2001.
External elector for the Chair in Theoretical Chemistry, University of Cambridge, 1995.
External reviewer for the Institute of Molecular Science, Okazaki, Japan, 1996.
Member, Committee on Committees, University of California, Berkeley, 1996-2000.
Vice-Chair, Chair-Elect, Chair of the Division of Chemical Physics of the American Physical Society, 1997-2000.
Co-Chairman, Pitzer Memorial Symposium on Theoretical Chemistry, Berkeley, CA, 9-13 January 2000.
External examiner, National University of Singapore, 1999-2001.
Secretary, International Academy of Quantum Molecular Science, Paris, France, 2000-2006.

Academic and Government Committee Service continued:

Member, Board of Directors, International Society for Theoretical Chemical Physics, 2000-present.

Member, Steering Group, American Association for the Advancement of Science, 2001-present.

Member, Review Committee of the Fritz Haber Minerva Center for Molecular Dynamics, Hebrew University of Jerusalem, 2002.

External Elector for the Coulson Chair in Theoretical Chemistry, University of Oxford, 2005.

Foreign Councilor, Institute of Molecular Science, Okazaki, Japan, 2007-2009.

Member of the International Advisory Committee, Center for Theoretical and Computational Chemistry, Dalian Institute if Chemical Physics, Chinese Academy of Sciences, 2009-present

Member, International Society for Theoretical Chemical Physics Honorary Board, 2012-present.

Named Lectureships and Lecture Series:

1. Series of five lectures, Freiburg University, Germany, 12-16 July 1971, "Molecular Collision Theory".

2. Sherwin-Williams Lecture, University of Illinois, Urbana, Illinois, 2 October 1974, "Transition State Theory Re-Visited".

3. Series of four lectures, Hahn Meitner Institute for Nuclear Physics, Berlin, Germany, 26-30 January 1976, "Semiclassical Scattering Theory".

4. Series of three lectures, Niels Bohr Institute, Copenhagen, Denmark, 11-13 February 1976, "Semiclassical Scattering Theory ".

5. Series of three lectures sponsored by the Nobel Institute of Physics, Quantum Chemistry Institute, Uppsala, Sweden, 19-21 May 1976, "Semiclassical Scattering Theory".

6. Specially Invited Chemical Physics Lecturer, University of Florida, Gainesville, 6-11 December 1978, "Semiclassical Quantum Mechanics".

7. Sherwin-Williams Lecture, University of Illinois, Urbana, 8 May 1979, "Classical Models for Electronically Non-Adiabatic Collision Processes".

8. Lecture Series on the Theory of Chemical Reactions, Department of Theoretical Chemistry, University of Sydney, Australia, July, 1979.

9. Invited Lecture Series, (five lectures), Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China, 6-10 August 1979, "Semiclassical Theory of Molecular Collision Processes".

10. Frontiers in Chemistry Lecture, Wayne State University, Detroit, 21 April 1980, "A New Classical Model for Electronically Non-Adiabatic Collision Processes."

11. The Camille and Henry Dreyfus Lecture, University of Kansas, 2 April 1981, "An Approach to Polyatomic Reaction Dynamics".

12. Distinguished Lecture Series in Chemistry, Indiana University, Bloomington, Indiana, 24 October 1984, "*Ab Initio* Reaction Dynamics in Polyatomic Systems".

13. W. Albert Noyes Memorial Lecture, Department of Chemistry, University of Rochester, 23-27 March 1987.

14. Distinguished Summer Lecturer, Department of Chemistry, Northwestern University, Evanston, Illinois, 24-26 June 1987.

15. NATO Advanced Study Institute on Collision Theory for Atoms and Molecules, Cortona, Italy, 14-26 September 1987, "Lectures on Reactive Scattering".

16. Arthur D. Little Lectures, Massachusetts Institute of Technology, Cambridge, 9-13 November 1987.

17. NATO Advanced Study Institute on New Theoretical Concepts for Understanding Organic Reactions, Sant Feliu de Guixols, Spain, 19 June-2 July 1988, "Theoretical Models for Reaction Dynamics in Polyatomic Molecular Systems".

18. Otto M. Smith Lecture, Oklahoma State University, Stillwater, 30 March 1989, "Quantum Mechanical Reactive Scattering: Nature's Most Precise Description of a Chemical Reaction".

19. Kistiakowsky Lecturer, Harvard University, Cambridge, MA, 24 February 1994, "Beyond Transition State Theory — a Rigorous Quantum Chemical Reaction Rates".

20. Charles A. Coulson Lecture, Center for Computational Quantum Chemistry, University of Georgia, 9 November 1995, "Quantum Theory of Chemical Reaction Rates".

21. Emerson Lecture, Emory University, 2 April 1996, "Quantum Theory of Chemical Reaction Rates".

22. Joseph O. Hirschfelder Lectures, University of Wisconsin, 14-16 October 1996.

23. Israel Pollak Distinguished Lecturer, Israel Institute of Technology (Technion), Haifa, Israel 3-10 January 1997.

24. Frontiers in Chemistry Lecture, Wayne State University, Detroit, MI, 21 April 1997, "Quantum and Semiclassical Theory of Chemical Reaction Rates".

25. Distinguished JILA Visitor, University of Colorado, May 1997.

26. Spiers Memorial Lecture, Faraday Discussion on Chemical Reaction Theory, St. Andrews, Scotland, July 1998, "Quantum and Semiclassical Theory of Chemical Reactions".

27. Moses Gomberg Lecture, University of Michigan, Ann Arbor, MI 3 April 2003, "Using Semiclassical Theory to Describe Quantum Effects in Molecular Dynamics Simulations of Chemical Reactions in Complex Systems".

28. Löwdin Lecture, University of Uppsala, Sweden, 24 October 2004, "The Quantum Instanton Model for Thermal Rates of Chemical Reactions".

29. 2004 Abbott Chemistry Lecturer, University of North Dakota, Grand Forks, ND, 29-30 April 2004, "Semiclassical and Quantum Theory of Chemical Reaction Rates".

30. 2005 G. Wilse Robinson Lecturer, Texas Tech University, Lubbock, TX, 26-28 April 2005, "The Remarkable Confluence of Theoretical Chemistry" and "Using the Initial Value Representation of Semiclassical Theory to Include Quantum Effects in Classical Molecular Dynamics Simulations".

31. Frontiers in Chemical Research Lecturer, Texas A & M University, College Station, TX, 10-12 October 2005, "Using the Initial Value Representation of Semiclassical Theory to Include Quantum Effects in Classical Molecular Dynamics Simulations".

32. P. C. Cross Lecturer, University of Washington, Seattle, 16 April 2008, "Using Semiclassical Theory to Add Quantum Effects to Classical Molecular Dynamics Simulations of Complex Systems".

33. 2009 William A. Chupka Lecturer, Yale University, New Haven, CT, 15 January 2009, "Using the Initial Value Representation of Semiclassical Theory to Add Quantum Effects to Classical Molecular Dynamics Simulations".

34. 48th Fritz London Memorial Lecturer, Duke University, Durham, NC, 7 April 2009, "Quantum Effects in the Dynamics of Complex Molecular Systems".

35. 8th Miller Lecturer at the Conference on Current Trends in Computational Chemistry, Jackson State University, Jackson, MS, 30 October 2009, "Using the Initial Value Representation of Semiclassical Theory to Add Quantum Effects to Classical Molecular Dynamics Simulations".

36. Ahmed Zewail Prize Symposium, 241st American Chemical Society National Meeting, Anaheim, CA, 26-30 March 2011.

37. The Pitzer Lecture in Theoretical Chemistry, Ohio State University, Columbus, OH, 9 November 2011, "Using Semiclassical Theory to Add Quantum Effects to Classical Molecular Dynamics Simulations of Large/Complex Molecular Systems".

38. The R. B. Woodward Lecture in the Chemical Sciences, Harvard-MIT, Cambridge, MA, 9 February 2012, "Semiclassical Description of Electronically Non-Adiabatic Processes".

39. The Seventy-Ninth Edgar Fahs Smith Memorial Lecture, University of Pennsylvania, Philadelphia, PA, 15 March 2012, "Semiclassical Theory of Electronically Non-Adiabatic Dynamics".

Invited Talks at National and International Meetings:

1. American Physical Society Symposium, Seattle, Washington, 23-25 November 1970, "Quantum, Classical and Semiclassical Methods of Calculations in Atomic and Molecular Collisions".

2. Rudolph Anderson Symposium in Chemistry, Potential Surfaces: Experiment and Theory, Yale University, New Haven, Connecticut, 6-7 May 1971, "The Semiclassical Nature of Atomic and Molecular Collisions".

3. Cambridge Conference on Molecular Energy Transfer, Cambridge, England, 19-23 July 1971, "The Semiclassical Nature of Atomic and Molecular Collisions".

4. American Chemical Society Symposium on Classical Dynamics, Washington, D.C., 12-17 September 1971, The Classical S-Matrix for Atomic and Molecular Collisions".

5. Conference on Theoretical Chemistry, Boulder, Colorado, 26-30 June 1972, "Reactive Tunneling in H + H2 Collisions".

6. German Symposium on Bimolecular Reactions as Elementary Processes, Oberwohlfach, Germany, 27-29 September 1972, "Semiclassical Theory of Inelastic and Reactive Scattering".

7. Faraday Discussion on Molecular Beams, London, England, 16-18 April 1973, "Partial Averaging in Classical S-Matrix Theory".

8. VIIIth International Conference on the Physics of Electronic and Atomic Collisions, Belgrade, Yugoslavia, 16-20 July 1973, "Semiclassical Methods in Reactive and Non-Reactive Collisions".

9. Symposium on Topics in Inelastic and Reactive Molecular Collisions, Weizmann Institute of Science, Rehovot, Israel, 21 August 1973, "The Classical S-Matrix in Molecular Collision Theory".

10. German Summer School on the Theory of Molecular Collisions, Garsam Inn, Germany, 2-15 September 1973, "Semiclassical Scattering Theory".

11. Atlas Laboratory Symposium, Quantum Chemistry – The State of The Art, Oxford, England, 8-10 April 1974, "Classical S-Matrix for Classically Forbidden Collision Processes".

12. Visiting Professor, Department of Physics, Bielefeld University, Germany, summer 1974.

13. Conference on the Dynamics of Molecular Collisions, Santa Cruz, California, 29 July-2 August 1974, "Theories of Reactive Scattering".

14. IIIrd International Workshop on Gross Properties of Nuclei, Hirschegg, Austria, 13-18 January 1975, "Semiclassical Methods in Inelastic and Reactive Scattering".

15. Organizer and participant in a Workshop on "Collisions on Potential Energy Surfaces of Excited States", Orsay, France, 7 July-5 September 1975.

16. 2nd International Congress of Quantum Chemistry, New Orleans, Louisiana, 19-24 April 1976, "Recent Developments in Semiclassical Mechanics".

17. Faraday Discussion on Potential Energy Surfaces, University of Sussex, Brighton, England, 8-10 September 1976, "Semiclassical Theory for Non-Separable Systems".

18. Germany Symposium on Energy Transfer Processes in Chemical Reactions, Konigstein, Germany, 13-16 September 1976, "Unified Statistical Model for 'Complex' and 'Direct' Reaction Mechanisms".

19. Canadian Symposium on Theoretical Chemistry, Fredericton, Canada, 19-25 June 1977, "Recent Developments in Semiclassical Scattering Theory".

20. Gordon Conference on Few Body Problems in Chemistry and Physics, Meriden, New Hampshire, 15-19 August 1977, "Semiclassical Theory of Collision Processes".

21. ACS National Meeting, Anaheim, California, 12-17 March 1978, "Infrared Laser Induced Chemical Reactions".

22. VIIth Soviet National Conference on Quantum Chemistry, Novosibirsk, USSR, 28 June-1 July 1978, "Semiclassical Theory of Molecular Collision Processes".

23. Eleventh International Symposium on Rarefied Gas Dynamics, Cannes, 3-8 July 1978, "Laser Induced Chemical Reactions".

24. Gordon Research Conference on Atomic and Molecular Interactions, Brewster Academy, Wolfeboro, New Hampshire, 24-28 July 1978, "A New Classical Model for Electronically Non-Adiabatic Collision Processes".

25. ACS National Meeting, Honolulu, 1-6 April 1979, "Recent Advances in the Semiclassical Theory of Electronically Non-Adiabatic Processes".

26. International Symposium on Reaction Dynamics and Energy Transfer in Systems with Many Accessible States, Munich, 26-30 March, 1979, "Recent Progress in the Semiclassical Theory of Non-Adiabatic Collision Processes".

27. Symposium on Atomic and Molecular Science, Taipei, Taiwan, 23-25 August 1979, "Laser Enhancement of Chemical Reactions".

28. International Symposium on Atomic, Molecular and Solid-State Theory, Collision Phenomena, and Computational Quantum Chemistry, in honor of Professor E. Bright Wilson, Daytona Beach, 10-15 March, 1980, "Reaction Path Hamiltonian for Polyatomic Molecules".

29. Symposium honoring Henry Eyring in his 80th year, Northwest Rocky Mountain Meeting of the American Chemical Society, Salt Lake City, 12-14 June, 1980, "Reaction Path Hamiltonian for Polyatomic Molecules".

30. Bielefeld Workshop on Energy Scrambling in Molecules, Bielefeld, Germany, 3-12 July, 1980, Model Studies of Mode-Specificity in Unimolecular Rate Constants".

31. Symposium on Potential Energy Surfaces and Dynamics Calculations, American Chemical Society National Meeting, Las Vegas, 24-29 August 1980, "Reaction Path Hamiltonian and its Application to Unimolecular Reaction Dynamics".

32. Conference on Theoretical Approaches to Dynamics, Austin, Texas, 1-4 March 1981, "Classical Valence Bond Model for Electronically Non-Adiabatic Collision Processes".

33. Sanibel Symposium on Atomic, Molecular, and Solid State Theory, Collision Phenomena, and Computational Quantum Chemistry, Daytona Beach, 8-13 March 1981, "Classical Valence Bond Model for Electronically Non-Adiabatic Collision Processes".

34. American Conference on Theoretical Chemistry, Boulder, Colorado, 22-26 June 1981, "A Reaction Path Model for Polyatomic Reaction Dynamics:" Tunneling, Vibrational Inelasticity, and Mode-Specificity".

35. Gordon Research Conference on Molecular Energy Transfer, Wolfeboro, New Hampshire, 29 June - 3 July 1981, "To What Extent Can Current Theoretical Models Accurately Describe the Dynamics of Electronic Energy Transfer in Gases?"

36. Austrian Workshop for Theoretical Chemistry, Mariapfarr, Austria, 16-19 February 1982, "On the Relation of Quasiperiodic on Chaotic Classical Mechanics to Semiclassical Eigenvalues of Polyatomic Molecules and to Mode-Specificity in Unimolecular Reaction Dynamics".

37. ACS National Meeting, Kansas City, Missouri, 12-17 September 1982, "Dynamical Effects of Reaction Path Symmetry".

38. International Conference on Photochemistry and Photobiology, Alexandria, Egypt, 5-10 January 1983, "On the Question of Mode-Specificity in Unimolecular Reaction Dynamics".

39. Symposium on Molecular Scattering Theory and Quantum Chemistry in honor of Professor David Bates, Palm Coast, Florida, 3-5 March, 1983, "Mode-Specificity in Unimolecular Reaction Dynamics".

40. International Workshop on Primary Photophysical Processes, 16-21 October 1983, Herrsching, West Germany, "Reaction Dynamics in Polyatomic Systems".

41. Sixth International Conference on Lasers and Applications, San Francisco, California, 12-16 December, 1983, "Classical and Semiclassical Methods for the Interaction of Molecular Systems with Strong Radiation Fields".

42. ACS National Meeting, St. Louis, Missouri, 8-13 April 1984, "Vinylidene: Potential Energy Surface and Unimolecular Reaction Dynamics".

43. American Conference on Theoretical Chemistry, Jackson, Wyoming, 15-20 June 1984, "Recent Developments in the Theory of Quantum Mechanical Reactive Scattering".

44. 8th International Symposium of Gas Kinetics, Nottingham (England), 16-21 July 1984, "Vinylidene: Potential Energy Surface and Unimolecular Reaction Dynamics".

45. International Workshop on Chemical Reaction Dynamics, Cambridge, England, 13-16 July 1984, "Some Recent Developments in Quantum Mechanical Reactive Scattering".

46. 5th European Conference on Dynamics of Molecular Collisions, Jerusalem, Israel, 3-7 September 1984, "Recent Progress in Quantum Mechanical Reactive Scattering".

47. Nobel Laureate Symposium, International Chemical Congress of Pacific Basin Societies, Honolulu, Hawaii, 16-21 December 1984, "Reaction Paths and Reaction Surfaces: an Approach to Reaction Dynamics in Polyatomic Systems".

48. Symposium on Semiclassical Descriptions of Atomic and Nuclear Collisions (Centenary of Niels Bohr), Copenhagen, 25-28 March 1985, "Classical-Limit Quantum Mechanics".

49. International Colloquium on Recent Advances in Molecular Reaction Dynamics, Aussois, France, 10-14 June 1985, "Some Recent Initiatives in Quantum Mechanical Reactive Scattering".

50. CECAM/NATO Advanced Research Workshop, Orsay, France, 17-28 June 1985, "Reaction Path Models for Polyatomic Reaction Dynamics – from Transition State Theory to Path Integrals".

51. Conference on the Dynamics of Molecular Collisions, Snowbird, Utah, 14-19 July 1985, "Overview of Reactive Scattering Theory".

52. Conference on Path Integrals from meV to MeV, Bielefeld, West Germany, 5- 9 August 1985, "Direct Calculation of Boltzmann Rate Constants by Path Integral Methods".

53. Symposium on Spectroscopy and Dynamics of Highly Vibrationally and Rotationally Excited Polyatomic Molecules, Chicago (National ACS Meeting), 9-13 September 1985, "Polyatomic Reaction Dynamics via a Reaction Surface Hamiltonian".

54. Symposium on Tunneling in Chemical Reactions, Chicago (National ACS Meeting), 8-13 September 1985, "'Direct' Calculation of Quantum Mechanical Reaction Rate Constants".

55. International CECAM Workshop on Intramolecular Vibrational Redistribution and Quantum Chaos, Rochester, New York, 3-5 October 1985, "Dynamics of Hydrogen Atom Transfer in Vinylidene and Malonaldehyde".

56. Nobel Laureate Signature Award Symposium, National ACS Meeting, New York, 13-18 April 1986, "Classical Models for Electronic Degrees of Freedom".

57. Jerusalem Symposium on Tunneling, 5-8 May 1986, "Reaction Paths and Reaction Surfaces for Hydrogen Atom Transfer Reactions".

58. Canadian Chemical Conference, Saskatoon, 1-4 June 1986, "Reaction Paths and Surfaces, and their Application to Reaction Dynamics in Polyatomic Systems".

59. NATO Advanced Research Workshop on Stochasticity and Intramolecular Redistribution Energy, Paris, 23 June 4 July 1986, "A New Strategy for Polyatomic Reaction Dynamics".

60. Symposium on State-to-State Chemistry, National ACS Meeting, Anaheim, California, 7-12 September 1986, "State Specific Reaction Dynamics in Polyatomic Molecules".

61. International Symposium "Chaos and Related Non-Linear Phenomena - Where Do We Go From Here?", 13-19 December 1986, Jerusalem, Israel, "Some New Approaches to Polyatomic Reaction Dynamics".

62. 14th Symposium on Quantum Chemistry of the Academy of Sciences of the German Democratic Republic, Kuhlungsborn, East Germany, 16-20 March 1987, "Recent Developments in Quantum Mechanical Reactive Scattering".

63. Symposium on Few-Body Systems and Multiparticle Dynamics, American Physical Society, Crystal City, Virginia, 20-24 April 1987, "Basis Set and Path Integral Methods for the Reactive Flux Correlation Function".

64. American Conference on Theoretical Chemistry, Gull Lake, Minnesota, 26-31 July 1987, "New Techniques in Time Dependent Dynamics".

65. 10th International Conference on Molecular Energy Transfer, Emmetten, Switzerland, 23-28 August 1987, "Hydrogen Atom Transfer in Polyatomic Molecules – a New Approach".

66. Faraday Discussion on Dynamics of Elementary Gas Phase Reactions, Birmingham, England, 14-16 September 1987, "The Reactive Flux Correlation Function for Collinear Reactions: H+H2, Cl+HCl, and F+H_2".

67. Faraday Symposium on Molecular Vibrations, Reading, England, 15-16 December 1987, "A New (Cartesian) Reaction Path Model for Dynamics in Polyatomic Systems".

68. Faraday Division High Resolution Spectroscopy Group, Reading, England, 17-18 December 1987, "Quantum Dynamics of Chemical Reactions".

69. Symposium on New Methods for Structures and Dynamics of Chemical Systems, American Physical Society National Meeting, New Orleans, 21-25 March 1988, "S-Matrix Version of the Kohn Variational Principle and its Application to Reactive Scattering".

70. Third Chemical Congress of North America and 195th ACS National Meeting, Toronto, Canada, 5-10 June 1988, "Hydrogen Atom Transfer in Polyatomic Molecules".

71. Sixth International Congress on Quantum Chemistry, Jerusalem, Israel, 21- 25 August 1988, "Quantum Theory of Chemical Dynamics: Reactive Scattering and Path Integrals".

72. Sanibel Symposium on Atomic, Molecular, and Condensed Matter, St. Augustine, FL, 1-8 April 1989, "Quantum Reactive Scattering via the S-Matrix Version of the Kohn Variational Principle".

73. Symposium on Relaxation and Dynamics in Complex Media, American Chemical Society National Meeting, Dallas, 9-14 April 1989, "Diabatic Reaction Path Hamiltonian".

74. Conference on Chaos and Quantum Mechanics, Institute for Theoretical Physics, Santa Barbara, 26-29 June 1989, "Topics in Semiclassical Scattering Theory".

75. International Conference on the Physics of Electronic and Atomic Collisions, New York, 26 July-1 August 1989, "Recent Developments in the Theory and Application of Quantum Scattering Theory for Chemical Reactions".

76. NATO Advanced Study Institute on Computational Advances in Organic Chemistry, Altinoluk, Turkey, 30 July-12 August 1989, " Reaction Dynamics of Polyatomic Molecular Systems".

77. Workshop on Quantum Simulations of Condensed Matter Phenomena, Center for Non-Linear Studies, Los Alamos, 8-11 August 1989, "Semiclassical and Quantum Mechanical Rate Constants for Chemical Reactions".

78. 3rd International Symposium on Elementary Processes and Chemical Reactivity, Liblice, Czechoslovakia, 4-8 September 1989, "Recent Developments in the Theory of Quantum Mechanical Reactive Scattering and its Application to Simple Chemical Reactions".

79. Adriatico Research Conference on Computation in Physics and Physics in Computation, International Centre for Theoretical Physics, Trieste, Italy, 5-8 September 1989, "Recent

Developments in the Theory of Quantum Mechanical Reactive Scattering and its Application to Simple Chemical Reactions".

80. Symposium on Novel Methods for Probing the Transition State (National ACS Meeting), Miami Beach, 10-15 September 1989, "Photodissociation and Continuum Resonance Raman Cross Sections from S-Matrix Kohn Scattering Calculations; Photoelectron Spectrum of $F^- - H_2 + hn \rightarrow F + H_2$, $HF+H + e^-$".

81. Symposium on Chemical Rate Processes in Condensed Phases: 100 Years After Arrhenius (National ACS Meeting), Miami Beach, 10-15 September 1989, "Hydrogen Atom Transfer Reactions in Polyatomic Molecules - Classical and Quantum Approaches".

82. Workshop on the Quantum Theory of Reactive Scattering, University of Cambridge, U.K., 25-27 March 1990, "S-Matrix Version of the Kohn Variational Principle: Recent Developments in Methodology and Applications".

83. Awards Symposium, ACS National Meeting, Boston, 22-27 April 1990, "Chemical Reaction Dynamics in Simple and Complex Systems".

84. Symposium on Large Amplitude Motions in Vibrationally Excited Molecules, ACS National Meeting, Boston, 22-27 April 1990, "Latest Developments in Quantum Mechanical Reactive Scattering Theory and its Application".

85. Symposium on Classical and Quantal Simulations for Reactive and Solvation Dynamics and Their Critical Experimental Tests, ACS National Meeting, Boston, 22-27 April 1990, "Some New Theoretical Methods for Reaction Dynamics in Polyatomic Systems: an Empirical Valence Bond Potential Surface and a Semiclassical Tunneling Model for Trajectory Simulations."

86. Second World Association of Theoretical Organic Chemists World Congress, Toronto, Canada, 8-14 July 1990, "A Transition State Theory for the Probability Distribution of State-Specific Unimolecular Rate Constants".

87. Frontiers of Theoretical Chemistry Symposium, 73rd Canadian Chemical Congress, Halifax, Nova Scotia, 15-20 July 1990, "Quantum Mechanical Reactive Scattering: Its Recent Developments and Applications to Simple Chemical Reactions".

88. American Conference on Theoretical Chemistry, 30 July-3 August 1990, San Diego, "Quantum Reactive Scattering".

89. Parallel Computing for Chemical Reactivity, Perugia, Italy, 31 August-1 September 1990, "Recent Developments in Quantum Mechanical Reactive Scattering Theory and its Application".

90. 8th European Conference on Dynamics of Molecular Collisions, Bernkastel-Kues, Germany, 10-14 September 1990, "Quantum Theory of Reactive Scattering".

91. NATO Advanced Research Workshop: Rate Processes in Dissipative Systems – 50 Years After Kramers, Tutzing, Germany, 10-13 September 1990, "Some New Aspects of Quantum Transition State Theory".

92. Kasha Conference on Proton Transfer Dynamics in Chemistry, Biology, and Physics, 6-9 January 1991, Tallahassee, Florida, "Some New Developments and Aspects of Transition State Theory".

93. Meeting on Chemical Dynamics in the Time Domain, 20-22 March 1991, Oxford, England, "Quantum Reactive Flux Correlation Functions – Some New Developments".

94. American Physical Society Spring Meeting, 22-25 April 1991, Washington, D.C., "Complex Kohn Variational Treatment of Reactive Scattering: Recent Advances and Applications".

95. Canadian Symposium on Computational Chemistry, 19-22 May 1991, Orford, Quebec, "Recent Developments and Applications of Quantum Mechanical Reactive Scattering".

96. NATO Advanced Research Workshop on the Role of Computational Models and Theories in Biotechnology, 13-19 June 1991, Saint Feliu de Guixols, Spain, "Reaction Dynamics in Polyatomic Molecular Systems: Some Approaches for Constructing Potential Energy Surfaces and Incorporating Quantum Effects in Classical Trajectory Simulations".

97. Meeting on Recent Methodological Advances in Dynamical and Correlation Calculations, 27-29 June 1991, Peyresq, France, "Some Recent Developments in Quantum Mechanical Reactive Scattering and in Quantum Transition State Theory".

98. Conference on the Dynamics of Molecular Collisions, 7-12 July 1991, Lake George, New York, "Quantum Theory of Chemical Reactions: Some Recent Developments in Reactive Scattering and in Transition State Theory".

99. NATO Advanced Study Institute on Methods in Computational Molecular Physics, 21 July-3 August 1991, Bad Windsheim, Germany, "Scattering Calculations Using Basis Set Expansions (4 Lectures)".

100. 4th Topsoe Summer School on Time Dependent Methods in Quantum Mechanics, 19-23 August 1991, Copenhagen, "Semiclassical Theory and Feynman Path Integrals".

101. Symposium on Comparison of *Ab Initio* Quantum Chemistry with Experiment (North American Chemical Congress), 25-30 August 1991, New York, "Quantum Theory of Chemical Reactions: Reactive Scattering and Transition State Theory".

102. 42nd Okazaki Conference, Molecular Science: Current Status and Future Prospects, 7-9 January 1992, Okazaki, Japan, "Recent Developments and Future Prospects in Rigorous Quantum Mechanical Descriptions of Chemical Reactions".

103. Joint US-Israel Workshop on Computational Chemistry, Berkeley, CA, 28-30 January 1992, "A Discrete Variable Representation for Quantum Reactive Scattering via the S-Matrix Kohn Method".

104. NATO Advanced Research Workshop on Time-Dependent Quantum Molecular Dynamics: Experiments and Theory, 30 March - 3 April, Snowbird, UT, "Quantum Mechanical Reactive Flux Correlation Functions".

105. Symposium of Frontiers of Molecular Simulations, ACS National Meeting, Washington, DC, 24-28 August 1992, "Direct Calculation of the Cumulative Reactive Probability".

106. NATO Advanced Research Workshop on Grid Methods in Atomic and Molecular Quantum Calculations, Corsica, France, 27 September - 3 October 1992, "Use of Discrete Variable Representative and Absorbing Boundary Conditions to Calculate State-to-State and Cumulative Reaction Probabilities".

107. Latsis Symposium on Intramolecular Kinetics and Reaction Dynamics, ETH Zürich, Switzerland, 20-23 October 1992, "Some Recent Developments Related to Quantum Mechanical Transition State Theory".

108. NATO Advanced Research Workshop on Orientation and Polarization Effects in Chemical Reaction Dynamics, Assisi, Italy, 20-25 November 1992, "Direct Calculation of Cumulative and State-to-State Reaction Probabilities".

109. Femtosecond Chemistry — The Berlin Conference, Berlin, Germany, 1-4 March 1993, "Cumulative and State-to-State Reaction Probabilities".

110. Symposium on Elementary to Complex Systems, American Physical Society Meeting, Seattle, WA, 22-26 March 1993, "Calculations of Cumulative and State-to-State Reaction Probabilities via an Absorbing Boundary Condition Green's Function".

111. 76th Canadian Society for Chemistry Conference, Sherbrooke, Quebec, 30 May - 3 June 1993, "Beyond Transition State Theory — a Rigorous Theory of Chemical Reaction Rates".

112. 8th American Conference on Theoretical Chemistry, Rochester, NY, 28 June - 2 July 1993, "Beyond Transition State Theory — a Rigorous Theory of Chemical Reaction Rates".

113. 14th European Conference on Few-Body Problems in Physics, Amsterdam, 22-27 August 1993, "Recent Advances in the Quantum Theory of Chemical Reaction Rates".

114. Nagoya Symposium on Chemical Reaction Theory, Nagoya, Japan, 15-18 November 1993, "Beyond Transition State Theory a Rigorous Quantum Theory for Chemical Reaction Rates".

115. Symposium on Future Challenges in Molecular Physics, Göttingen, Germany) 25-27 November 1993, "Chemical Reaction Dynamics — Where Are We and Where Are We Going?"

116. Awards Symposium, ACS National Meeting, San Diego, CA, 12-15 March 1994, "Beyond Transition State Theory, A Rigorous Quantum Theory for Chemical Reaction Rates".

117. Symposium on Quantum Reactive Scattering, American Physical Society National Meeting, 18-22 April 1994, Crystal City, VA, "Semiclassical Corrections to Quantum Mechanical Scattering".

118. Workshop on Quantum Mechanical Treatment of Atom Exchange Processes in Molecular Collisions, Harvard-Smithsonian Center for Astrophysics, Cambridge, MA, 30 June - 2 July 1994, "Direct Calculation of the Cumulative Reaction Probability".

119. International Discussion Meeting of the Deutsche Bunsengesellschaft für Physikalische Chemie, Molecular Spectroscopy and Molecular Dynamics: Theory and Experiment, Grainau, Bavarian Alps, Germany, 28 August - 1 September 1994, "A Random Matrix/Transition State Model for the Probability Distribution of State-Specific Unimolecular Decay Rates".

120. NATO Advanced Study Institute on Frontiers of Chemical Dynamics, Antalya, Turkey, 5-17 September 1994, "Chemical Reaction Rate Theory — From Transition State Theory to Rigorous Quantum Approaches".

121. Welch Conference on Chemical Dynamics of Transient Species, Houston, TX, 24-25 October 1994, "Quantum Theory of Chemical Reactions".

122. Conference on Stereodynamics and Active Control in Chemical Reactions, Gif-sur-Yvette, France, 11-15 December 1994, "Random Matrix/Transition State Theory Model for the Probability Distribution of Unimolecular Decay Rates".
123. Sixth Australian Conference on Chemical Reaction Dynamics, Canberra, Australia, 12-16 February 1995, "Quantum Theory of Chemical Reaction Rates".

124. XIVth International Conference on Molecular Energy Transfer, Bamberg, Germany, 25-30 June 1995, "Quantum Theory of Chemical Reaction Rates".

125. Conference on the Dynamics of Molecular Collisions, 16-21 July 1995, Pacific Grove, California, "Quantum Theory of Chemical Reaction Rates".

126. 12th Canadian Symposium on Theoretical Chemistry, Fredericton, Canada, 6-11 August 1995, "Quantum Theory of Chemical Reaction Rates".

127. 35th International Union of Pure and Applied Chemistry (IUPAC) Congress, Istanbul, Turkey, 14-19 August 1996, "Semiclassical Corrections for Quantum Reaction Dynamics".

128. Conference on Reaction Dynamics, Nottingham, England, 29 August - 1 September 1995, "Quantum and Semiclassical Theories for Chemical Reactions".

129. 4th Conference on Current Trends in Computational Chemistry, Vicksburg, Mississippi, 3-4 November 1995, "Quantum Theory of Chemical Reaction Rates".

130. XXth Solvay Conference on Chemistry, Brussels, Belgium, 28 November - 2 December 1995, "Quantum and Semiclassical Theories of Chemical Reaction Rates".

131. Faraday Discussion on Unimolecular Reaction Dynamics, Oxford, England, 19-21 December 1995, "On the Quantum Mechanical Theory of Collisional Recombination Rates. II. Beyond the Strong Collision Approximation".

132. Symposium on Transition States, American Chemical Society National Meeting, New Orleans, LA, 24-19 March 1996, "Quantum Theory of Chemical Reactions Rates".

133. 11th European Conference on Dynamics of Molecular Collisions (MOLEC), Hotel Nyborg Strand, Denmark, 1-6 September 1996, "Quantum and Semiclassical Reaction Dynamics".

134. 14th International Symposium on Gas Kinetics, Leeds, England, 7-12 September 1996, "Quantum Theory of Collisional Recombination".

135. Charles Coulson Summer School, Oxford, England, 8-18 September 1996, "Lectures on Quantum Scattering Theory".

136. Conference on Stereodynamics of Chemical Reactions, 1-5 December 1996, Bielefeld, Germany, "Quantum and Semiclassical Theory of Chemical Reaction Rates".

137. Euroconference on Computer Simulation of Rare Events and the Dynamics of Classical and Quantum Condensed Phase Systems, 7-18 July 1997, Lerici, Italy, "A Revival of Interest in Semiclassical Methods for Simulating Chemical Dynamics: The Initial Value Representation".

138. XXth International Conference on the Physics of Electronic and Atomic Collisions, 23-29 July 1997, Vienna, Austria, "Quantum and Semiclassical Descriptions of Reactive Scattering and Reaction Rates".

139. 5th Chemical Congress of North America, 11-15 November 1997, Cancun, Mexico, "Semiclassical Initial Value Representation for Electronically Non-Adiabatic Dynamics".

140. Symposium on Combustion Processes, Am. Chem. Soc. National Meeting, 29 March - 3 April 1997, Dallas, TX, "Quantum and Semiclassical Theory of Chemical Reaction Rates".

141. Faraday Discussion on Chemical Reaction Theory, 1-3 July 1998, St. Andrews, Scotland, "Quantum Theory of Chemical Reaction Dynamics".

142. Celebration of 20 Years of the Subdivision of Theoretical Chemistry, American Chemical Society National Meeting, 23-27 August 1998, Boston, MA, "Quantum and Semiclassical Theory of Chemical Reactions Rates".

143. International CECAM Workshop on Computational Methods for Studying the Dynamics of Quantum Systems, 28 September - 1 October 1998, Lyon, France, "Semiclassical Description of Chemical Reaction Rates".

144. XIVth Winter School Workshop on Theoretical Chemistry, 14-17 December 1998, Helsinki, Finland, four lectures on "Quantum and Semiclassical Theory of Chemical Reaction Dynamics".

145. Winter School and Workshop on Resonance Phenomena in Chemical Reactions, 14-19 February 1999, Haifa, Israel, "Reaction Rate Theory".

146. Invited lecture series, National University of Singapore, 9-17 April 1999, Singapore, "Quantum and Semiclassical Theory of Chemical Reaction Dynamics".

147. International Workshop and Seminar on Dynamics of Complex Systems, 11-15 May 1999, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany, "Semiclassical Approach for Including Quantum Effects in Simulations of Complex Molecular Systems".

148. In the Frontiers of Quantum Chemistry and Chemical Reactions, 21-22 May 1999, Emory University, Atlanta, GA, "Semiclassical Approximations for Quantum Reaction Rates".

149. XVI International Conference on Molecular Energy Transfer. 20-25 June 1999, Assisi, Italy, "Recent Developments in Semiclassical Approximations for Quantum Dynamics in Complex Molecular Systems."

150. Workshop on Quantum Reactive Scattering, 25-27 June 1999, Perugia, Italy, "Flux Correlation Functions via the Semiclassical Initial Value Representation".

151. American Conference on Theoretical Chemistry, 27 June - 2 July 1999, Boulder, CO, "Recent Developments in Semiclassical Theory for Reaction Dynamics."

152. Symposium on Photo-Dynamics and Reaction Dynamics of Molecules, 31 July - 2 August 1999, Okazaki, Japan, "On Use of the Semiclassical Initial Value Representation for Including Quantum Effects in Molecular Dynamics Simulations".

153. American Chemical Society National Meeting, Electronically Non-Adiabatic Symposium, 22-26 August, 1999, New Orleans, LA, "Electronically Non-Adiabatic Dynamics via the Semiclassical Initial Value Representation".

154. III Congress of the International Society for Theoretical Chemical Physics, 8-13 November 1999, Mexico City, Mexico, "Use of the Semiclassical Initial Value Representation to Include Quantum Effects in Molecular Dynamics Simulations".

155. American Physical Society National Meeting, Symposium on Experimental and Theoretical Frontiers in Molecular Quantum Dynamics, 19-23 March 2000, "Semiclassical Initial Value Representation for Including Quantum Effects in Classical Molecular Dynamics Simulations".

156. International Workshop on Quantum Dynamics in Terms of Phase-Space Distributions, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany, 22-26 May 2000, "Semiclassical Approximations for Molecular Dynamics — What Can and Cannot Describe Quantum Effects".

157. DYNAM 2000 — Reactive and Non-reactive Quantum Dynamics, 31 May - 3 June 2000, Arcachon, France, "The Semiclassical Initial Value Representation: a Way to Include Quantum Effects into Molecular Dynamics Simulations".

158. Fourth Asian International Seminar on Atomic and Molecular Physics, 13-18 October 2000, Taipei, Taiwan, "Including Quantum Effects into Molecular Dynamics Simulations via the Semiclassical Initial Value Representation".

159. Pacific Chem Symposium on New Frontiers in Chemical Reaction Dynamics, 14-19 December 2000, Hawaii, "Semiclassical Description of Diffraction and its Quenching by an Environment".

160. Fourth Symposium on Molecular Physical Chemistry, 11-13 January 2001, Kumamoto, Japan, "Including Quantum Effects in Classical Molecular Dynamics Simulations via the Semiclassical Initial Value Representation".

161. 38th Congress of the International Union of Pure and Applied Chemistry, Frontiers in Chemistry, 1-6 July 2001, Brisbane, Australia, "Using Semiclassical Theory to Include Quantum Effects into Classical Molecular Dynamics Simulations".

162. Charles Coulson Summer School, Oxford, England, 14-24 August 2001, "Lectures on Semiclassical Theory".

163. Annual Meeting of the American Institute of Chemical Engineers, Reno, NV, 17-20 September 2001, "Using Semiclassical Theory to Include Quantum Effects into Classical Molecular Dynamics Simulations".

164. 10th Conference on Current Trends in Computational Chemistry, Jackson, MS, 1-3 November 2001, "Using Semiclassical Theory to Add Quantum Effects to Classical Molecular Dynamics Simulations".

165. CCP6 Workshop on Wide-Amplitude Rovibrational States in Polyatomic Molecules, 15-18 December 2001, University of Manchester, UK, "Using Semiclassical Theory to Include Quantum Effects into Classical Molecular Dynamics Simulations".

166. Spring School on Semiclassical and Quantum Multibody Problems, University of Warwick, UK, 18-22 March 2002, "Semiclassical Methods in Chemical Dynamics (three lectures)".

167. 2nd Southern School on Computational Chemistry, 22-23 March 2002, Orange Beach, AL, "Using Semiclassical Theory to Include Quantum Effects in Classical Molecular Dynamics Simulations of Chemical Processes".

168. International Seminar and Workshop on Quantum Dynamics Concepts: from Diatomics to Biomolecules, 15-19 April 2002, Max-Planck-Institut, Dresden, Germany, "Implementing the Semiclassical Initial Value Representation: Filtering, Phase Distributions, and Time-Averaging".

169. CECAM (European Center for Atomic and Molecular Calculations) Workshop on Methods for Computer Simulation of Non-Adiabatic Charge Transfer Processes in the Condensed Phase, Lyon, France, 22-24 April 2002, "Using the Semiclassical Initial Value Representation to Add Quantum Effects to Classical Molecular Dynamics Simulations".

170. Conference on Quantum Dynamics of Condensed Phase Systems, 24-28 June 2002, Rethimno, Crete, "Using Semiclassical Theory to Add Quantum Effects to Classical Molecular Dynamics Simulations of Complex Processes".

171. 4th International Congress on Theoretical Chemical Physics, 9-16 July 2002, Marly-le-Roi, France, "Using Semiclassical Theory to Include Quantum Effects in Classical Molecular Dynamics Simulations".

172. Conference on the Kinetics and Dynamics of Elementary Gas Phase Reactions, 16-18 September 2002, University of Birmingham, UK, "Using Semiclassical Theory to Include Quantum Effects in Classical Molecular Dynamics Simulations".

173. Trends in Theoretical Chemistry, 17-19 January 2003, Calcutta, India, "Using Semiclassical Theory to Include Quantum Effects in Classical Molecular Dynamics Simulations".

174. 50th Annual Western Spectroscopy Association Conference, 29-31 January 2003, Asilomar, CA, "Using Semiclassical Theory to Include Quantum Effects in Classical Molecular Dynamics Simulations".

175. American Chemical Society National Meeting, Awards Symposium, 23-27 March 2003, New Orleans, LA, "Using Semiclassical Theory to Add Quantum Effects to Classical Molecular Dynamics Simulations".

176. Frontiers in Computational Chemistry, 12 April 2003, Emory University, Atlanta, GA, "Using Semiclassical Theory to Add Quantum Effects to Classical Molecular Dynamics Simulations".

177. NATO Advanced Research Workshop on the Dynamics of Elementary Chemical Reactions, 8-12 June 2003, Balatonfold var, Hungary, "Using the Semiclassical Initial Value Representation to Add Quantum Effects to Classical Molecular Dynamics Simulations".

178. Joint SIAM (Society for Industrial and Applied Mathematics) – CRM (Centre de Recherches Mathematiques) Symposium on "Numerical Methods for Multidimensional Schrödinger Equations," 16-20 June 2003, Montreal, Canada, "Using the Semiclassical Initial Value Representation to Add Quantum Effects to Classical Molecular Dynamics Simulations".

179. International Complutense Seminar on Quantum Reactive Scattering, 20-23 June 2003, El Escorial, Spain, "Quantum Instanton Approximation for Thermal Rate Constants of Chemical Reactions".

180. Second European School on Computational Chemistry, Reaction and Molecular Dynamics, 23-29 June 2003, Barcelona, Spain, "Semiclassical Dynamics".

181. Multidimensional Quantum Reaction Dynamics, 16-17 July 2003, Berlin, Germany, "Semiclassical Theory of Chemical Reaction Rates".

182. Moscow-Chernogolovka Workshop, 4-5 August 2003, Moscow, Russia, "Using the Semiclassical Initial Value Representation to Add Quantum Effects to Classical Molecular Dynamics Simulations".

183. G. D. Billing Memorial Symposium, 10-13 August 2003, Copenhagen, Denmark, "Quantum Instanton Approximation for Thermal Rate Constants of Chemical Reactions".

184. 39th Symposium on Theoretical Chemistry, Molecular Spectroscopy and Dynamics, 28 September - 2 October 2003, Gwatt, Switzerland, "Using the Initial Value Representation of Semiclassical Theory to Add Quantum Effects to Classical Molecular Dynamics Simulations".

185. Löwdin-Forelasningar 2003, Quantum Chemistry - Theory, Models, and Computations Symposium, 22-26 October 2003, Uppsala, Sweden, "The Quantum Instanton Model for Thermal Rates of Chemical Reactions".

186. Theory and Applications of Computational Chemistry Conference, 15-20 February 2004, Gyeongju, Korea, "The Quantum Instanton Model for Thermal Rates of Chemical Reactions".

187. 44th Sanibel Symposium, 28 February - 5 March 2004, St. Augustine, Florida, "The Quantum Instanton Model for Thermal Rates of Chemical Reactions".

188. Joint Harvard-MIT-BU Theoretical Chemistry Seminar, 17 March 2004, Cambridge, MA, "Quantum Theory of Chemical Reaction Rates".

189. Theory of Chemical Dynamics, a Symposium in Honour of Professor Mark S. Child, 25-26 March 2004, University of Oxford, UK, "The Quantum Instanton Model for Thermal Rates of Chemical Reactions".

190. 227th American Chemical Society National Meeting (Symposium on Mixed Quantum, Classical and Semiclassical Dynamics), 28-31March 2004, Anaheim, CA, "The Quantum Instanton Model for Thermal Rates of Chemical Reactions".

191. 2004 Abbott Chemistry Lectures, 29-30 April 2004, University of North Dakota, Grand Forks, ND, "Semiclassical and Quantum Theory of Chemical Reaction Rates".

192. Physical Chemistry Seminar, 20 May 2004, Brown University, Providence, RI, "Using the Initial Value Representation of Semiclassical Theory to Add Quantum Effects to Classical Molecular Dynamics Simulations".

193. 25th Annual Department of Energy, Combustion Research Conference, 1-4 June 2004, Warrenton, VA, "The Quantum Instanton Model for Thermal Rates of Chemical Reactions".

194. 15th Canadian Symposium on Theoretical Chemistry, 10-14 July 2004, Sainte-Adèle, Québec, Canada, "Beyond the Quantum Instanton Model: Computing Thermal Reaction Rates from Higher Derivatives of the Zero Time Flux Correlation Function".

195. Molecular Quantum Mechanics: The No Nonsense Path to Progress, 24-29 July 2004, Cambridge University, UK, "Beyond the Quantum Instanton: A More Rigorous Approach to Quantum Reaction Rates".

196. 228th American Chemical Society National Meeting, 22-26 August 2004, Philadelphia, PA, "Semiclassical Correction to Quantum Energy Levels".

197. CECAM Workshop: Quantum MD for Condensed Phase Applications, 16-18, September 2004, Lyon, France "Beyond the Quantum Instanton Model: Computing Thermal Reaction Rates from Higher Derivatives of the Zero Time Flux Correlation Function".

198. Theoretical Chemistry Seminar, 28 October 2004, University of Illinois at Urbana-Champaign, "Using Semiclassical Theory to Include Quantum Effects into Classical Molecular Dynamics Simulations of Complex Systems".

199. 20th Annual Symposium on Chemical Physics, 29-31 October 2004, University of Waterloo, Ontario, Canada, "Some Recent Applications of the Semiclassical Initial Value Representation".

200. International Workshop on Theoretical and Computational Chemistry of Complex Systems in Conjunction with the 3rd T&CC Conference, 2-6 January 2005, Hong Kong, "Using the Initial Value Representation of Semiclassical Theory to Include Quantum Effects in Classical Molecular Dynamics".

201. 229th American Chemical Society National Meeting (John Pople Memorial Symposium), 14-16 March 2005, San Diego, CA, "Thermal Reaction Rates from Higher Derivatives of the Flux-Flux Autocorrelation Function at Time Zero".

202. Keynote speaker at the CCP6 Workshop, 1-5 April 2005, Belfast, Ireland, "Semiclassical and Other Methods for Understanding Molecular Collisions and Chemical Reactions".

203. Workshop on Quantum Dynamics of Complex Molecular Systems, 16-20 May 2005, Paris, France.

204. Workshop on Molecular Dynamics: Chemistry and Mathematics, 16-18 June 2005, Blaubeuren, Germany.

205. Workshop on Complexified Dynamics, Chaos, and Tunneling, 25 August – 1 September 2005, Kusatsu, Japan, "Semiclassical Scattering Theory, Analytic Continuation and Initial Value Representation".

206. Symposium on Atomic and Molecular Chemistry and Physics, 23-24 September 2005, Los Angeles, CA, "Using the Initial Value Representation of Semiclassical Theory to Include Quantum Effects in Classical Molecular Dynamics Simulations".

207. International Chemical Congress of Pacific Basin Societies, 14-18 December 2005, Honolulu, Hawaii, "Quantum Instanton Model for Thermal Reaction Rates: Theory and Applications" and "Using the Initial Value Representation of Semiclassical Theory to Include Quantum Effects in Classical Molecular Dynamics Simulations".

208. 46th Sanibel Symposium, 25 February – 3 March 2006, St. Simons Island, Georgia.

209. 231st American Chemical Society National Meeting, 27-29 March 2006, Atlanta, GA, "Some Recent Developments in Using the Initial Value Representation of Semiclassical Theory to Add Quantum Effects to Time Correlation Functions".

210. XIIth International Congress of Quantum Chemistry, 21-16 May 2006, Kyoto, Japan, "Using the Initial Value Representation of Semiclassical Theory to include Quantum Effects in Classical Molecular Dynamics Simulations".

211. Gordon Research Conference on Atomic and Molecular Interactions, 9-14 July 2006, Colby-Sawyer College, New London, NH, "Using the Initial Value Representation of Semiclassical Theory as a Way for Adding Quantum Effects to Classical Molecular Dynamics Simulations".

212. 232nd American Chemical Society National Meeting, 10-14 September 2006, San Francisco, CA, "New Developments in the Application of the Semiclassical Initial Value Representation for Describing Quantum Effects in Large Molecular Systems".

213. 2006 Dalian Institute of Chemical Physics Symposium on Molecular Dynamics, 12-15 October 2006, Dalian, China, "Using the Initial Value Representation of Semiclassical Theory as a Way for Adding Quantum Effects to Classical Molecular Dynamics Simulations".

214. Trends in Chemical Dynamics: from Small Molecules to Biomolecules, 9-15 December 2006, Chiao-His, Taiwan.

215. Competence Centre for Computational Chemistry (C4) / Kenneth S. Pitzer Center Workshop, 4-6 January 2007, ETH, Zürich, Switzerland, "Using the Initial Value Representation of Semiclassical Theory to Include Quantum Effects in Classical Molecular Dynamics Simulations".

216. Symposium in Honor of William A. Lester, Jr.'s 70th Birthday, 28-31 March 2007, University of California, Berkeley, "Using the Initial Value Representation of Semiclassical Theory to Include Quantum Effects in Classical Molecular Dynamics Simulations".

217. 100 Years of Chemistry at Georgia Tech, 18-19 April 2007, Atlanta, Georgia.

218. XXI Dynamics of Molecular Collisions Meeting, 8-13 July 2007, Santa Fe, NM, "Using the Initial Value Representation of Semiclassical Theory to Include Quantum Effects in Classical Molecular Dynamics Simulations",

219. CECAM Workshop on Theoretical and Experimental Studies of Quantum Dynamics in Condensed Phase Chemical Systems, 7-10 August 2007, Dublin, Ireland.

220. 234th American Chemical Society National Meeting, 19-22 August 2007, Boston, MA, "Vibronic Dynamics via the Semiclassical (SC) Initial Value Representation (IVR) ".

221. Symposium in Honor of Wolfgang Domcke's 60th Birthday, 30 May 2008, Technical University of Munich, "Using Semiclassical Theory to Add Quantum Effects to Classical Molecular Dynamics Simulations".

222. Meeting of the 6th Congress of the International Society for Theoretical Chemical Physics, 19-24 July 2008,Vancouver, Canada.

223. 236th American Chemical Society National Meeting, 17-19 August 2008, Philadelphia, PA, "Using Semiclassical Theory to Add Quantum Effects to Classical Molecular Dynamics Simulations".

224. International Seminar and Workshop on Quantum Dynamical Concepts: From Path Integrals to Semiclassics, 20-24 August 2008, Dresden, Germany, "Using the Initial Value Representation of Semiclassical Theory to Add Quantum Effects to Classical Molecular Dynamics Simulations".

225. Latsis-Symposium on Intramolecular Dynamics, Symmetry and Spectroscopy, 6-10 September 2008, Zurich, Switzerland, "Using the Initial Value Representation of Semiclassical Theory to Add Quantum Effects to Classical Molecular Dynamics Simulations".

226. IMA Workshop on Coherence, Control, and Dissipation, 2-6 March 2009, University of Minnesota, Minneapolis, "Electronically Non-Adiabatic Dynamics via Semiclassical Initial Value Methods".

227. Xth International Workshop on Quantum Reactive Scattering, 6-10 June 2009, Dalian, China, "Using Semiclassical Theory to Add Quantum Effects to Classical Molecular Dynamics Simulations".

228. Telluride Workshop on Nonequilibrium Phenomena and Nonadiabatic Dynamics and Spectroscopy, 19-25 July 2009, Telluride, CO.

229. 50th Sanibel Symposium, 26 February – 3 March 2010, St. Simons Island, GA, "Electronically Non-Adiabatic Dynamics via Semiclassical Initial Value Methods".

230. Workshop on Quantum-Classical Modeling of Chemical Phenomena, 8-11 March 2010, College Park, MD, "Electronically Non-Adiabatic Dynamics via Semiclassical Initial Value Methods".

231. Workshop on Multiscale Molecular Modelling: Molecular Dynamics, Computational Statistical Mechanics, and Simulation Algorithms, 30 June – 2 July 2010, Edinburgh, Scotland, "Electronically Non-Adiabatic Dynamics via Semiclassical Initial Value Methods".

232. Telluride Workshop on Condensed Phase Dynamics, 19-23 July 2010, Telluride, CO.

233. 240th American Chemical Society National Meeting, 21-25 August 2010, Boston, MA, "Electronically Non-Adiabatic Dynamics via Semiclassical Initial Value Methods".

234. XVth International Workshop on Quantum Systems in Chemistry and Physics, 1-5 September 2010, Cambridge, UK, "Electronically Non-Adiabatic Dynamics via Semiclassical Initial Value Methods".

235. 43rd Midwest Theoretical Chemistry Conference, 9-11 June 2011, Notre Dame, IN, "Classical Models for Electronic Degrees of Freedom".

236. 11th Workshop on Quantum Reactive Scattering, 17-21 July, 2011, Santa Fe, "Electronically Non-Adiabatic Dynamics via Semiclassical Initial Value Methods".

237. International Conference on Theoretical and High Performance Computational Chemistry, 11-14 August 2011, Xi'an, China, "Electronically Non-Adiabatic Dynamics via Semiclassical Initial Value Methods".

238. DICP Symposium on Theoretical and Computational Chemistry, 16-19 August 2011, Dalian, China, "Semiclassical Theory of Electronically Non-Adiabatic Dynamics".

239. 20th Conference on Current Trends in Computational Chemistry, 27-29 October 2011, Jackson, MS, "Electronically Non-Adiabatic Dynamics via Semiclassical Initial Value Methods".

240. 5th Asian Pacific Conference of Theoretical and Computational Chemistry, 9-13 December 2011, Rotorua, New Zealand.

241. 243rd American Chemical Society National Meeting, 25-29 March 2012, San Diego, CA.

242. 33rd Annual Combustion Research Meeting, 29 May – 1 June 2012, Potomac, MD, "Reaction Dynamics in Polyatomic Molecular Systems".

243. 14th International Congress of Quantum Chemistry, 23-26 June 2012, Boulder, CO.

244. Telluride Science Research Workshop on Condensed Phase Dynamics, 26-30 June 2012, Telluride, CO.

245. Joint CHARMM/AMBER Meeting, 10-12 July 2012, Washington, DC, "Using Semiclassical Theory to Add Quantum Effects to Classical MD Simulations".

246. National Academy of Sciences Meeting, 26-28 April 2013, Washington, DC.

247. Mathematical Methods in Quantum Molecular Dynamics Workshop, 28 April – 3 May 2013, Banff, Canada.

248. Quantum Reactive Scattering (QRS 12), 10-14 June, 2013, Bordeaux University, France, "Semiclassical Theory of Electronically Non-Adiabatic Dynamics".

249. CECAM, Many-Dimensional Quantum Dynamics with (non) Classical Trajectories, 17-21 June, 2013, EPFL, Lausanne, Switzerland, "Semiclassical Theory of Electronically Non-Adiabatic Dynamics".

250. Telluride Science Research Workshop on Quantum Effects in Condensed-Phase Systems, 8-12 July 2013, Telluride, CO.

251. Fundamentals in Chemistry and Applications – A Conference in Honor of Rudy Marcus on his 90th Birthday, Nanyang Tech University, Singapore, 22-24 July 2013, "Using Semiclassical Theory to Add Quantum Effects to Classical Molecular Dynamics Simulations of Complex Molecular Systems".

252. 246th American Chemical Society National Meeting, Chemistry in Motion, 8-12 September 2013, Indianapolis, IN, "Using Semiclassical Theory to Add Quantum Effects to Classical Molecular Dynamics Simulations".