

## Curriculum Vitae

James T. Hynes

### Educational Background

A.B. Catholic University (with honors)	1965
Ph.D. Princeton University (Physical Chemistry)	1969

### Academic Positions

NIH Postdoctoral Fellow, M.I.T.	1969-70
Assistant Professor, University of Colorado	1/71-76
Associate Professor, University of Colorado	1976-79
Visiting Associate Professor, University of Toronto	9/78-5/79
Full Professor, University of Colorado	1979-
Stanley J. Cristol Distinguished Professor, University of Colorado	2012-
Visiting Senior Research Fellow, University of Oxford	6/85-8/85
Visiting Professor, Laboratoire de Physique Théorique des Liquides, University of Paris VI	9/85
Visiting Professor, Theoretical Chemistry Department, University of Oxford	1/87-8/87
Visiting Professor, Laboratoire de Physique Théorique des Liquides, University of Paris VI	9/87
Visiting Professor, Quantum Chemistry, Universita Autonoma de Barcelona	5/95-8/95
Visiting Professor, ENS, Paris, France	5/97
Visiting Professor, Univ. Paris Sud, Orsay, France	6/97
CNRS Directeur de Recherche, Première Classe, Département de Chimie, Ecole Normale Supérieure, Paris, France (Emeritus)	10/99 –9/08 0/08-10/13;10/13-
Professeur associé honoraire du Département de Chimie de l'ENS	12/13-12/14

### Honors and Awards

War Memorial Fellow, Catholic University	1961-65
NSF Undergraduate Summer Research Fellow, Catholic University	1964
American Can Predoctoral Fellow, Princeton	1967-69
NIH Postdoctoral Fellow, M.I.T.	1969-70
Alfred P. Sloan Foundation Fellow	1975-77
University of Colorado Faculty Foundation Fellow	9/78-8/79
John Simon Guggenheim Fellow	9/78-8/79
ACS Nobel Laureate Signature Award (w/ D. J. Nesbitt and S. R. Leone)	1983

Boulder Faculty Assembly Teaching Excellence Award	1983
SERC Fellow at Oxford University	6/85-8/85
University of Colorado Faculty Fellow	9/86-8/87
University of Colorado Council on Research and Creative Work Research Lecturer	1988
Catholic University Distinguished Alumnus Award in Research & Scholarship	1988
Texas A&M Frontiers in Chemistry Lecturer	1991
NSF Creativity Award	1991
Iberdrola Foundation Invited Visiting Professor, Barcelona, Spain	5/95-8/95
CEA Invited Scientist, Service de Photochimie Moléculaire, Centre d'Etudes de Saclay, France	8/95, 12/95-1/96
Directeur de Recherche Associé, GdR "Acte Chimique Elémentaire", Service de Photochimie Moléculaire, Centre d'Etudes de Saclay, France	5/96-8/96
ACS Lecturer, Chemistry Department, University of Wisconsin	2/97
Invited Visiting Professor, ENS, Paris, France	5/97
Invited Visiting Professor, Univ. Paris Sud, Orsay, France	6/97
CNRS Poste Rouge, Univ. Paris Sud, Orsay, France	6/97-8/97
University of Colorado Faculty Fellow	9/97-8/98
Condorcet Chair, ENS, Paris, France	5/99-7/99
Laboratory for Molecular Sciences Distinguished Visiting Scholar, California Institute of Technology	Spring 2000
Frederick Kaufman Lecturer, Department of Chemistry, University of Pittsburgh	Fall 2000
Fellow, American Physical Society	2000-
Merck-Frosst Lecturer, Concordia University, Montreal, Quebec, CA	1/2001
ISI Highly Cited Researcher for 1980-1999	2002-
Who's Who in America	2003-
Hirschfelder Prize in Theoretical Chemistry	2004
ACS Hildebrand Award in the Theoretical and Experimental Chemistry of Liquids	2005
Frontier Lecturer, Indian Inst. Of Science and Nehru Center for Advanced and Scientific Research, Bangalore, India	1/2006
Davidson Lecturer, Univ. of Kansas	3/2006
Welch Lecturer	2,3/2007
Hynes Special Issue J. Phys. Chem. B	1/2008
American Academy of Arts and Sciences	2008-
Greater Boston Area Theory Lecturer	2009
National Academy of Sciences	2011-
Who's Who in the World	2011-
Invited Visiting Professor, Harvard Univ.	9,10/2011
Distinguished Professor, University of Colorado	2012-
John A. Pople Lecture, Carnegie-Mellon Univ.	2013
American Chemical Society Fellow	2013-
Invited Autobiographical Article, Ann Rev Phys Chem, Vol. 66	2014
Oscar K. Rice Lecture, Univ. North Carolina, Chapel Hill, NC	9/2014
Heinemann Hall Lecturer, Bowling Green Univ., OH	6/2016

### Professional Memberships

American Physical Society  
American Chemical Society  
French Chemical Society

### Major Professional Activities

ACS Phys. Chem. Grad. Exam Com.	1975-78
ACS Speakers Bureau	1983-87
ACS Examination Committee	1983-90
ACS Theoretical Division, Vice Chairman	1984
Chairman-Elect,	1985
Chairman	1986
ACS, Chair, Hildebrand Award Nomination Committee	1987-88
ACS Phys. Chem. Division, Executive Committee	1989-91
Advisory Board, Journal of Physical Chemistry	1990-98
Editorial Board, Journal of Molecular Liquids	1991-
Advisory Editorial Board, International Journal of Quantum Chemistry	1993-97
Advisory Board, TRIUMF Muon Facility, (Vancouver, BC, Canada)	1993-97
Organizer or co-organizer of 16 international and ACS Symposia	1982-
Co-chair, Editorial Board, ChemPhysChem-A European Journal	1999-2010
American Editor, Progress in Reaction Kinetics and Mechanism	1999-2006
Editorial Advisory Board, Chemical Physics Letters	2003-08
Member, Editorial Board, Journal of Chemical Physics	1/03-12/05
Member, International Advisory Board, Chemical Society Reviews	2005-07
Member, Editorial Board, Interdisciplinary Sciences: Computational Life Sciences	2009-
Member, Editorial Board, Journal of Chemical Physics	1/14-12/16

### Publication and Lecture Activities

Author or co-author of over 315 research articles. 3 books co-edited.  
Over 400 invited lectures and seminars. (As of Jan 2018: h index 83)

### Research Interests

Theoretical Chemistry, Dynamics of Chemical Reactions and Energy Relaxation in Solution, Reactions at Interfaces of Atmospheric Relevance, Intramolecular Energy Flow, Chemical Reactions in Enzymes and Other Biomolecules, Electronic Structure in Condensed Phases, Catalytic Reactions related to Solar Energy.

## PUBLICATIONS

James T. Hynes

1. James T. Hynes, J. M. Deutch, Chin Hsien Wang and Irwin Oppenheim, "Quantum Corrections to Time Correlation Functions," *J. Chem. Phys.* **48(7)**, 3085-3091 (1968).
2. Bruce J. Berne, J. M. Deutch, James T. Hynes, and H. L. Frisch, "Light Scattering from Chemically Reacting Mixtures," *J. Chem. Phys.* **49(6)**, 2864-2865 (1968).
3. James T. Hynes and J. M. Deutch, "Quantum Corrections to the Momentum Relaxation Time of a Brownian Particle," *J. Chem. Phys.* **50(7)** 3015-3023 (1969).
4. James T. Hynes and J. M. Deutch, "Generalized Linear Trajectory Approximations and the Constant Acceleration Approximation," *J. Chem. Phys.* **53(12)**, 4705-4709 (1970).
5. James T. Hynes, "On Hydrodynamic Models for Brownian Motion," *J. Chem. Phys.* **57(12)**, 5612-5613 (1972).
6. James T. Hynes, "Transient Initial Condition Effects for Brownian Particle Motion," *J. Chem. Phys.* **59(7)**, 3459-3467 (1973).
7. E. L. Chang, R. M. Mazo and James T. Hynes, "On the Fokker-Planck Equation for the Linear Chain," *Mol. Phys.* **28(4)**, 997-1004 (1974).
8. James T. Hynes, "Initial Condition Effects for a Brownian Particle in a Harmonic Chain," *J. Stat. Physics* **11(3)**, 257-275 (1974).
9. James T. Hynes, "Nonlinear Fluctuations in Master Equation Systems. I. Velocity Correlation Function for the Rayleigh Model," *J. Chem. Phys.* **62(8)**, 2972-2981 (1975).
10. James T. Hynes and J. M. Deutch, "Non-Equilibrium Problems - Projection Operator Techniques," Chap. 11 in *Physical Chemistry, an Advanced Treatise*, H. Eyring, W. Jost and D. Henderson, eds., Vol. 11-B-Mathematical Methods, pp. 153-239 (1975).
11. James T. Hynes, Raymond Kapral and Michael Weinberg, "Microscopic Theory of Brownian Motion: Mori Friction Kernel and Langevin Equation Derivation," *Physica* **80A**, 105-127 (1975).
12. James T. Hynes, Raymond Kapral and Michael Weinberg, "Nonlinear Momentum Relaxation for a Particle in a Harmonic Chain," *J. Stat. Phys.* **13(5)** 425-449 (1975).
13. James T. Hynes, Raymond Kapral and Michael Weinberg, "Microscopic Theory of Brownian Motion. II. Nonlinear Langevin Equations," *Physica* **81A**, 485-508 (1975).
14. James T. Hynes, Raymond Kapral and Michael Weinberg, "Microscopic Theory of Brownian Motion. III. The Nonlinear Fokker-Planck Equation," *Physica* **81A**, 509-521 (1975).
15. James E. Clauter and James T. Hynes, "Rotational Relaxation for a Rough Particle Model," *Chem. Phys. Letters* **38(2)**, 248-252 (1976).
16. R. I. Cukier and James T. Hynes, "On Exponential Time Decay in Relaxation," *J. Chem. Phys.* **64(6)**, 2674-2683 (1976).
17. James T. Hynes, Raymond Kapral and Michael Weinberg, "Slip Boundary Condition for Rough Sphere Rotation," *Chem. Phys. Letters* **46(3)**, 463-466 (1977).

18. James T. Hynes, Raymond Kapral and Michael Weinberg, "Slip Boundary Condition for Rough Sphere Angular Velocity Correlations," *Chem. Phys. Lett.* **47(3)**, 575-77 (1977).
19. James T. Hynes, Raymond Kapral and Michael Weinberg, "Particle Rotation and Translation in a Fluid with Spin," *Physica* **87A**, 427-452 (1977).
20. James T. Hynes, "Statistical Mechanics of Molecular Motion in Dense Fluids," *Ann. Rev. Phys. Chem.* **28**, 301-321 (1977).
21. James T. Hynes, Raymond Kapral and Michael Weinberg, "Microscopic Boundary Layer Effects and Rough Sphere Rotation," *J. Chem. Phys.* **67(7)**, 3256-3267 (1977).
22. Scott H. Northrup and James T. Hynes, "Coupling of Translational and Reactive Dynamics for a Simple Lattice Model," *J. Stat. Phys.* **18(1)**, 91-105 (1978).
23. Scott H. Northrup and James T. Hynes, "Coupling of Translational and Reactive Dynamics for a Fokker-Planck Model," *J. Chem. Phys.* **68(7)**, 3203-3216 (1978).
24. Scott H. Northrup and James T. Hynes, "On the Description of Reactions in Solution," *Chem. Phys. Letters* **54(2)**, 244-247 (1978).
25. Scott H. Northrup and James T. Hynes, "On Reaction Rate Constants and Rate Kernels," *Chem. Phys. Letters* **54(2)**, 248-252 (1978).
26. James T. Hynes, Raymond Kapral and Michael Weinberg, "Molecular Rotation and Reorientation: Microscopic and Hydrodynamic Contributions," *J. Chem. Phys.* **69(6)**, 2725-2733 (1978).
27. Scott H. Northrup and James T. Hynes, "Reaction Dynamics for Diffusive Barrier Crossing," *J. Chem. Phys.* **69(12)** 5246-5260 (1978).
28. Scott H. Northrup and James Y. Hynes, "Initial Condition Effects for Diffusive Barrier Crossing," *J. Chem. Phys.* **69(12)** 5261-5266 (1978).
29. James T. Hynes, Raymond Kapral and Michael Weinberg, "Molecular Theory of Translational Diffusion: Microscopic Generalization of the Normal Velocity Boundary Condition," *J. Chem. Phys.* **70(3)** 871-883 (1979).
30. Scott H. Northrup and James T. Hynes, "Short Range Caging Effects for Reactions in Solution. I. Reaction Rate Constants and Short Range Caging Picture," *J. Chem. Phys.* **71(2)**: 871-883 (1979).
31. Scott H. Northrup and James T. Hynes, "Short Range Caging Effects for Reactions in Solution. II. Escape Probability and Time Dependent Reactivity," *J. Chem. Phys.* **71(2)**, 884-893 (1979).
32. Michael Pagitsas, James T. Hynes, and Raymond Kapral, "Kinetic Energy Relaxation of a Test Particle in a Dense Fluid," *J. Chem. Phys.* **71(11)**, 4492-4501 (1979).
33. James T. Hynes, "Dynamical Aspects of Reactions in Liquids," *J. Jpn. Chem.* **33**, 893-896 (1979).
34. James T. Hynes, "Some Dynamical Aspects of Reactions in Liquids" *Proceedings, Photochemistry with Lasers*, J. Troe, ed., Gottingen, W. Germany pp.1-4 (1979).
35. James T. Hynes, Raymond Kapral, and Glenn M. Torrie, "Stochastic Trajectory

- Simulation of Iodine Recombination in Liquids," *J. Chem. Phys.* **72(1)**, 177-188 (1980).
36. Scott H. Northrup and James T. Hynes, "The Stable States Picture of Chemical Reactions. I. Formulation for Rate Constants and Initial Condition Effects," *J. Chem. Phys.* **73(6)**, 2700-2714 (1980).
  37. Richard F. Grote and James T. Hynes, "The Stable States Picture of Chemical Reactions.II. Rate Constants for Condensed and Gas Phase Reaction Models," *J. Chem. Phys.* **73(6)**, 2715-2732 (1980).
  38. Richard F. Grote and James T. Hynes, "Reactive Modes in Condensed Phase Reactions," *J. Chem. Phys.* **74(8)**, 4465-4475 (1981).
  39. James T. Hynes, "Reaction Rate Constant for the BGK Model," *Chem. Phys. Lett.* **79(2)** 344-346 (1981).
  40. James T. Hynes and Peter G. Wolynes, "Continuum Model for Quadrupole Relaxation of Ions in Solution," *J. Chem. Phys.* **75(1)**, 395-401 (1981).
  41. Richard F. Grote and James T. Hynes, "Saddle Point Model for Atom Transfer Reactions in Solution," *J. Chem. Phys.* **75(5)**, 2191-2198 (1981).
  42. David J. Nesbitt and James T. Hynes, "Vibrational-Translational Energy Transfer from Highly Excited Anharmonic Oscillators," *Chem. Phys. Lett.* **82(2)**, 252-254 (1981).
  43. Gert van der Zwan and James T. Hynes, "Dynamical Polar Solvent Effects on Solution Reactions: A Simple Continuum Model," *J. Chem. Phys.* **76(6)**, 2993-3001 (1982).
  44. David J. Nesbitt and James T. Hynes, "Vibrational Energy Transfer from Highly Excited Anharmonic Oscillators. Dependence on Quantum State and Interaction Potential," *J. Chem. Phys.* **76(12)**, 6002-6014 (1982).
  45. Gert van der Zwan and James T. Hynes, "Reactive Paths in the Diffusion Limit," *J. Chem. Phys.* **77(13)**, 1295-1301 (1982).
  46. David J. Nesbitt and James T. Hynes, "Slow Vibrational Relaxation in Picosecond Iodine Recombination in Liquids," *J. Chem. Phys.* **77(4)**, 2130-2143 (1982).
  47. Edwin L. Sibert, III, William P. Reinhardt and James T. Hynes, "Classical Dynamics of Energy Transfer between Bonds in ABA Triatomics," *J. Chem. Phys.* **77(7)**, 3583-3594 (1982).
  48. Edwin L. Sibert, III, James T. Hynes and William P. Reinhardt, "Quantum Mechanics of Local Mode ABA Triatomic Molecules," *J. Chem. Phys.* **77(7)**, 3595-3604 (1982).
  49. Richard F. Grote and James T. Hynes, "Energy Diffusion-Controlled Reactions in Solution," *J. Chem. Phys.* **77(7)**, 3736-3743 (1982).
  50. Branka Ladanyi and James T. Hynes, "Hydrodynamic Interaction Effects on Isomerization Rates in Chain Molecules," *J. Chem. Phys.* **77(9)**, 4739-4746 (1982).
  51. Edwin L. Sibert, John S. Hutchinson, William P. Reinhardt and James T. Hynes, "Local Mode Energy Transfer: Ebb and Flow," *Int. J. Quant. Chem., Quant. Biol. Symp.* **9**, 375-383 (1982).
  52. Edwin L. Sibert, III, William P. Reinhardt and James T. Hynes, "Intramolecular Vibrational Relaxation of CH Overtones in Benzene," *Chem. Phys. Lett.* **92(5)**, 455-458 (1982).

53. Gert van der Zwan and James T. Hynes, "Nonequilibrium Solvation Dynamics in Solution Reactions," *J. Chem. Phys.* **78(6)**, Part II, 4174-4185 (1983).
54. Edwin L. Sibert, III, James T. Hynes, and William P. Reinhardt, "Fermi Resonance from a Curvilinear Perspective," *J. Phys. Chem.* **87**, 2032-2037 (1983).
55. Donald G. Truhlar, William L. Hase and James T. Hynes, "The Current Status of Transition State Theory," *J. Phys. Chem.* **87**, 2664-2682 (1983).
56. Gert van der Zwan and James T. Hynes, "Polarization Diffusion and Dielectric Friction," *Physica* **121A**, 227-252 (1983).
57. John S. Hutchinson, William P. Reinhardt and James T. Hynes, "Nonlinear Resonances and Vibrational Energy Flow in Model Hydrocarbon Chains," *J. Chem. Phys.* **99(9)**, 4247-4260 (1983).
58. Gert van der Zwan and James T. Hynes, "Polarization Diffusion Effects on Reaction Rates in Polar Solvents," *Chem. Phys. Lett.* **101(4)**, 367-371 (1983).
59. James T. Hynes, "The Theory of Reactions in Solution," in *The Theory of Chemical Reaction Dynamics*, Vol. IV, M. Baer, ed., CRC Press, Boca Raton, FL., 1985, pp 171-234.
60. John S. Hutchinson, Edwin L. Sibert III and James T. Hynes, "Quantum Dynamics of Energy Transfer in Coupled Morse Oscillator Systems," *J. Chem. Phys.* **81**, 1314-1326 (1984).
61. John S. Hutchinson, James T. Hynes and William P. Reinhardt, "Quantum Dynamic Analysis of Energy Transfer in Model Hydrocarbons," *Chem. Phys. Lett.* **108**, 353-358 (1984).
62. Edwin L. Sibert III, William P. Reinhardt and James T. Hynes, "Intramolecular Vibrational Relaxation and Spectra of CH and CD Overtones in Benzene and Perdeuterobenzene", *J. Chem. Phys.* **81**, 1115-1134 (1984).
63. Edwin L. Sibert III, James T. Hynes and William P. Reinhardt, "Classical Dynamics of Highly Excited CH and CD Overtones in Benzene and Perdeuterobenzene" *J. Chem. Phys.* **81**, 1135-1144 (1984).
64. Richard F. Grote, Gert van der Zwan and James T. Hynes, "Frequency Dependent Friction and Solution Reaction Rates", *J. Phys. Chem.* **88**, 4676-4684 (1984).
65. Gert van der Zwan and James T. Hynes, "A Simple Dipole Isomerization Model for Nonequilibrium Solvation Dynamics in Reactions in Polar Solvents," *Chem. Phys.* **90**, 21-35 (1984).
66. Edwin L. Sibert III, John S. Hutchinson, James T. Hynes and William P. Reinhardt, "Energy Flow from Highly Excited CH Overtones in Benzene and Alkanes," in *Ultrafast Phenomena IV*, 336-340, D. H. Auston and K. B. Eisenthal, eds., Springer-Verlag, New York, 1984.
67. Gert van der Zwan and James T. Hynes, "Time Dependent- Fluorescence Solvent Shifts, Dielectric Friction, and Nonequilibrium Solvation in Polar Solvents," *J. Phys. Chem.* **89**, 4181-4188 (1985).
68. Anthony G. Zawadzki and James T. Hynes, "Double Well Isomerization Rate Constants in Solution," *Chem. Phys. Lett.* **113(5)**, 476-482 (1985).

69. T. Uzer and James T. Hynes, "A Model Study of Overtone-Induced Isomerization: The Role of Nonlinear Resonances," *Chem. Phys. Lett.* **113(5)**, 483-488 (1985).
70. T. Uzer, James T. Hynes and William P. Reinhardt, "Overtone-Induced Dissociation of Hydrogen Peroxide: A Classical Trajectory Study," *Chem. Phys. Lett.* **117(6)**, 600-605 (1985).
71. David J. Nesbitt and James T. Hynes, "Probability Oscillations in Single Pass Curve Crossings: Semiclassical Predictions of Nonmonotonic Dependence on Crossing Velocity," *J. Chem. Phys.* **84(3)**, 1554-64 (1986).
72. Branka M. Ladanyi and James T. Hynes, "Transition-State Solvent Effects on Atom Transfer Rates in Solution", *J. Amer. Chem. Soc.* **108**, 585-593 (1986).
73. John S. Hutchinson, James T. Hynes and William P. Reinhardt, "A Mechanism for CH Vibrational Relaxation in Alkanes," *J. Phys. Chem.* **90**, 3528-3532 (1986).
74. James T. Hynes, "Chemical Reaction Dynamics in Solution," *Ann. Rev. Phys. Chem.* **36**, 573-597 (1985).
75. James T. Hynes, "Chemical Reaction Rates and Solvent Friction," *J. Stat. Phys.* **42**, 149-168 (1986).
76. T. Uzer, G. Natanson, and James T. Hynes, "Coriolis-Induced Intramolecular Vibrational Energy Flow between Anharmonic Normal Modes", *Chem. Phys. Lett.* **122(1,2)**, 12-18 (1985).
77. John P. Bergsma, Pamela M. Edelsten, Brad J. Gertner, Kevin R. Huber, Jeffrey R. Reimers, Kent R. Wilson, Samuel M. Wu and James T. Hynes, "Dynamics of the A + BC Reaction in Solution", *Chem. Phys. Lett.* **123**, 394-398 (1986).
78. T. Uzer and James T. Hynes, "Intramolecular Energy Transfer in Simple Model Organometallics," *J. Phys. Chem.* **90**, 3524-3527 (1986).
79. James T. Hynes, "Outer Sphere Electron Transfer Reactions and Frequency-Dependent Friction," *J. Phys. Chem.* **90**, 3701-3706 (1986).
80. Domenic P. Ali and James T. Hynes, "Activated Hydrogen Atom Tunneling Reactions in Solution," in *Tunneling*, J. Jortner and B. Pullman, eds., D. Reidel Publishing Company, 1986. pp, 203-212.
81. John P. Bergsma, Jeffrey R. Reimers, Kent R. Wilson and James T. Hynes, "Molecular Dynamics of the A + BC Reaction in Rare Gas Solution," *J. Chem. Phys.* **85(10)**, 5625-5643 (1986).
82. T. Uzer, James T. Hynes and William P. Reinhardt, "Classical Dynamics of Intramolecular Energy Flow and Overtone-Induced Dissociation in HOOH and HOOD," *J. Chem. Phys.* **85(10)**, 5791-5804 (1986).
83. John P. Bergsma, Bradley J. Gertner, Kent R. Wilson and James T. Hynes, "Molecular Dynamics of a Model S<sub>N</sub>2 Reaction in Water," *J. Chem. Phys.* **86(3)**, 1356-1376 (1987).
84. Bradley J. Gertner, John P. Bergsma, Kent R. Wilson, Sangyoub Lee and James T. Hynes, "Nonadiabatic Solvation Model for S<sub>N</sub>2 Reactions in Polar Solvents," *J. Chem. Phys.* **86(3)**, 1377-1386 (1987).
85. James T. Hynes, "Cages, Crossings and Correlations—Theoretical Perspectives on

- Solution Reaction Dynamics," in *Ultrafast Phenomena*, G. R. Fleming and A. E. Siegman, eds., V, Springer-Verlag, 288-292 (1986).
86. T. Uzer and James T. Hynes, "Theoretical Studies of Overtone-Induced Chemical Reactions," in *Stochasticity and Intramolecular Redistribution of Energy*, R. Lefebvre and S. Mukamel, eds. NATO ASI SERIES, 1987, pp 273-283.
  87. Dominic A. Zichi and James T. Hynes, "A Dynamical Theory of Unimolecular Dissociation Reactions in Polar Solvents," *J. Chem. Phys.* **88**(4), 2513-2525 (1988).
  88. Sangyoub Lee and James T. Hynes, "Solution Phase Reaction Path Hamiltonian. I. Formulation," *J. Chem. Phys.*, **88**, 6853-6862 (1988).
  89. Sangyoub Lee and James T. Hynes, "Solution Phase Reaction Path Hamiltonian.II. Applications," *J. Chem. Phys.*, **88**, 6863-6870 (1988).
  90. James T. Hynes, "Theory of Association and Substitution Reactions", in *Chemical Reactivity in Liquids. Fundamental Aspects*, M. Moreau and P. Turq, eds., (Plenum, New York, 1988), pp 221-28.
  91. Giovanni Ciccotti, Mauro Ferrario, James T. Hynes and Raymond Kapral, "Molecular Dynamics Simulation of Ion Association Reactions in a Polar Solvent", *J. de Chimie Phys.* (Paris), **85**, 925-929 (1988).
  92. Bradley, J. Gertner, Kent R. Wilson, Dominic A. Zichi, Sangyoub Lee and James T. Hynes, "Nonequilibrium Solvation in  $S_N1$  and  $S_N2$  Reactions in Polar Solvents," *Faraday Disc. Chem. Soc.*, **85**, 297-308 (1988).
  93. Terumitsu Morita, Branka M. Ladanyi and James T. Hynes, "Polar Solvent Contributions to Activation Parameters for Model Ionic Reactions," *J. Phys. Chem.*, **93**, 1386-1392 (1989).
  94. Bernard Gaveau, James T. Hynes, Raymond Kapral and Michel Moreau, "A Stochastic Theory of Chemical Reaction Rates. I. Formalism", *J. Stat. Phys.*, **56**, (5/6), 879-893 (1989).
  95. Bernard Gaveau, James T. Hynes, Raymond Kapral and Michel Moreau, "A Stochastic Theory of Chemical Reaction Rates. II. Applications", *J. Stat. Phys.*, **56**, (5/6), 895-910 (1989).
  96. Giovanni Ciccotti, Mauro Ferrario, James T. Hynes and Raymond Kapral, "Constrained Molecular Dynamics and the Mean Potential for an Ion Pair in a Polar Solvent", *Chem. Phys.*, **129**, 241-251 (1989).
  97. Daniel Borgis and James T. Hynes, "Proton Transfer Reactions," in *The Enzyme Catalysis Process*, NATO ASI Series, A. Cooper, J.L. Houben and L.C. Chien, eds., (Plenum, New York, 1989). pp 293-303.
  98. James T. Hynes, "The Role of the Environment in Chemical Reactions," in *The Enzyme Catalysis Process*, NATO ASI Series, A. Cooper, J.L. Houben and L.C. Chien, eds., (Plenum, New York, 1989). pp 283-292.
  99. Bradley J. Gertner, Kent R. Wilson and James T. Hynes, "Nonequilibrium Solvation Effects on Reaction Rates for Model  $S_N2$  Reactions in Water.," *J. Chem. Phys.*, **90** (7), 3537-3558 (1989).
  100. Emily A. Carter, Giovanni Ciccotti, James T. Hynes and Raymond Kapral, "Constrained Reaction Coordinate Ensemble for Molecular Dynamics Simulation of Rare Events,"

- Chem. Phys. Lett.*, **156** (5) 472-477 (1989).
101. James T. Hynes, "Charge Transfer Reaction Dynamics in Solution," *New Perspectives in Quantum Chemistry*, J. Jortner and B. Pullman, eds., (Kluwer, Dordrecht, 1989), pp. 83-95.
  102. Sally Chapman, Dominic P. Ali and James T. Hynes, "Collinear Proton Transfer in a Symmetric Bihalide System," *Chem. Phys.*, **136** (2), 297-309 (1989).
  103. Emily A. Carter and James T. Hynes, "Solute-Dependent Solvent Force Constants For Ion Pairs and Neutral Pairs in a Polar Solvent," *J. Phys. Chem.*, **93**, 2184-2187 (1989).
  104. Dominic A. Zichi, Giovanni Ciccotti, James T. Hynes and Mauro Ferrario, "Molecular Dynamics Simulation of Electron Transfer Reactions in Solution," *J. Phys. Chem.*, **93**, 6261-65 (1989).
  105. Anthony G. Zawadzki and James T. Hynes, "Radical Recombination Rates from Gas to Liquid Phase," *J. Phys. Chem.*, **93**, 7031-7036 (1989).
  106. James T. Hynes, Emily A. Carter, Giovanni Ciccotti, Hyung J. Kim, Dominic A. Zichi, Mauro Ferrario and Raymond Kapral, "Environmental Dynamics and Electron Transfer Reactions" in *Perspectives in Photosynthesis*, J. Jortner and B. Pullman, Eds., (Kluwer, Dordrecht) 1990, pp. 133-148.
  107. Daniel J. Borgis, Sangyoub Lee and James T. Hynes, "A Dynamical Theory of Nonadiabatic Proton and Hydrogen Atom Transfer Reaction Rates in Solution", *Chem. Phys. Lett.*, **162** (1,2), 19-26 (1989).
  108. Turgay Uzer and James T. Hynes, "Dissociation of Remote Bonds by Overtone Excitation: A Model Study", *Chem. Phys.*, **139**, 163-169 (1989).
  109. Hyung J. Kim and James T. Hynes, "The Role of Solvent Electronic Polarization in Electron Transfer Processes," *J. Phys. Chem.*, **94**, 2736-2740 (1990).
  110. Anthony G. Zawadzki and James T. Hynes, "Molecular Solvent Vibrational Effects on the Friction for Barrier Crossing Reactions," *J. Molec. Liquids*, **48**, 197-209 (1991).
  111. Daniel Borgis and James T. Hynes, "Nonadiabatic Proton Transfer Reaction Rates in Solution: A Semiclassical Microscopic Formalism", *J. Chim. Phys. (Paris)*, **87**, 819-829 (1990).
  112. Giovanni Ciccotti, Mauro Ferrario, James T. Hynes and Raymond Kapral, "Dynamics of Ion Pair Interconversion in a Polar Solvent", *J. Chem. Phys.*, **93** (10), 7137-7147 (1990).
  113. Hyung J. Kim and James T. Hynes, "Equilibrium and Nonequilibrium Solvation and Solute Electronic Structure. I. Formulation", *J. Chem. Phys.*, **93** (7), 5194-5210 (1990).
  114. Hyung J. Kim and James T. Hynes, "Equilibrium and Nonequilibrium Solvation and Solute Electronic Structure. II. Strong Coupling Limit", *J. Chem. Phys.*, **93** (7), 5211-23 (1990).
  115. Hyung J. Kim and James T. Hynes, "Equilibrium and Nonequilibrium Solvation and Solute Electronic Structure", *Int. J. Quant. Chem.: Quantum Chemistry Symposium*, **24**, 821-833 (1990).
  116. Bradley J. Gertner, Robert M. Whitnell, Kent R. Wilson and James T. Hynes, "Activation to the Transition State: Reactant and Solvent Energy Flow for a Model  $S_N2$

- Reaction in Water", *J. Amer. Chem. Soc.*, **113**, 74-87 (1991).
117. Daniel Borgis and James T. Hynes, "Molecular Dynamics Simulation for a Model Nonadiabatic Proton Transfer Reaction in Solution", *J. Chem. Phys.*, **94**, 3619-3628 (1991).
  118. Gert van der Zwan and James T. Hynes, "Chemical Reaction Rates and Solvation Dynamics in Electrolyte Solutions: Ion Atmosphere Friction," *Chem. Phys.*, **152**, 169-183 (1991).
  119. Emily A. Carter and James T. Hynes, "Solvation Dynamics for an Ion Pair in a Polar Solvent: Time Dependent Fluorescence and Photochemical Charge Transfer", *J. Chem. Phys.*, **94**, 5961-5979 (1991).
  - 120.. Stephen K. Klippenstein and James T. Hynes, "Direct and Indirect Solvent Coupling Mechanisms for Vibrational Dephasing in Hydrogen—Bonded Molecules", *J. Phys. Chem.*, **95**, 4651-4659 (1991).
  - 121.. Robert M. Whitnell, Kent R. Wilson and James T. Hynes, "Fast Vibrational Relaxation for a Dipolar Molecule in a Polar Solvent", *J. Phys. Chem.*, **94**, 8625-8628 (1990).
  122. Hyung J. Kim and James T. Hynes, "A Theoretical Model for S<sub>N</sub>1 Ionic Dissociation in Solution I. Activation Free Energetics and Transition State Structure", *J. Amer. Chem. Soc.*, **114**, 10508-10528 (1992).
  123. Hyung J. Kim and James T. Hynes, "A Theoretical Model for S<sub>N</sub>1 Ionic Dissociation in Solution II. Nonequilibrium Solvation Reaction Path and Reaction Rate", *J. Amer. Chem. Soc.*, **114**, 10528-10537 (1992).
  124. William P. Kierstead, Kent R. Wilson and James T. Hynes, "Molecular Dynamics of a Model S<sub>N</sub>1 Reaction in Water", *J. Chem. Phys.*, **95** (7), 5256-5267 (1991).
  125. Hyung J. Kim and James T. Hynes, "Equilibrium and Nonequilibrium Solvation and Solute Electronic Structure. III. Quantum Theory", *J. Chem. Phys.*, **96** (7), 5088-5110 (1992).
  126. J. Juanos-i-Timoneda and James T. Hynes, "Nonequilibrium Free Energy Surfaces for Hydrogen-Bonded Proton Transfer Complexes in Solution", *J. Phys. Chem.*, **95**, 10431-10442 (1991).
  127. John Gehlen, David Chandler, Hyung J. Kim and James T. Hynes, "Free Energies of Electron Transfer", *J. Phys. Chem.*, **96**, 1748-1753 (1992).
  128. Barton B. Smith and James T. Hynes, "Electron Transfer Reactions in Solution: The Role of Solvation Dynamics", in *Condensed Matter Physics Aspects of Electrochemistry*, M.P. Tosi and A.A. Kornyshev, eds., (World Scientific, 1991).
  129. Barton B. Smith, Hyung J. Kim, Daniel Borgis and James T. Hynes, "Solvent Dynamics and Charge Transfer Reactions", in *Dynamics and Mechanisms of Photoinduced Electron Transfer and Related Phenomena*, N. Mataga, T. Okada and H. Masuhara, eds., (Elsevier, Amsterdam, 1992). pp. 39-56.
  130. Teresa Fonseca, Branka M. Ladanyi and James T. Hynes, "Solvation Free Energies and Solvent Force Constants", *J. Phys. Chem.*, **96**, 4085-4093 (1992).
  131. Margaret Bruehl and James T. Hynes, "Dielectric Friction and Solvation Dynamics: A Molecular Dynamics Study", *J. Phys. Chem.*, **96**, 4068-4074 (1992).

132. Robert M. Whitnell, Kent R. Wilson and James T. Hynes, "Vibrational Relaxation of a Dipolar Molecule in Water", *J. Chem. Phys.*, **96** (7), 5354-5369 (1992).
133. Michel Moreau, Daniel Borgis, Bernard Gaveau, James T. Hynes, Raymond Kapral and Ewa Gudowska-Nowak, "Reactive Processes in a Fluctuating Medium", *Acta. Phys. Pol.* **Bb23**, 367-88 (1992).
134. James T. Hynes, Hyung J. Kim, Jeffery R. Mathis and J. Timoneda, "Solute Electronic Structure and Solvation in Chemical Reactions in Solution", *J. Molec. Liquids*, **57**, 53-73 (1993).
135. Barton B. Smith and James T. Hynes, "Electronic Friction and Electron Transfer Rates at Metallic Electrodes", *J. Chem. Phys.*, **99**, 6577-90 (1993).
136. Hyung J. Kim, Roberto Bianco, Bradley J. Gertner and James T. Hynes, "A Simple Basis Set Approach to Solute Electronic Structure and Free Energy in Solution", *J. Phys. Chem.* **97**, 1723-27 (1993).
137. Daniel Borgis and James T. Hynes, "Dynamical Theory of Proton Tunnelling Transfer Rates in Solution: General Formulation", *Chem. Phys.*, **170** (3), 315-346 (1993).
138. Arnulf Staib and James T. Hynes, "Vibrational Predissociation in Hydrogen-Bonded OH . . . O Complexes via OH Stretch—OO Stretch Energy Transfer", *Chem. Phys. Lett.* **204**, 197-203 (1993).
139. Jeffery R. Mathis, Hyung J. Kim and James T. Hynes, "A Theoretical Model for S<sub>N</sub>1 Ionic Dissociations in Solution. III. Analysis of t-Butyl Halide", *J. Am. Chem. Soc.* **115**, 8248-62 (1993).
140. Margaret Bruehl and James T. Hynes, "Vibrational Relaxation Times for a Model Hydrogen-Bonded Complex in a Polar Solvent", *Chem. Phys.* **175**, 205-21 (1993).
141. Barton B. Smith, Arnulf Staib and James T. Hynes, "Well and Barrier Dynamics and Electron Transfer Rates. A Molecular Dynamics Study", *Chem. Phys.* **176**, 521-37 (1993).
142. James T. Hynes, "Charge Transfer Reactions and Solvation Dynamics", in *Ultrafast Spectroscopy*, J. Simon, Ed. (Kluwer, Dordrecht, 1994). pp. 345-381.
143. Bradley J. Gertner, Koji Ando, Roberto Bianco and James T. Hynes, "Bihalide Ion Combination Reactions in Solution: Electronic Structure and Solvation Effects", *Chem. Phys.* **183**, 309-23 (1994).
144. Jeffrey R. Mathis, Roberto Bianco and James T. Hynes, "On the Activation Free Energetics of the Cl<sup>-</sup> + CH<sub>3</sub>Cl S<sub>N</sub>2 reaction in Solution", *J. Molec. Liquids*, **61**, 81-102 (1994).
145. Teresa Fonseca, Hyung J. Kim and James T. Hynes, "Dynamics of Twisted Intramolecular Charge Transfer Complexes in Polar Solvents", *J. Molec. Liquids*, **60**, 161-200 (1994).
146. Teresa Fonseca, Hyung J. Kim, and James T. Hynes, "TICT Dynamics in Polar Solvents", *J. Photochem. Photobiol. A: Chem.* **82**, 67-79 (1994).
147. Arnulf Staib, Rossend Rey and James T. Hynes, "Ultrafast Vibrational Predissociation and Relaxation in Hydrogen-Bonded Systems", in *Ultrafast Reaction Dynamics and Solvent Effects*, Y. Gauduel and P. Rossky, Eds. (AIP Press, New York, 1994), pp. 173-190.

148. James T. Hynes, Hyung J. Kim, Jeffery R. Mathis, Roberto Bianco, Koji Ando and Bradley J. Gertner, "Electronic Structure and Chemical Reactions in Solution", in *Reaction Dynamics in Solution and in Clusters*, B. Pullman and J. Jortner, Eds. (Reidel, Dordrecht, 1994), pp. 289-309.
149. Jeffery R. Mathis and James T. Hynes, "Solvent Barriers in Unimolecular Ionizations. I. Solution Reaction Path Analysis for Alkyl Iodides", *J. Phys. Chem.* **98**, 5445-59 (1994).
150. Jeffery R. Mathis and James T. Hynes, "Solvent Barriers in Unimolecular Ionizations. II. Electron Transfer Perspective for Alkyl Iodide Ionization", *J. Phys. Chem.* **98**, 5460-70 (1994).
151. James T. Hynes, "Wet Chemistry", *Nature*, 439-40 (1994).
152. Koji Ando and James T. Hynes, "How Do Acids Ionize in Water?" in *Structure, Energetics and Reactivity in Aqueous Solution*, C.J. Cramer and D.G. Truhlar, Eds. (ACS Publications, Washington, D.C., 1994), pp. 143-153.
153. Roberto Bianco, J. Juanos-i-Timoneda, and James T. Hynes, "Equilibrium and Nonequilibrium Solvation and Solute Electronic Structure. IV. Quantum Theory in a Multi-Diabatic State Formulation", *J. Phys. Chem.* **98**, 12103-12107 (1994).
154. Arnulf Staib, James T. Hynes and Daniel Borgis, "Proton Transfer in Hydrogen-Bonded Acid-Base Complexes in Polar Solvents", *J. Chem. Phys.* **102**, 2487-2505 (1995).
155. Roberto Bianco and James T. Hynes, "VB Resonance Theory in Solution. I. Multi-state Formulation", *J. Chem. Phys.*, **102**, 7864-7884 (1995).
156. Roberto Bianco and James T. Hynes, "VB Resonance Theory in Solution. II.  $I_2^- \leftrightarrow I + I^-$  in Acetonitrile", *J. Chem. Phys.* **102**, 7885-7901 (1995).
157. Ilan Benjamin, Paul Barbara, Bradley J. Gertner and James T. Hynes, "Nonequilibrium Free Energy Functions, Recombination Dynamics and Vibrational Relaxation of  $I_2^-$  in Acetonitrile: Molecular Dynamics of Charge Flow in the Electronically Adiabatic Limit", *J. Phys. Chem.* **99**, 7557-7567 (1995).
158. Koji Ando and James T. Hynes, "HCl Acid Ionization in Water: A Theoretical Molecular Modelling", *J. Molec. Liquids*, **64**, 25-34 (1995).
159. James T. Hynes, "Twisted Intramolecular Charge Transfer Reactions: The Role of the Solvent", *Portuguese Chemical Reviews*, **2**, 12-17 (1995).
160. Koji Ando, Arnulf Staib and James T. Hynes, "Acid-Base Proton Transfer in Solution", in *Femtochemistry II*, M. Cergui, Ed. (World Scientific, Singapore, 1996), pp. 534-539.
161. Rossend Rey and James T. Hynes, "Energy Relaxation Time and Pathway for HOD in Liquid  $D_2O$ ", *J. Chem. Phys.*, **104**, 2356-2368 (1996).
162. James T. Hynes, "Crossing the Transition State in Solution", in *Solvent Effects and Chemical Reactivity*, O. Tapia and J. Bertran, Eds. (Kluwer, Amsterdam, 1996), pp 231-258.
163. Roberto Bianco and James T. Hynes, "Valence Bond Multistate Approach to Chemical Reactions in Solution", in *Solvent Effects and Chemical Reactivity*, O. Tapia and J. Bertran, Eds. (Kluwer, Amsterdam, 1996), 259-281.
164. Daniel Borgis and James T. Hynes, "A Curve Crossing Approach for Proton Transfer

- Reactions in Solution”, *J. Phys. Chem.*, **100**, 1118-1128 (1996).
165. Bradley J. Gertner and James T. Hynes, “HCl Acid Ionization at the Surface of Stratospheric Ice”, *Science*, **271**, 1563-1566 (1996).
  166. Koji Ando, Arnulf Staib and James T. Hynes, “Adiabatic Acid-Base Proton Transfer in Solution”, in *Fast Elementary Processes in Chemical and Biological Systems*, A. Tramer, Ed., (AIP, New York, 1996) pp. 326-332.
  167. Rossend Rey and James T. Hynes, “Hydration Shell Exchange Kinetics: an MD Study for Na<sup>+</sup> (aq)”, *J. Phys. Chem.*, **100**, 5611-5615 (1996).
  168. Koji Ando and James T. Hynes, "HF Acid Ionization in Water: The First Step", *Faraday Society Discussions 1995*, **102**, 435-441 (1996).
  169. Koji Ando, Arnulf Staib, and James T. Hynes, “Ultrafast Proton Transfer in Aqueous Solution”, in *Femtochemistry II*, M. Cergui, Ed., (World Scientific, Singapore, 1996), pp 534-539.
  170. Rossend Rey and James T. Hynes, "Vibrational Phase and Energy Relaxation of the Cyanide Ion in Water", in *Ultrafast Phenomena*, P. Barbara, J. G. Fujimoto, W.H. Knox, and W. Zinth, Eds., (Springer-Verlag, Berlin, 1996), 294-295.
  171. Sangyoub Lee and James T. Hynes, "Intramolecular Hydrogen Atom Transfer Rates in Solution", *J. de Chimie Physique*, **99**, 7557-7567 (1996).
  172. Rossend Rey and James T. Hynes, “Hydration Shell Exchange Dynamics for Na<sup>+</sup> in Water”, *J. Phys. Condensed Matter*, **8**, 9411-9416 (1996).
  173. Hyung Kim and James T. Hynes, “Excited State Intramolecular Charge Transfer Rates for DMABN in Solution: A Two-Dimensional Dynamics Perspective”, *J. Photochem. Photobiol. A: Chemistry*, **105**, 337-343 (1997).
  174. Gilles H. Peslherbe, Roberto Bianco, Branka M. Ladanyi, and James T. Hynes, “On the Photoionization of Alkali-Metal Halides in Solution”, *J. Chem. Soc. Faraday Trans.*, **93** (5), 977-988 (1997).
  175. Koji Ando and James T. Hynes, "Molecular Mechanism of HCl Acid Ionization in Water. *Ab initio* Potential Energy Surfaces and Monte Carlo Simulations", *J. Phys. Chem.B*, **101**, 10464-10478 (1997).
  176. Hyung J. Kim, Arnulf Staib, and James T. Hynes, “Ultrafast Dynamics at the Transition State in Solution”, *Ultrafast Reaction Dynamics at Atomic-Scale Resolution Femtochemistry and Femtobiology*, Nobel Symposium 101, Villy Sundstrom, Ed., (Imperial College Press, London, 1998) pp. 510-527.
  177. Rossend Rey and James T. Hynes, “Vibrational Phase and Energy Relaxation of CN<sup>-</sup> in Water”, *J. Chem. Phys.*, **108**, 142-153 (1998).
  178. Roberto Bianco and James T. Hynes, “Ab Initio Model Study of the Mechanism of ClONO<sub>2</sub> Hydrolysis on Ice”, *J. Phys. Chem. A*, **102**, 309-314 (1998).
  179. Dario Baksic, Juan Bertran, J. M. Lluich, and James T. Hynes, "An Ab Initio Study of Nitromethane Deprotonation by OH •nH<sub>2</sub>O Clusters", *J. Phys. Chem., A* **102**, 3977-3984 (1998).
  180. Gilles H. Peslherbe, Branka Ladanyi, and James T. Hynes, "Trajectory Study of Photodissociation Dynamics in the NaI-H<sub>2</sub>O Cluster system", *J. Phys. Chem., A* **102**,

- 4100-4110 (1998).
181. Roberto Bianco, Bradley J. Gertner, and James T. Hynes, "Proton Transfer Reactions at the Surface of Ice. Heterogeneous Reactions Involved in Stratospheric Ozone Depletion," *Berichte der Bunsen-Gesellschaft für Physikalische Chemie*, **102**, 518-526 (1998).
  182. Bradley J. Gertner and James T. Hynes, "Model Molecular Dynamics Simulation of Hydrochloric Acid Ionization at the Surface of Stratospheric Ice," *Faraday Society Discussions*, **110**, 301-322 (1998).
  183. Ward Thompson, Mireille Blanchard-Desce, and James T. Hynes, "Two Valence Bond State Model for Molecular Nonlinear Optical Properties. Nonequilibrium Solvation Formulation", *J. Phys. Chem. A.*, **102**, 7712-7722 (1998).
  184. Gilles H. Peslherbe, Branka M. Ladanyi, and James T. Hynes, "Cluster Ion Thermodynamic Properties: Predictions of the Liquid Drop Model and Rate of Convergence to the Bulk Limit Revisited", *J. Phys. Chem. A*, **103**, 2561-2571 (1999).
  185. Bradley J. Gertner, Gilles H. Peslherbe, and James T. Hynes, "Acid Ionized HBr in a Four Water Cluster", *Isr. J. Chem.*, **39**, 273-281, (1999).
  186. Koji Ando and James T. Hynes, "Acid-Base Proton Transfer and Ion Pair Formation in Solution", *Adv. Chem. Phys.*, **110**, 381-430 (1999).
  187. Ward H. Thompson, Mireille Blanchard-Desce, Valérie Alain, Jacques Muller, Alain Fort, Marguerite Barzoukas, and James T. Hynes, "Two Valence Bond State Model for Molecular Nonlinear Optical Properties. Comparison with Push-Pull Polyene Solution Measurements", *J. Phys. Chem. A.*, **103**, 3766-3771 (1999).
  188. James T. Hynes, "The Protean Proton in Water", *Nature*, **397**, 565 (1999).
  189. Roberto Bianco and James T. Hynes, "A Theoretical Study of the Reaction of ClONO<sub>2</sub> with HCl on Ice", *J. Phys. Chem. A*, **103**, 3797-3801 (1999).
  190. Roberto Bianco and James T. Hynes, "Theoretical Studies of Heterogeneous Reaction Mechanisms Relevant for Stratospheric Ozone Depletion", *Int. J. Quantum Chem.*, **75**, 683-692 (1999).
  191. Koji Ando and James T. Hynes, "Acid Ionization of HF in Water, an Electronic Structure and Monte Carlo Study", *J. Phys. Chem. A*, **103**, 10398-10408 (1999).
  192. Pascal Plaza, Damien Laage, Monique M. Martin, Valerie Alain, Mireille Blanchard-Desce, Ward H. Thompson, and James T. Hynes, "Excited State Dynamics in Polar Solvents of Push-Pull Polyenes Designed for Nonlinear Optics", *J. Phys. Chem. A*, **104:11**, 2396-2401 (2000).
  193. Ward H. Thompson and James T. Hynes, "Frequency Shifts in the Hydrogen-Bonded OH Stretch in Water-Halide Clusters. The Importance of Charge Transfer", *J. Am. Chem. Soc.*, **122**, 6278-6286 (2000).
  194. Giovanni Granucci, James T. Hynes, Philippe Millie, Thu-Hoa Tran-Thi, "A Theoretical Investigation of Excited State Acidity of Phenol and Cyanophenols", *J. Am. Chem. Soc.*, **122**, 12235-12245 (2000).
  195. Gilles H. Peslherbe, Branka M. Ladanyi, and James T. Hynes, "Free Energetics of NaI Contact Ion Pairs in Water Clusters. A Theoretical Study," *J. Phys. Chem. A*, **104**, 4533-4548 (2000)..

196. Gilles H. Peslherbe, Branka M. Ladanyi, and James T. Hynes, "Structure of NaI Ion Pairs in Water Clusters", *Chem. Phys.*, **258**, 201-224 (2000).
197. Akihiro Morita and James T. Hynes, "A Theoretical Analysis of the Sum Frequency Generation Spectrum of the Water Surface", *Chem. Phys.*, **258**, 371-390 (2000).
198. Thu-Hoa Tran-Thi, Thomas Gustavsson, Cécile Prayer, Stanislas Pommeret, and James T. Hynes, "Primary Ultrafast Events Preceding the Photoinduced Proton Transfer from Pyranine to Water", *Chem. Phys. Lett.*, **329**, 421-430 (2000).
- Roberto Bianco and James T. Hynes, "Theoretical Chemistry for Heterogeneous Reactions of Atmospheric Importance. The HCl + ClONO<sub>2</sub> Reaction on Ice", *Theoretical Methods in Condensed Phase Chemistry*, S.D. Schwartz, ed. (Kluwer, Dordrecht, Netherlands, 2000), pp. 235-245.
199. Roberto Bianco, Ward H. Thompson, Akihiro Morita, and James T. Hynes, "Is the H<sub>2</sub>OCl<sup>+</sup> Ion a Viable Intermediate for the Hydrolysis of ClONO<sub>2</sub> on Ice Surfaces?", *J. Phys. Chem. A*, **105**, 3132-3139 (2001).
- 201 Rossend Rey and James T. Hynes, "Coulomb Force and Intramolecular Energy Flow Effects for Vibrational Energy Transfer for Small Molecules in Polar Solvents", *Ultrafast Infrared and Raman Spectroscopy*, M.D. Fayer, editor. (Marcel Dekker, New York, 2001). pp. 593-624
202. Ward H. Thompson and James T. Hynes, "A Model Study of the Acid-Base Proton Transfer Reaction of the ClH...OH<sub>2</sub> Pair in Low Polarity Solvents", *J. Phys. Chem. A*, **105**, 2582-2590 (2001).
203. Ward H. Thompson, Philip M. Kiefer, and James T. Hynes, "Transition State Theory and Reaction Dynamics-An Overview", *Femtochemistry IV*, F. C. De Schryver, S. De Feyter, G. Schweitzer, eds. (Wiley-VCH, Weinheim, 2001), pp. 87-96.
204. Thu-Hoa Tran-Thi, Cecile Prayer, Philippe Millie, Pavel Uznanski, and James T. Hynes, "Effect of Sulfonate Groups and Solvents on the Nature of the Transitions of Pyrenol and Pyranine. Identification of an Intermediate in the ESPT Reaction", *J. Phys. Chem., A*, **106**, 2244-2255, (2002).
205. Akihiro Morita and James T. Hynes, "A Theoretical Analysis of the Sum Frequency Generation Spectrum of the Water Surface II. Time-Dependent Approach", *J. Phys. Chem B*, **106**, 673-685 (2002).
- 206 Philip M. Kiefer and James T. Hynes, "Free Energy Relationship for Adiabatic Proton Transfer Reactions in a Polar Environment. I. Fixed Proton Donor-Acceptor Separation", *J. Phys. Chem A.*, **106**, 1834-1849 (2002).
- 207 Philip M. Kiefer and James T. Hynes, "Free Energy Relationship for Adiabatic Proton Transfer Reactions in a Polar Environment. II. Inclusion of the Hydrogen Bond Vibration", *J. Phys. Chem. A*, **106**, 1850-1861 (2002).
- 208 Ayman S. Al-Halabi, Roberto Bianco, and James T. Hynes, "Acid Dissociation of HBr on a Model Ice Surface", *J. Phys. Chem, A*, **106**, 7639-7645 (2002).
- 209 Giovanni Grannucci, Thu-Hoa Tran-Thi, Thomas Gustavsson, Philippe Millie and James T. Hynes, "New Theoretical Ideas for Excited State Proton Transfer in

- Solution", *Femtochemistry and Femtobiology*, ed. A. Douhal and J. Santamaria, 158-168 (2002).
- 210 Rossend Rey, Klaus Moller, and James T. Hynes, "Hydrogen Bond Dynamics in Water and Ultrafast Infrared Spectroscopy", *J. Phys. Chem. A*, **106**, 11993-11996 (2002).
- 211 James T. Hynes, Thua-Hoa Tran-Thi, and Giovanni Granucci, "Intermolecular Photochemical Proton Transfer in Solution: New Insights and Perspectives", *J. Photochem. And Photobiology; A. Photochemistry*, **154**, 3-11 (2002).
- 212 Philip Kiefer and James T. Hynes, "Proton Transfer Reactions and Hydrogen Bonding in Solution", in *Ultrafast Hydrogen Bonding Dynamics and Proton Transfer Processes in the Condensed Phase*, T. Elsaesser and H. Bakker, eds. (Kluwer, Dordrecht, 2002), pp.73-90.
- 213 Damien Laage, Irene Burghardt, Thomas Sommerfeld and James T. Hynes, "On the Dissociation of Aromatic Radical Anions in Solution", *ChemPhysChem*, **4**, 61-66 (2003).
- 214 C. Toubin, S. Picaud, P.N.M. Hoang, C. Girardet, R.M. Lynden-Bell, and James T. Hynes, "Adsorption of HF and HCl Molecules on Ice at 190K and 235K from Molecular Dynamics Simulations: Free Energy Profiles and Residence Times", *J. Chem. Phys* **118** , 9814-9823 (2003).
- 215 Daniel Spangberg, Rossend Rey, James T. Hynes, and Kersti Hermansson, "The Rate and Mechanisms for Water Exchange around Li+(aq) from MD Simulations", *J. Phys Chem B.*, **107**, 4470-4477 (2003).
- 216 Damien Laage, Ward H. Thompson, Mireille Blanchard-Desce, and James T. Hynes, "Charged Push-Pull Polyenes in Solution: Anomalous Solvatochromism and Nonlinear Optical Properties", *J. Phys. Chem. A* , **107**, 6032-6046 (2003).
- 217 Philip M. Kiefer and James T. Hynes, "Kinetic Isotope Effects for Adiabatic Proton Transfer Reactions in a Polar Environment", *J. Phys. Chem A*, **107** , 9022-9039 (2003).
- 218 Roberto Bianco and James T. Hynes, "A Theoretical Study of  $\text{ClONO}_2 + \text{Cl}^- \rightarrow \text{Cl}_2 + \text{NO}_3^-$  on Ice", *J. Phys. Chem. A* , **107**, 5253-5257 (2003).
- 219 Philip M. Kiefer and James T. Hynes, "Adiabatic and Nonadiabatic Proton Transfer Rate Constants in Solution", *Solid State Ionics*, **168**, 219-224 (2004).
- 220 Roberto Bianco, A. Al-Halabi and James T. Hynes, "Theoretical Studies of Heterogeneous Reactions Important in Atmospheric Ozone Depletion", *Advanced Topics in Theoretical Chemical Physics*, J. Maruani et al. (eds.), p. 379-390, 2003, Kluwer Academic Publishers, Netherlands.
- 221 Rossend Rey, Klaus B. Moller and James T. Hynes, "On Hydrogen Bond Dynamics in Water and Ultrafast Infrared Spectroscopy. A Theoretical Study", *J. Phys. Chem. A*, **108**, 1275-1289 (2004).
222. Roberto Bianco and James T. Hynes, "A Theoretical Study of the  $\text{H}_2\text{SO}_4 + \text{H}_2\text{O} \rightarrow \text{HSO}_4^- + \text{H}_3\text{O}^+$  Reaction at the Surface of Aqueous Aerosols", *Theoretical Chemistry Accounts*, **111**, 182-187 (2004).
223. Damien Laage, Irene Burghardt, Thomas Sommerfeld, and James T. Hynes , « On the

- Dissociation of Aromatic Radical Anions in Solution. I. Formulation and Application to p-Cyanochlorobenzene Radical Anion » *J. Phys. Chem. A*, **107**, 11271-11291 (2003).
224. Irene Burghardt, Damien Laage, and James T. Hynes, « On the Dissociation of Aromatic Radical Anions in Solution. II. Reaction Path and Rate Constant Analysis » *J. Phys. Chem., A*, **107**, 11292-11306 (2003).
225. Philip M. Kiefer and James T. Hynes, « Temperature Dependent Solvent Polarity Effects on Proton Transfer Rate Constants and Kinetic Isotope Effects » *Israel J. Chem.*, **44**, 171-184 (2004).
226. Rossend Rey, Klaus B. Moller and James T. Hynes, « Ultrafast Vibrational Population Dynamics of Water and Related Systems : A Theoretical Perspective' , *Chem. Rev.*, **104**, 1915-1928 (2004).
227. Philip M. Kiefer and James T. Hynes, “Kinetic Isotope Effects for Nonadiabatic Proton Transfer Reactions in a Polar Environment. I. Interpretation of Tunneling Kinetic Isotope Effects”, *J. Phys. Chem. A*, **108**, 11793-11808 (2004).
228. Philip M. Kiefer and James T. Hynes, « Kinetic Isotope Effects for Nonadiabatic Proton Transfer Reactions in a Polar Environment. II. Comparison with an Electronically Nonadiabatic Perspective. » *J. Phys. Chem. A*, **108**, 11809-11818 (2004).
229. Klaus B. Moller, Rossend Rey and James T. Hynes, « Theoretical Perspectives for Ultrafast IR Spectroscopy in Water », in Time Resolved Spectroscopy, *Proceedings of the XIth TRVS International Conference*, eds. S. Califano, P. Foggi and R. Righini (Olschki, Florence, 2005). 195-201.
230. Klaus B. Møller, Rossend Rey, and James T. Hynes, "On Ultrafast IR Spectroscopy in Water", *Femtochemistry and Femtobiology : Ultrafast Events in Molecular Science*, eds. M. Martin and J.T. Hynes, (Elsevier, Amsterdam, 2004). Pp. 177-180.
231. Irene Burghardt, Lorenz S. Cederbaum and James T. Hynes, ‘Environmental Effects on a Conical Intersection: a Model Study’, *Faraday Discuss.* **127**, 395- 411(2004)
232. Klaus.B. Moller, Rossend Rey, Marco Masia and James T. Hynes, ‘On the Coupling Between Molecular Diffusion and Solvation Shell Exchange’ *J. Chem. Phys.*, **122**, 114508-114519 (2005).
233. Philip M. Kiefer and James T. Hynes, “ Interpretation of Primary Kinetic Isotope Effects for Adiabatic and Nonadiabatic Proton Transfer Reactions in a Polar Environment », H. Limbach and A. Kohen, eds. *"Isotope Effects in the Biological and Chemical Sciences"*. (CRC Press, Boca Raton, 2005).PP. 549-578
234. Irene Burghardt, Lorenz S. Cederbaum and James T. Hynes, “Ultrafast Excited State

- Charge Transfer at a Conical Intersection: Effects of an Environment”, *Comp. Phys..Commun.* **169**, 95-98 (2005)
235. Damien Laage, Hagop Demirdjian and James T. Hynes, « Intermolecular Vibration-Vibration Energy Transfer in Solution: Hydrogen Fluoride in Water ». *Chem. Phys. Lett.*, **405**, 453-458 (2005)..
236. Roberto Bianco, Shuzhi Wang and James T. Hynes, “ Theoretical Study of the First Acid Dissociation of H<sub>2</sub>SO<sub>4</sub> at a Model Aqueous Surface”, *J. Phys. Chem. B* , **109**, 21313-21321 (2005).
- 237.. Philip Kiefer, Damien Laage and James T. Hynes, ‘Une Vision Non Traditionnelle du Transfert de Proton en Solution’ in Réactions ultrarapides en solution. Approches expérimentales et théoriques’ eds. T. Gustavsson, M. Mostafavi (CNRS Press, Paris, 2006).pp.283-300.
238. Roberto Bianco and James T. Hynes, « Heterogeneous Reactions Important in Atmospheric Ozone Depletion; A Theoretical Perspective », *Accts. Chem. Res.*, **39**, 150-165 (2006)
239. Riccardo Spezia, Irene Burghardt and James T. Hynes. “Conical Intersections in Solution: Nonequilibrium versus Equilibrium Solvation”, *J. Molec. Phys.* (Robb Issue), **104**, 903-914 (2006).
240. Bruno Nigro, Suyong Re, Damien Laage , Rossend Rey and James T. Hynes, « On the Ultrafast Infrared Spectroscopy of Anion Hydration Shell Hydrogen Bond Dynamics », *J. Phys. Chem. A*, **110**, 11237-11243 (2006).
241. Denise M. Koch, Qadir K. Timerghazin, Gilles H. Peslherbe, Branka M. Ladanyi and James T. Hynes, “Nonadiabatic Trajectory Studies of NaI(H<sub>2</sub>O)<sub>n</sub> Photodissociation Dynamics”, *J. Phys. Chem.A*, **110**, 1438-1454 (2006)
242. Irene Burghardt, James T. Hynes, E. Gindensperger, and L. S. Cederbaum, “Ultrafast Excited-State Dynamics at a Conical Intersection: the Role of Environmental Effects,” *Physica Scripta* **73**, C42-C46 (2006).
243. Damien Laage and James T. Hynes, “A Molecular Jump Mechanism of Water Reorientation”, *Science*, **311**, 832-835 (2006).
244. Maite Roca, Vicente Moliner, Inaki Tunon, and James T. Hynes, “Coupling Between Protein and Reaction Dynamics in Enzymatic Processes. Application of Grote-Hynes Theory to Catechol O-Methyltransferase”, *J. Am. Chem. Soc.*, **128**, 6186-6193 (2006).
245. Irene Burghardt, Riccardo Spezia and James T. Hynes, “Solvation and Photochemical Funnels: Environmental Effects on Conical Intersection Structure and Dynamics”, in *Femtochem VII: Fundamental Ultrafast Processes in Chemistry, Physics and Biology* (Elsevier, Amsterdam, 2006). Pp. 143-151.
246. Irene Burghardt and James T. Hynes, “Excited-State Charge Transfer at Conical Intersections: Effect of an Environment”, *J. Phys.. Chem. A*, **110**, 11411-11423 (2006)

247. Biman Jana, Subrata Pal, Prabal K. Maiti, Shiang-Tai Lin, James T. Hynes and Biman Bagchi, « Entropy of Water in the Hydration Layer of Major and Minor Grooves of DNA », *J. Phys. Chem. B*, **110**, 19611-19618 (2006)
248. Subrata Pal, Prabal K. Maiti, Biman Bagchi and James T. Hynes, “Multiple Timescales in Solvation Dynamics of DNA in Aqueous Solution: Role of Water, Counterions, and Cross-Correlations », *J. Phys. Chem. B*, **110**, 26396-26402 (2006)
249. Philip M. Kiefer and James T. Hynes, « Proton Transfer Reactions in a Polar Environment », in Vol. 1, *Hydrogen Transfer Reactions*, James T. Hynes and Hans Limbach, editors, R.Schowen, general editor. (Wiley-VCH, Weinheim, 2007). Pp. 307-348.
250. Damien Laage and James T. Hynes, “Do More Strongly Hydrogen-Bonded Water Molecules Reorient More Slowly?” *Chem. Phys. Lett.* **433**, 80-85 (2006).
251. Damien Laage, Irene Burghardt and James T. Hynes, “Nonequilibrium Solvation and Conical Intersections”, in *Continuum Solvation Models in Chemical Physics: Theory and Application*, B. Mennucci R. Cammi and R. Cammi, eds. (Wiley-VCH, Weinheim, 2007).pp. 429-449.
252. James T. Hynes, “The Peripatetic Proton”, *Nature*, **446**, 270-272 (2007).
253. Damien Laage and James T. Hynes, “Reorientational Dynamics of Water Molecules in Anionic Hydration Shells”, *Proc. Natl. Acad. Sci.*, **104**, 11167-11172 (2007)
254. Evgeniy V. Gromov, Irene Burghardt, James T. Hynes, Horst Koppel and Lorenz Cederbaum, “Electronic Structure of the Photoactive Yellow Protein Chromophore: Ab Initio Study of the Low-Lying Excited Singlet States”, *J. Photochem. Photobiol. A: Chem.* **190**, 241-257 (2007).
255. Roberto Bianco, Shuzhi Wang and James T. Hynes, “Theoretical Study of the Dissociation of Nitric Acid HNO<sub>3</sub> at a Model Aqueous Surface”, *J. Phys. Chem.A*, **111**, 11033-11042 (2007).
256. Sai G.Ramesh, Suyong Re and James T. Hynes, “Charge Transfer and Hydrogen-Bonded OH Frequency Shifts in Nitrate Ion Water Clusters”, *J. Phys. Chem. A*, **112**, 3391-3398 (2008).
257. Roberto Bianco, Shuzhi Wang and James T. Hynes, “Theoretical Studies of the Dissociation of Sulfuric Acid and Nitric Acid at a Model Aqueous Surface”, *Adv. Quant. Chem.*, **55**, 387-405 (2008).
258. Denise M. Koch, Celine Toubin, Sichuan Xu, Gilles H. Peslherbe and James T. Hynes, « Concerted Proton Transfer Mechanism and Solvation Effects in the HNC-HCN Isomerization on the Surface of Icy Grain Mantles in the Interstellar Medium », *J. Phys. Chem. C*, **111**, 15026-15033 (2007).
259. Joao P. Malhado and James T. Hynes, « On the Landau-Zener Approach to Nonadiabatic

Transitions for a Vertical Conical Intersection » *Chemical Physics*, **347**, 39-45 (2008).

260. Denise M. Koch, Celine Toubin, Gilles H. Peslherbe and James T. Hynes, “Theoretical Study of the Formation of the AminoAcetonitrile Precursor of Glycine on Icy Grain Mantles in the Interstellar Medium”, *J. Phys. Chem. C*, **112** 12972 –12980 (2008).

261. Arnab Mukherjee, Richard Lavery, Biman Bagchi and James T. Hynes, « On the Molecular Mechanism of Drug Intercalation into DNA : A Simulation Study of the Intercalation Pathway, Free Energy and DNA Structural Changes», *J. Amer. Chem. Soc.*, **130**, 9747-9755 (2008).

262 José Ruiz-Pernía, Iñaki Tuñón, Vicente Moliner, James T. Hynes and Maite Roca , « Dynamic Effects on Reaction Rates in a Michael Addition Catalyzed by Chalcone Isomerase. Beyond the Frozen Environment Approach » *J. Amer. Chem. Soc.* **130**, 7477-7488 (2008).

263. Roberto Bianco, Shuzhi Wang and James T. Hynes, « Infrared Signatures of HNO<sub>3</sub> and NO<sub>3</sub> at a Model Aqueous Surface. A Theoretical Study, » *J. Phys. Chem. A*, **112**, 9467-9476 (2008).

264. Damien Laage and James T. Hynes, « On the Residence Time for Water in a Solute Hydration Shell. Application to Aqueous Halide Solutions”, *J. Phys. Chem.,B*, **112**, 7697-7701 (2008).

265. Damien Laage and James T. Hynes, “On the Molecular Mechanism of Water Reorientation” *J. Phys. Chem.,B*, **112**, 1430-1442 (2008).

266. Damien Laage, Guillaume Stirnemann and James T. Hynes, “Why water reorientation slows down without iceberg formation around hydrophobic solutes”, *J. Phys. Chem.,B*, **113**, 2428-2435 (2009).

267. Arnab Mukherjee, Richard Lavery, Biman Bagchi and James T. Hynes, « Simulation Study of the Molecular Mechanism of Intercalation of the Anti-Cancer Drug Daunomycin into DNA », in Energy transfer dynamics in biomaterial systems, Eds, I. Burghardt, V. May, D. A. Micha, and E.R. Bittner, Lecture Notes in Chemical Physics, Vol. 93 (Springer-Verlag, Heidelberg/Berlin (2009). Pp. 165-180.

268. Shuzhi Wang, Roberto Bianco and James T. Hynes, “Depth-Dependent Dissociation of Nitric Acid at an Aqueous Surface: Car-Parrinello Dynamics”, *J. Phys. Chem.A*, **113**, 1295-1307 (2009).

269. Shuzhi Wang, Roberto Bianco and James T. Hynes, “Nitric Acid Dissociation at an Aqueous Interface: Occurrence and Mechanism”, *Isr. J. Chem.* **49**, 251-259 (2009).

270, Damien Laage and James T. Hynes, “Echoes of a Salty Exchange”, *Proc. Nat. Acad. Sci. (US)*, **106**, 967-968 (2009).

271. Francesca Ingrosso, Rossend Rey, Thomas Elsaesser and James T. Hynes, “Ultrafast Energy Transfer from the Intramolecular Bending Vibration to Librations in Liquid Water:”, *J. Phys. Chem A*, **113** , 6657-6665 (2009).

272. Rossend Rey, Francesca Ingrosso, Thomas Elsaesser and James T. Hynes, "Pathways for H<sub>2</sub>O Bend Vibrational Relaxation in Liquid Water". *J. Phys. Chem A*, **113**, 8949-8962 (2009).
273. Sai G. Ramesh, Suyong Re, Jean Boisson and James T. Hynes, "Vibrational Symmetry-Breaking of NO<sub>3</sub><sup>-</sup> in Aqueous Solution: NO Asymmetric Stretch Frequency Distribution and Mean Splitting", *J. Phys. Chem A*, **114**, 1255-1269 (2010).
274. Philip M. Kiefer and James T. Hynes, "Theoretical Aspects of Tunneling Proton Transfer Reactions in a Polar Environment", Special Issue on Tunneling, *J. Phys. Org. Chem.*, **23**, 632-646 (2010).
275. Guillaume Stirnemann, James T. Hynes and Damien Laage, "Water Hydrogen Bond Dynamics in Aqueous Solutions of Amphiphiles", *J. Phys. Chem B*, **114**, 3052-3059 (2010).
276. Fabio Sterpone, Guillaume Stirnemann, James T. Hynes and Damien Laage, "Water Hydrogen Bond Dynamics around Amino Acids: the Key Role of Hydrophilic Hydrogen-Bond Acceptor Groups", *J. Phys. Chem B*, **114**, 2083-2089 (2010).
277. Damien Laage, Guillaume Stirnemann and James T. Hynes. "Water Reorientation in the Hydration Shells of Hydrophilic and Hydrophobic Solutes", *Science in China, Series G.*, **53**, 1068-1072 (2010).
278. Guillaume Stirnemann, Peter J. Rossky, James T. Hynes, and Damien Laage, « Water Hydrogen-bond Dynamics and 2D-IR Spectroscopy next to an Extended Hydrophobic Surface », *Faraday Disc.*, **146**, 263-281 (2010).
279. Shuzhi Wang, Roberto Bianco and James T. Hynes, « Dissociation of Nitric Acid at an Aqueous Surface: Large Amplitude Motions in the Contact Ion Pair to Solvent-Separated Ion Pair Conversion », *PhysChemChemPhys*, **12**, 8241-8249 (2010).
280. Joao Malhado, Riccardo Spezia and James T. Hynes, « Dynamical Friction Effects on the Photoisomerization of a Model Protonated Schiff Base in Solution », *J. Phys. Chem. A*, **115**, 3720-3735 (2011).
281. Damien Laage, Guillaume Stirnemann, Fabio Sterpone, Rossend Rey and James T. Hynes, « Reorientation and Allied Dynamics in Water and Aqueous Solutions », *Annu. Rev. Phys. Chem.*, **62**, 395-416 (2011).
282. Inaki Tunon and James T. Hynes, "A Simple Model for Barrier Frequencies for Enzymatic Reactions", *ChemPhysChem*, **12**, 184-190 (2011).
283. Shuzhi Wang, Roberto Bianco and James T. Hynes, "An Atmospherically Relevant Acid: HNO<sub>3</sub>", *Comp. & Theor. Chem* **965**, 340-345 (2011). (Special Issue: Theoretical chemistry of atmospheric processes.)
284. Roberto Bianco, P. Jeffrey Hay and James T. Hynes, "Theoretical Study of O-O Single Bond Formation in the Oxidation of Water by the Ruthenium Blue Dimer", *J. Phys. Chem. A*, **115**, 8003-8016 (2011).

285. Damien Laage, Guillaume Stirnemann, Fabio Sterpone and James T. Hynes, "Water Jump Reorientation: from Theoretical Prediction to Experimental Observation", *Accts Chem Res*, **45**, 53-62 (2012).
286. Jean Boisson, Guillaume Stirnemann, Damien Laage and James T. Hynes, "Water Reorientation Dynamics in the First Hydration Shells of F<sup>-</sup> and I<sup>-</sup>", *Phys.Chem.Chem.Phys*, **13**, 19895-19901 (2011).
287. Guillaume Stirnemann, Santiago Romero-Vargas Castrillon, James T. Hynes, Peter J. Rossky, Pablo G. Debenedetti and Damien Laage, "Non-monotonic dependence of water reorientation dynamics with surface hydrophilicity: competing effects of hydration structure and hydrogen-bond strength", *Phys. Chem. Chem.Phys*, **13**, 19911-19917 (2011).
288. Roberto Bianco, P. Jeffrey Hay and James T. Hynes, "Proton Relay and Electron Flow in the O-O Single Bond Formation in Water Oxidation by the Ruthenium Blue Dimer", *Energy Environ. Sci.*, **5**, 7741-7746 (2012). DOI: 10.1002/qua.24095
289. Damien Laage, Guillaume Stirnemann, and James T. Hynes, "Water Jump Reorientation and Ultrafast Vibrational Spectroscopy", *J. Photochem. PhotoBio. A: Chemistry*, **234**, 75-82 (2012).
290. Rossend Rey and James T. Hynes, "Tracking energy transfer from excited to accepting modes: application to water bend vibrational relaxation", *Phys. Chem. Chem. Phys*, **14**, 6332-6342 (2012).
291. Matthieu Wilhelm, Arnab Mukherjee, Benjamin Bouvier, Krystyna Zakrzewska, James T. Hynes, Richard Lavery, "Multistep drug intercalation: molecular dynamics and free energy studies of daunomycin binding to DNA" *J. Am. Chem. Soc.* **134**, 8588-8596 (2012).
292. Joao Malhado and James T. Hynes, "Photoisomerization for a Model Protonated Schiff Base in Solution: Sloped/Peaked Conical Intersection Perspective", *J. Chem. Phys.* **137**, 22A543 (2012).
293. Joao Malhado, Riccardo Spezia and James T. Hynes, "Conical Intersection Structure and Dynamics for a Model Protonated Schiff Base Photoisomerization in Solution", *Int. J. Quantum Chem.* **113**, 296-305 (2013). DOI :10.1002/qua.24095
294. Damien Laage and James T. Hynes, "Water Reorientation and Ultrafast Infrared Spectroscopy, in M. Fayer, ed, Ultrafast Infrared Vibrational Spectroscopy (CRC Press, Boca Raton, FL 2013). Pp. 77-98.
295. Jakob Petersen, Klaus Moller, Rossend Rey and James T. Hynes, "Ultrafast Librational Relaxation of H<sub>2</sub>O in Liquid Water", *J. Phys. Chem. B*, **117**, 4541-4552 (2013).
296. Aoife C.Fogarty, Elise Duboue-Dijon, Fabio Sterpone, James T. Hynes, Damien Laage "Biomolecular hydration dynamics: a jump model perspective", *Chem. Soc. Rev.*, **42**, 5672-5683 (2013)
297. Chern-Hooi Lim, Aaron M. Holder, James T. Hynes and Charles B. Musgrave, "What

are the Roles of the Lewis Acids and Base in the Chemical Reduction of CO<sub>2</sub> by Frustrated Lewis Pairs?' *Inorg. Chem.*, **52**, 10062-10066 (2013).DOI: <http://dx.doi.org/10.1021/ic4013729>

298. Xinliang Xu, Hao Ge, Chan Gu, Yi Qin Gao, Siyuan S. Wang, Beng Joo Reginald Thio, James T. Hynes, X. Sunney Xie, and Jianshu Cao, "Modeling Spatial Correlation of DNA Deformation: DNA Allostery in Protein Binding", *J. Phys. Chem. B*, **117**, 13378–13387 (2013). DOI: 10.1021/jp4047243

299. Roberto Bianco, P. Jeffrey Hay, and James T. Hynes, "Theoretical Study of Water Oxidation by the Ruthenium Blue Dimer. II. Proton relay chain mechanism for the step [bpy<sub>2</sub>(HOO)RuIVORuIV(OH)bpy<sub>2</sub>]<sup>4+</sup> → [bpy<sub>2</sub>(O<sub>2</sub>)RuIVORuIII(OH<sub>2</sub>)bpy<sub>2</sub>]<sup>4+</sup>", *J. Phys. Chem. B*, **117**, 15761-15763 (2013). DOI:<http://dx.doi.org/10.1021/jp406504h>

300. Chern-Hooi Lim, Aaron M. Holder, James T. Hynes, and Charles M. Musgrave, "Reduction of CO<sub>2</sub> to methanol catalyzed by a biomimetic organo-hydride produced from pyridine", *J. Am. Chem. Soc.* **136**, 16081–16095 (2014) DOI: <http://dx.doi.org/10.1021/ja510131a>

301. Philip M. Kiefer, Ehud Pines, Dina Pines, and James T. Hynes, 'Solvent-Induced Red-Shifts for the Proton Stretch Vibrational Frequency in a Hydrogen-Bonded Complex. I. A Valence Bond-Based Theoretical Approach', *J. Phys. Chem. B*, **118**, 8330-8351 (2014) DOI: 10.1021/jp501815j

302. Joao Malhado, Michael J. Bearpark, and James T. Hynes, "Non-adiabatic dynamics close to conical intersections and the surface hopping perspective", *Frontiers in Chemistry: Theoretical and Computational Chemistry*, 2014, *Front. Chem.*2:97. doi:10.3389/fchem.2014.00097

303. Dina Pines, Sharon Keinan, Philip M. Kiefer, James T. Hynes, and Ehud Pines. "Effect of Solvent Dielectric Constant and Acidity on the OH Vibration Frequency in Hydrogen-bonded Complexes of Fluorinated Ethanol", *J. Phys. Chem B*, **119**, 9278-9286 (2015). Web Publication Date (Web): November 24, 2014 DOI: 10.1021/jp509914w

304. Rossend Rey and James T. Hynes, "Solvation Dynamics in Liquid Water. I. Ultrafast Energy Fluxes", *J. Phys. Chem. B*, **119**, 7558-7570 (2015). <http://dx.doi.org/10.1021/jp5113922>

305. Sharon Keinan, Dina Pines, Philip M. Kiefer, James T. Hynes, and Ehud Pines, "Solvent Induced O-H Vibration Red-shifts in Hydrogen-Bonded Acid-Base Complexes", *J. Phys. Chem. B*, **119**, 679–692 (2015). DOI: 10.1021/jp502553r

306. James T. Hynes, "Molecules in Motion: Chemical Reaction and Allied Dynamics in Solution and Elsewhere", *Annual Review of Physical Chemistry*, **66**, 1-20 (2015). DOI: 10.1146/annurev-physchem-040214-121833

307. Inaki Tunon, Damien Laage, and James T. Hynes, "Are There Dynamical Effects in Enzyme Catalysis? Some Thoughts Concerning the Enzymatic Chemical Step", *Arch. Biochem., Biophys.*, **582**, 42–55. (2015). doi: [10.1016/j.abb.2015.06.004](http://dx.doi.org/10.1016/j.abb.2015.06.004)

308. Chern-Hooi Lim, Aaron M. Holder, James T. Hynes, and Charles B. Musgrave, “Catalytic Reduction of CO<sub>2</sub> by Renewable Organo-Hydrides “. *J. Phys. Chem. Lett.*, 2015, 6 (24), pp 5078–5092. DOI: 10.1021/acs.jpcelett.5b01827
309. Chern-Hooi Lim, Brady T. Worrell, Samuel S. Bacon, Christopher N. Bowman, James T. Hynes, and Charles B. Musgrave, “A Recyclable Metal-Free Organo-Hydride for CO<sub>2</sub> Reduction”, submitted 2015.
310. Dina Pines, Julia Ditkovich, Tzah Mukra, Yifat Miller, Philip M. Kiefer, Snehasis Daschakraborty, James T. Hynes, and Ehud Pines, “How acidic is carbonic acid?”, *J. Phys. Chem. B*, 120, 2440-2451 (2016). DOI: **10.1021/acs.jpccb.5b12428**
311. Elise Duboue-Dijon, Aoife, C. Fogarty, James T. Hynes and Damien Laage, “Dynamical Disorder in the DNA Hydration Shell” *J. Amer. Chem. Soc.*, **138** (24), pp 7610–7620 (2016). DOI: 10.1021/jacs.6b02715
312. Snehasis Daschakraborty, Philip M. Kiefer, Yifat Miller, Yair Motro, Dina Pines, Ehud Pines, and James T. Hynes, “Direct Proton Transfer from Carbonic Acid to a Strong Base in Aqueous Solution I: Acid and Base Coordinate and Charge Dynamics”, *J. Phys. Chem. B*, **120**, 2271-2280 (2016). DOI: **10.1021/acs.jpccb.5b12742** 2016.
313. Snehasis Daschakraborty, Philip M. Kiefer, Yifat Miller, Yair Motro, Dina Pines, Ehud Pines, and James T. Hynes, “Direct Proton Transfer from Carbonic Acid to a Strong Base in Aqueous Solution II: Solvent Coordinate-Dependent Reaction Path”, *J. Phys. Chem. B*, **120**, 2281-2290 (2016). DOI: **10.1021/acs.jpccb.5b12744**.
314. James T. Hynes, Damien Laage, Iñaki Tuñón, Vicent Moliner” “A Transition State Theory Perspective for Enzymatic Reactions: Fundamentals and Applications”, in *Simulating Enzymatic Reactivity*, I. Tunon and V. Moliner, eds., Royal Society of Chemistry, Cambridge UK, pp 54-88 2016, <http://pubs.rsc.org/en/content/ebook/9781782626831>.
315. Joao Malhado and James T. Hynes, ‘Non-adiabatic Transition Probability Dependence on Conical Intersection Topography’, *J. Chem. Phys.*, **145** 194104 (2016). DOI: <http://dx.doi.org/10.1063/1.4967259>
316. Rossend Rey and James T. Hynes, “Solvation Dynamics in Water. 2. Energy Fluxes on excited and ground state surfaces”, *J. Phys. Chem B*, **120**,11287-11297 (2016). <http://dx.doi.org/10.1021/acs.jpccb.6b08965>
317. Rossend Rey and James T. Hynes, “Solvation Dynamics in Liquid Water. III. Energy Fluxes and Structural Changes”, *J Phys Chem B*, **121**, 1377-1385 (2017). DOI: 10.1021/acs.jpccb.6b11805.
318. Damien Laage, Thomas Elsaesser, and James T. Hynes, “Water Dynamics in the Hydration Shells of Biomolecules”, *Chem. Rev.*, **117**, 10694-10725 (2017). DOI: 10.1021/acs.chemrev.6b00765
319. Rossend Rey and James T. Hynes, “Translational versus Rotational Energy Flow in Water Solvation Dynamics”, *Chem. Phys Lett* (Zewail Memorial Issue) **683**, 483-487 (2017).

<https://doi.org/10.1016/j.cplett.2017.02.064>

320. Chern-Hooi Lim, Aaron M. Holder, James T. Hynes and Charles B. Musgrave, "Dihydropteridine/Pteridine as a  $2\text{H}^+/2\text{e}^-$  Redox Mediator for the Reduction of  $\text{CO}_2$  to Methanol: A Computational Study", *J. Phys Chem. B*, **121** 4158-4167 (2017). DOI: 10.1021/acs.jpccb.7b01224

321. Damien Laage, Thomas Elsaesser, and James T. Hynes, "Perspective: Structure and ultrafast dynamics of biomolecular hydration shells", *Structural Dynamics*, 4, 044018 (2017). doi: 10.1063/1.4981019 (online: <http://dx.doi.org/10.1063/1.4981019>).

322. David M. Wilkins, David E. Manolopoulos, Silvio Pipolo, Damien Laage, and James T. Hynes, "Nuclear Quantum Effects in Water Reorientation and Hydrogen-Bond Dynamics", *J. Phys. Chem. Lett.* **8**, 2602-2607 (2017). DOI: 10.1021/acs.jpcclett.7b00979

323. Abdulaziz Alherz, Chern-Hooi Lim, James T. Hynes, and Charles B. Musgrave "Predicting Hydride Donor Strength Via Quantum Chemical Calculations of Hydride Transfer Activation Free Energy", *J Phys Chem B*, **122**, 1278-1288 (2018)  
DOI: 10.1021/acs.jpccb.7b12093

### Books Edited

1. Monique M. Martin and James T. Hynes, Editors, *Femtochemistry and Femtobiology. Ultrafast Events in Molecular Science* (Femtochemistry VI) Elsevier B.V., Amsterdam, 2004

2,3. James T. Hynes and Hans Limbach, editors, "Hydrogen Transfer: Chemical and Physical Aspects", Vols. 1 and 2 of the 4 volumes of *Hydrogen Transfer Reactions*, R.Schowen, general editor. (Wiley-VCH, Weinheim, 2007)

### Other

235 "thought" questions for *Physical Chemistry*", G. W. Castellan (Addison-Wesley) 3rd Edition.

James T. Hynes, "Autobiography of James T. (Casey) Hynes, *J. Phys. Chem. B*, **122**, 191-194 (2008)

### In Preparation

James T. Hynes, *The Theory of Chemical Reaction Dynamics in Solution*, Oxford University Press.



## Invited Lectures and Seminars

(20 previous)

- 8/78 Invited Lecture, Gordon Conference on Dielectrics.
- 10/78 Invited Lecture, ACS Miami Meeting, Symposium on Liquids.
- 10/78 Lecture, Canadian Conference on Theoretical Chemistry, Kingston, Ont.
- 11/78 Seminar, Physics Dept., University of Toronto.
- 1/79 Seminar, Chem. Dept., University of Toronto.
- 2/79 Seminar, Chem. Dept., University of Toronto.
- 3/79 Seminar, Chem. Dept., University of Minnesota.
- 3/79 Seminar, Chem. Dept, Michigan State University.
- 4/79 Invited Lecture, ACS Honolulu Meeting, Symposium on Dynamics in Liquids.
- 4/79 Seminar, Chem. Dept., University of California, Los Angeles.
- 4/79 Seminar, Chemical Physics, University of Colorado, Boulder.
- 5/79 Seminar, Chem. Dept., Harvard University.
- 8/79 Invited Lecture, Gordon Conference on Liquids.
- 10/79 Invited Lecture, Conference on Photochemistry, University of Gottingen.
- 1/80 Seminar, Physics Dept., University of Colorado, Boulder.
- 2/80 Seminar, Chem. Dept., University of California San Diego, La Jolla.
- 8/80 Contrib. Lecture, ACS San Francisco Mtg., Symposium on Potential Energy Surfaces.
- 11/80 Seminar, Chem. Dept., Illinois Institute of Technology, Chicago.
- 11/80 Seminar, Chem. Dept., Colorado State University.
- 12/80 Seminar, Chem. Physics, University of Colorado, Boulder.
- 1/81 Seminar, Physics Dept., University of Colorado, Boulder.
- 4/81 Invited Lecture, ACS Atlanta Meeting, Symposium on Equilibrium and Dynamic Properties of Solutions.
- 8/81 Invited Lecture, IUPAC, Vancouver Meeting, Symposium on Lasers in Chemistry.

- 11/81 Seminar, Chem. Dept., University of Denver.
- 12/81 Seminar, Chem. Dept., Texas Tech.
- 12/81 Seminar, Chem. Dept., University of Houston.
- 1/82 Seminar, Chem. Physics, University of Colorado, Boulder.
- 3/82 Symposium Organizer and Chair, "Chemical Processes in Solution," APS Meeting  
Dallas, TX.
- 3/82 Invited Lecture, Joe Mayer Sanibel Symposium, Palm Coast, FL.
- 3/82 Seminar, Chem. Dept., MIT.
- 3/82 Seminar, Chem. Dept., Harvard University.
- 9/82 Invited Lecture, ACS, Kansas City Meeting, Symposium on Transition State Theory.
- 10/82 Invited Lecture, CECAM Meeting on Simulation of Rare Events in Physics and  
Chemistry, Zwolle, Netherlands.
- 11/82 Seminar, Chem. Dept., University of Utah.
- 3/83 Seminar, Chem. Dept., University of Chicago.
- 3/83 Seminar, Chem. Dept., Northwestern University.
- 6/83 Invited Lecture, Canadian Chemical Conference, Symposium on Light Atom Kinetics  
and Reaction Dynamics, Calgary.
- 6/83 Invited Lecture, Conference on Molecular Dynamics of Collisions, Gull Lake, MN.
- 8/83 Invited Lecture, Gordon Conference on Liquids.
- 8/83 Discussion Leader, Reactions in Solution, NSF Workshop on Dynamics in Liquids,  
Penn State.
- 10/83 Seminar, Physics Dept., Colorado School of Mines.
- 11/83 Seminar, Chem. Dept., Colorado State University.
- 12/83 Seminar, Chem. Depts., Harvard University/MIT.
- 1/84 Seminar, Chem. Dept., University of Oregon.
- 1/84 Seminar, Chem. Dept., University of British Columbia.
- 1/84 Seminar, Chem. Dept., Simon Fraser University.

- 1/84 Invited Lecture, Conference on Chemical Reactions - New Concepts and Methods, Institute for Molecular Science, Okazaki, Japan.
- 1/84 Seminar, Chem. Dept., University of California Los Angeles.
- 1/84 Seminar, Chem. Dept., USC.
- 2/84 Invited Lecture, Colorado Section ACS Meeting, Denver.
- 3/84 Seminar, Chem. Dept., Columbia University.
- 3/84 Invited Lecture, California Conference on Statistical Mechanics, Davis, CA.
- 3/84 Contributed Lecture, California Conference on Statistical Mechanics, Davis, CA.
- 4/84 Seminar, Chem. Dept., University of MD.
- 4/84 Seminar, Bell Labs, Murray Hill, NJ.
- 6/84 Invited Lecture, Chemical Institute of Canada, Symposium on Photodissociation and Related Spectroscopy, Montreal.
- 7/84 Seminar, Chem. Dept., University of California, San Diego.
- 7/84 Invited Lecture, G. W. Robinson Conference on Molecular Dynamics and Spectroscopy, Lubbock, TX.
- 8/84 Invited Lecture, ACS Philadelphia Mtg., Symposium on Radical Reaction Kinetics.
- 10/84 Seminar, Chem. Dept., University of California, San Diego.
- 10/84 Seminar, Chem. Dept., University of Colorado, Boulder.
- 11/84 Invited Lecture, NSF/CECAM Workshop on Reaction Dynamics in Condensed Phases, Purdue University.
- 11/84 Seminar, Chem. Dept., Rice University.
- 3/85 Seminar, Chem. Dept., University of Rochester.
- 3/85 Seminar, Chem. Dept., University of Toronto.
- 3/85 Invited Lecture, Sanibel Symposium on Quantum Chemistry, St. Augustine, FL.
- 4/85 Invited Lecture, ACS Miami Meeting, Symposium on Theoretical Chemistry, sponsored by Chem. Educ. Division.
- 5/85 Invited Lecture, NIH Symposium on Rate Processes and First Passage Times, Bethesda, MD.
- 6/85 Seminar, Math. Institute University of Oxford.

- 7/85 Invited Lecture, Gordon Conference on Molecular Energy Transfer, Wolfboro, NH.
- 9/85 Invited Lecture, ACS Chicago Meeting, Symposium on Intramolecular Dynamics.
- 9/85 Invited Lecture, ACS Chicago Meeting, Symposium on Tunneling in Chemical Reactions (presented by D. Ali).
- 9/85 Seminar, Chem. Dept., University of Minnesota.
- 9/85 Invited Lecture, CECAM Workshop on Chemical Reactions in Solution, Paris, France.
- 10/85 Invited Lecture, CECAM Workshop on Intramolecular Vibrational Redistribution, Rochester, NY.
- 11/85 Seminar, Chem. Dept., University of California, San Diego.
- 1/86 Seminar, Chem. Dept., University of Colorado., Colorado Springs.
- 3/86 Invited Lecture, West Coast Theoretical Chemistry Conference, Santa Barbara, CA.
- 4/86 Invited Lecture, ACS New York Meeting, Symposium on the Role of the Solvent in Charge Transfer Reactions.
- 4/86 Invited Lecture, Sanibel Theoretical Chemistry Conference, Snowbird, UT.
- 5/86 Seminar, Chem. Depts., Harvard University/MIT.
- 5/86 Invited Lecture, Jerusalem International Symposium on Tunneling, Jerusalem, Israel.
- 6/86 Invited Lecture, Optical Society Meeting on Ultrafast Phenomena, Snowmass, CO.
- 6/86 Invited Lecture, Canadian Theoretical Chemistry Conference, Toronto, Canada.
- 7/86 Invited Lecture, NATO Advanced Workshop on Stochasticity and Intramolecular Redistribution of Energy, Orsay, France.
- 7/86 Invited Lecture, Symposium on Lasers, Molecules and Methods, Los Alamos, NM.
- 7/86 Seminar, Laboratoire Physique Théorique des Liquides, University of Paris VI, Paris.
- 9/86 Invited Lecture, CECAM Workshop on Molecular Dynamics Simulation of Solution Reactions, Orsay, France.
- 10/86 Seminar, Chemistry Department, University of Houston.
- 10/86 Seminar, Chemistry Department, University of Texas.
- 11/86 Seminar, Chemistry Department, Stanford University.

- 11/86 Plenary Lecture, Australian Conference on Chemical Kinetics, Leura, Australia.
- 11/86 Seminar, Chemistry Department, Australian National University, Canberra.
- 12/86 Seminar, Chemistry Department, Brookhaven National Laboratory.
- 12/86 Seminar, Chemistry Department, University of Sherbrooke, Canada.
- 12/86 Seminar, Chemistry Department, University of Toronto.
- 12/86 Seminar, Physics Department, University of Colorado, Boulder.
- 2/87 Seminar, Chemistry Department, University of Manchester, UK.
- 2/87 Seminar, Physical Chemistry Department, University of Oxford, UK.
- 3/87 Seminar, Theoretical Chemistry Department, University of Cambridge, UK.
- 4/87 Seminar, Theoretical Chemistry Department, University of Oxford, UK
- 5/87 Invited Lecture, Quantum Electrochemistry Symposium, Electrochemical Society Meeting, Philadelphia, PA.
- 5/87 Invited Lecture, Symposium on Intramolecular Kinetics, Royal Society, London.
- 5/87 Seminar, Laboratoire de Physique Théorique des Liquides, Université P. et M. Curie, Paris.
- 7/87 Seminar, Chemistry Department, University Autònoma, Barcelona.
- 8/87 Seminar, CECAM Workshop on Reactions in Solution, Orsay, France.
- 9/87 Invited Lecture, French Physical Chemistry Society Meeting on Chemical Reactions in Solution, Paris.
- 9/87 Invited Lecture, EPS Conference on Liquids of Small Molecules, Santa Trada, Italy (presented by M. Ferrario).
- 10/87 Seminar, Chemistry Department, University of California, San Diego.
- 10/87 Seminar, Chemistry Department, University of Pittsburgh.
- 11/87 Seminar, Chemistry Department, California Institute of Technology.
- 3/88 Invited Lecture, Faraday Symposium on Solvation, Durham, UK.
- 3/88 Seminar, Chemistry Department, York University, York, UK.
- 6/88 Invited Lecture, ACS Toronto Meeting, Symposium on Muonium Kinetics.

- 7/88 3 Invited Lectures, NATO Summer School on Enzyme Catalysis, Barga, Italy.
- 8/88 Invited Lecture, Gordon Conference on Water and Aqueous Solutions, Holderness, NH.
- 8/88 Plenary Lecture, International Conference on Quantum Chemistry, Jerusalem, Israel.
- 8/88 Seminar, CECAM Workshop on Reactions in Solution, Orsay, France.
- 9/88 Invited Lecture, ACS Los Angeles Meeting, Symposium on Dynamics in Condensed Media.
- 9/88 Seminar, Chemistry Department, University of California, Irvine.
- 10/88 Seminar, Chemistry Department, Penn State University.
- 10/88 Seminar, Chemistry Department, Catholic University.
- 11/88 Seminar, Chemistry Department, University of Washington.
- 1/89 Seminar, Chemistry Department, University of Wisconsin.
- 2/89 Seminar, Chemistry Department, Colorado State University.
- 3/89 Seminar, Physical Chemistry, University of California, San Diego.
- 3/89 Seminar, Chemistry Department, University of California, Berkeley.
- 3/89 Seminar, Chemistry Department, University of Puerto Rico, San Juan.
- 4/89 Seminar, Chemical Engineering Department, University of Colorado, Boulder.
- 4/89 Invited Lecture, ACS Dallas Meeting, Symposium on Computational Modeling of Molecular Systems.
- 4/89 Invited Lecture, ACS Dallas Meeting, Symposium on Relaxation and Dynamics in Complex Media.
- 5/89 CRCW Research Lecture, University of Colorado, Boulder.
- 5/89 Invited Lecture, Electrochemical Society, Symposium on Electron Transfer in Extended Systems, Los Angeles, CA.
- 5/89 Invited Lecture, Jerusalem Symposium on Quantum Chemistry and Biochemistry, Perspectives in Photosynthesis, Jerusalem, Israel.
- 5/89 Invited Lecture, CECAM Discussion Meeting on Computer Simulation of Quantum Reactions in Solution, Paris, France.
- 7/89 Invited Lecture, CECAM Discussion Meeting on Simulation of Proton Transfer

Reactions in Solution, Paris, France.

- 7/89 Invited Lecture, Gordon Conference on Molecular Energy Transfer, Wolfeboro, NH.
- 8/89 Discussion Leader, Gordon Conference on Physics and Chemistry of Liquids, Holderness, NH.
- 9/89 Invited Lecture, Symposium on Femtosecond Chemistry, ACS Miami Meeting, Miami, FL.
- 9/89 Invited Lecture, ACS Miami Meeting, Symposium on Chemical Kinetics, Miami, FL.
- 9/89 Invited Lecture, Conference on H Atom and Proton Transfer Reactions in Solution, West Germany.
- 9/89 Seminar, Physical Chemistry Department, Technical University, Munich, West Germany.
- 10/89 Invited Lecture, Conference on Chemical Reactions in Condensed Phases, Irvine, CA.
- 11/89 Seminar, Chemistry Department, University of North Carolina, Chapel Hill, NC.
- 12/89 Invited Lecture, Pacific Basin ACS Meeting, Symposium on Structure and Dynamics in Solution, Honolulu, HI.
- 3/90 Plenary Lecture, Sanibel Symposium on Quantum Chemistry, Solid-State Theory and Quantum Biology, St. Augustine, FL (delivered by H.J. Kim).
- 4/90 Invited Lecture, ACS Boston Meeting, Symposium on Classical and Quantum Simulation of Reactions and Solvation Dynamics, Boston, MA.
- 4/90 Invited Lecture, ACS Boston Meeting, Symposium on Reaction Paths in Chemistry, Boston, MA.
- 6/90 Invited Lecture, Regional ACS Meeting, Symposium on Inhomogeneous Reaction Kinetics, Salt Lake City, UT.
- 6/90 Invited Lecture, Lab. de Physique Théorique des Liquides, Univ. Paris VI, Paris, France.
- 7/90 Invited Lecture, Symposium on the Frontiers of Theoretical Chemistry, Chemical Institute of Canada, Halifax, NS, Canada.
- 7/90 Invited Lecture, Physical Electrochemistry Gordon Conference, New London, NH.
- 7/90 Invited Lecture, American Theoretical Chemistry Conference, San Diego, CA.
- 8/90 Invited Lecture, ACS Washington Meeting, Symposium on Electron Transfer Reactions, Washington, DC.
- 8/90 Plenary Lecture, International Conference on Atomic, Molecular and Structural

Aspects of Electrochemistry, Trieste, Italy.

- 9/90 Invited Lecture, Interdisciplinary Conference on Electrified Interfaces, Asilomar, CA.
- 9/90 Plenary Lecture, NATO Advanced Research Workshop/Discussion Meeting of Deutsche Bunsengesellschaft für Physicalische Chemie "Rate Processes in Dissipative Systems: 50 years after Kramers", Tutzing, Bavaria.
- 9/90 Lecture, International Conference on Industrial Applications of Natural, Modified and Artificial Enzymes, Pisa, Italy.
- 9/90 Seminar, Chemistry Dept., University of Pisa, Pisa, Italy.
- 10/90 Invited Lecture, CECAM Workshop on "Quantum Chemistry and Chemical Reactions in Solution", Orsay, France.
- 10/90 Seminar, Chemistry Department, Harvard University.
- 10/90 Seminar, Chemistry Department, Brown University.
- 1/91 Invited Lecture, Kasha Symposium on Hydrogen Transfer Dynamics in Chemistry, Physics and Biology, Tallahassee, FL.
- 2/91 Invited Lecture, AAAS Symposium on the Revolution in Kinetics, Washington, DC.
- 2/91 Seminar, Chemistry Department, University of Pennsylvania.
- 3/91 Seminar, Chemical Physics, University of Colorado, Boulder.
- 3/91 Seminar, Chemical Physics Department, University of California, Riverside, CA.
- 3/91 Seminar, Chemistry Department, University of California, Riverside, CA.
- 4/91 Seminar, Condensed Phase Theory Division, Battelle, Northwest, Richland, WA.
- 5/91 Plenary Lecture, International Conference on Photoinduced Electron Transfer, Osaka, Japan.
- 5/91 Invited Lecture, Symposium on Ultrafast Processes in Solution, University of Kyoto, Japan.
- 6/91 Invited Lecture, International Symposium on Computer Simulation of Biomolecular Systems and Mechanism, Menton, France.
- 6/91 Plenary Lecture, Conference on Electron Transfer, Sophia Antipolis, France.
- 8/91 Invited Lecture, Symposium on Energy Transfer and Relaxation in Condensed Phases, ACS New York Meeting.
- 1/92 Invited Lecture, DOE Joint Israel-U.S. Workshop on Computational Chemistry, Berkeley, CA.

- 2/92 Seminar, Chemistry Department, Northwestern University, Evanston, IL.
- 4/92 Invited Lecture, Second Conference on Chemical Dynamics in Condensed Phases, University of California, Irvine, CA.
- 6/92 Seminar, Theoretical Chemistry Department, University Autònoma, Barcelona, Spain.
- 6/92 Invited Lecture, European Science Foundation Conference on Electronic Structure, Costa Brava, Spain.
- 7/92 Invited Lecture, Telluride Workshop on Large Amplitude Motion in Chemistry, Telluride, CO.
- 8/92 Plenary Lecture, Gordon Conference on Electron Donor-Acceptor Interactions, Plymouth, NH.
- 8/92 Invited Lecture, Symposium on Photochemistry, DC ACS Meeting, Washington, DC.
- 9/92 Plenary Lecture, International Conference of Excited State Electron Transfer, Warsaw, Poland.
- 9/92 Seminar, Chemistry Department, MIT, Cambridge, MA.
- 10/92 Seminar, Chemistry Department, University of Chicago, Chicago, IL.
- 2/93 Seminar, Chemistry Department, University of California at Davis.
- 2/93 Seminar, Chemistry Department, University of California at Santa Cruz.
- 2/93 Seminar, Chemistry Department, Texas A&M University.
- 3/93 Seminar, Chemistry Department, Purdue University.
- 5/93 Invited Lecture, Symposium on Ultrafast Processes in Solution, Paris, France.
- 5/93 Seminar, Quantum Chemistry Department, University of Paris VI, Paris, France.
- 5/93 Invited Lecture, Jerusalem Conference on Reaction Dynamics, Jerusalem, Israel.
- 5/93 Seminar, Chemistry Department, University of Pisa, Pisa, Italy.
- 7/93 Invited Lecture, Gordon Conference on Energy Transfer, NH.
- 7/93 Invited Lecture, American Conference on Theoretical Chemistry, Rochester, NY.
- 8/93 Invited Lecture, Symposium on Tunneling, Chicago ACS Meeting, Chicago, IL.
- 9/93 Invited Lecture, NATO Advanced Study Workshop on Photoinduced Electron

Transfer, Algarve, Portugal.

- 10/93 Seminar, Chemistry Department, Iowa State University, Ames, IA.
- 10/93 Seminar, Chemistry Department, University of Illinois, Urbana, IL.
- 12/93 Seminar, Chemistry Department, Carnegie-Mellon University, Pittsburgh, PA.
- 3/94 Invited Lecture, Symposium on Reactions in Aqueous Solutions, ACS Meeting, San Diego, CA.
- 4/94 Seminar, Chemistry Department, University of Rochester, Rochester, NY.
- 4/94 Seminar, Chemistry Department, Cornell University, Ithaca, NY.
- 4/94 Seminar, Chemistry Department, SUNY at Buffalo, Buffalo, NY.
- 4/94 Seminar, Chemistry Department, Louisiana State University, Baton Rouge, LA.
- 8/94 Invited Lecture, IUPAC Symposium on Physical Organic Chemistry, Padova, Italy.
- 9/94 Invited Lecture, International Symposium on Ultrafast Processes, Zakopane, Poland.
- 10/94 Seminar, Chimie Moléculaire, Saclay, France.
- 10/94 Invited Lecture, Workshop on Computer Simulation of Reactions, CECAM, Lyons, France.
- 10/94 Seminar, Chemistry Department, Argonne National Laboratory, Argonne, Illinois.
- 10/94 "Mr. Wizard" Science Series, Boulder, CO.
- 11/94 Seminar, Chemistry Department, Georgia Tech, Atlanta, GA.
- 11/94 Seminar, Chemistry Department, University of Minnesota.
- 2/95 Seminar, Chemistry Department, Boston College, Boston, MA.
- 3/95 Seminar, Chemistry Department, Notre Dame University, IN.
- 3/95 Invited Lecture, Symposium on Gas Phase and Condensed Phase Reactions, American Physical Society, San Jose, CA.
- 5/95 Invited lecture, Jerusalem Symposium on Electron Transfer Processes, Jerusalem, Israel, (delivered by H. Kim).
- 5/95 Two invited lectures, International School on Quantum Simulation Methods for Biological Systems, Les Houches, France.
- 6/95 Two seminars, Quantum Chemistry Department, Univ. Autònoma, Barcelona, Spain.

- 7/95 Invited Lecture, Portuguese Chemical Society, Porto, Portugal.
- 7/95 Invited Lecture, Catalan Quantum Chemistry Society, Barcelona, Spain.
- 7/95 Invited Lecture, French Physical Chemistry Society, Lille, France.
- 8/95 Invited Lecture, Canadian Conference on Theoretical Chemistry, New Brunswick, Canada.
- 9/95 Invited Lecture, International Symposium on Femtochemistry, Lausanne, Switzerland.
- 10/95 Two seminars, Service de Chimie Moléculaire, Saclay, France.
- 10/25 Seminar, Laboratoire de Photophysique Moléculaire, Orsay, France.
- 10/95 Seminar, Physics Department, Polytechnical University, Barcelona, Spain
- 11/95 Seminar, Service de Chimie Moléculaire, Saclay, France.
- 11/95 Seminar, Laboratoire d' Electrochimie, Université de Paris VII, France.
- 12/95 Invited Lecture, Faraday Discussion on Unimolecular Reactions, Oxford, England.
- 1/96 "Mr. Wizard" Science Series, Boulder, CO.
- 1/96 Invited Lecture, Gordon Research Conference on Isotopes in Chemistry and Biology, Ventura, CA.
- 3/96 Invited Lecture, American Chemical Society Meeting, Symposium on the Transition State, New Orleans, LA.
- 5/96 Invited Lecture, Ultrafast Phenomena Conference, American Optical Society, San Diego, CA.
- 7/96 Invited Lecture, European Physical Society Meeting on Dynamics in Excited Organic Molecules, Riccione, Italy.
- 9/96 Plenary Lecture, Royal Society Meeting on Fast Reaction Dynamics, Graz, Austria.
- 9/96 Invited Lecture, Nobel Symposium on Femtochemistry, Bjorkborn, Sweden.
- 10/96 Seminar, Service de Chimie Moléculaire, CEA, Saclay, France.
- 10/96 Seminar, Chemistry Department, Ecole Normale Supérieure, Paris, France.
- 10/96 Seminar, Service de Chimie Moléculaire, CEA, Saclay, France.
- 10/96 "Mr. Wizard" Science Series, University of Colorado, Boulder.
- 11/96 Invited Lecture, 250 Years of Chemistry at Princeton, Princeton University, NJ.

- 2/97 Invited Lecture, Mesilla Workshop on Dynamics, Mesilla, NM.
- 2/97 ACS Lecturer, Chemistry Department, University of Wisconsin, Madison, WI.
- 2/97 Seminar, Chemistry Department, University of Wisconsin, Madison, WI.
- 3/97 Seminar, Chemistry Department, California Institute of Technology, Pasadena, CA.
- 3/97 Invited Lecture, Symposium on Vibrational Energy Transfer, American Physical Society, Kansas City, MO.
- 6/97 Two Seminars, Chemistry Department, Ecole Normale Supérieure, Paris, France.
- 10/97 Seminar, Photochimie Moleculaire, Saclay, France.
- 8/97 Invited Lecture, International Conference on Photochemistry, Warsaw, Poland.
- 8/97 Invited Lecture, International Conference on Femtochemistry, Lund, Sweden.
- 9/97 Plenary Lecture, International Conference on Proton Transfer, Berlin, Germany.
- 10/97 Three seminars, Laboratoire de Photophysique Moleculaire, Orsay, France.
- 11/97 Plenary Lecture, Korea Institute of Advanced Studies Conference on Theoretical Chemistry, Seoul, Korea.
- 11/97 Seminar, Chemistry Department, Seoul National University, Seoul, Korea.
- 11/97 Seminar, French/German GDR Meeting on Ultrafast Phenomena, Munich, Germany.
- 3/98 Invited Lecture, Japanese Physical Society Meeting, Japan.
- 3/98 Invited Lecture, International Conference on Nonadiabatic Transitions, Okazaki, Japan.
- 6/98 Invited Lecture, Annual Meeting, French Photochemistry Group, Paris, France.
- 6/98 Seminar, Theoretical Chemistry Department, University of Nancy, France.
- 6/98 Invited Lecture, International Conference on Water in the Gas Phase, Paris, France
- 7/98 Invited Lecture, Faraday Society Discussion on Chemical Reaction Theory, St. Andrews, Scotland.
- 8/98 Invited Lecture, Symposium on 20 Years of Theoretical Chemistry, ACS Meeting, Boston, MA.
- 10/98 Invited Talk, Workshop on Computer Modelling and Simulation, University of Colorado, Boulder, CO.

- 10/98 Invited Lecture, International Conference on Proton Transfer, Jerusalem, Israel.
- 12/98 Seminar, Environmental Molecular Sciences Lab, PNNL, Richland, WA.
- 2/99 Invited Lecture, Conference on Molecular Reaction Dynamics in Condensed Media, Newport Beach, CA.
- 2/99 Seminar, Physics Department, University of Colorado, Boulder, CO
- 3/99 Plenary Lecture, Sanibel Symposium, St. Augustine, FL.
- 3/99 Invited Lecture, Liquid Chemical Dynamics Symposium, American Physical Society, Atlanta, GA.
- 4/99 Seminar, NOAA Aeronomy Laboratory, Boulder, CO.
- 6/99 Invited Lecture, American Conference on Theoretical Chemistry, Boulder, CO.
- 6/99 Invited Lecture, Gordon Conference on Physical Organic Chemistry, Holderness, NH.
- 7/99 Seminar, Chemistry Department, Ecole Normale Supérieure, Paris.
- 7/99 Plenary Lecture, Femtochemistry IV, Leuven, Belgium.
- 8/99 Plenary Lecture, International Conference on Photochemistry, Durham, NC.
- 10/99 Seminar, Harvard/MIT, Cambridge, MA.
- 10/99 Invited Lecture, Symposium on Interfacial Phenomena, SWARM ACS Meeting, El Paso, TX.
- 11/99 Seminar, CNRS Division 17 Meeting, Paris, France.
- 11/99 CU Wizard Show, Boulder, CO.
- 11/99 Plenary Lecture, Southwest Theoretical Chemistry Conference, Lubbock, TX.
- 1/00 Invited Lecture, Gordon Conference on Isotope Effects in Chemistry and Biochemistry, Ventura, CA.
- 1/00 Plenary Lecture, Symposium on Reactivity on Ice, Vars, France.
- 2/00 Invited Lecture, Mesilla Workshop on Dynamics of Enzyme-Catalyzed Reactions, Mesilla, NM.
- 3/00 Invited Lecture, Computational Chemistry Award Symposium, American Chemical Society National Meeting, San Francisco, CA
- 4/00 Invited Lecture, Annual Meeting, French Photochemistry Group, Paris, France.
- 5/00 Four invited lectures as Distinguished Laboratory for Molecular Sciences Lecturer,

Cal Tech, Pasadena, CA.

- 6/00 Invited Lecture, French Gas Phase Kinetics Group, Paris, France.
- 8/00 Invited Lecture, Symposium on Hydrogen Transfer Reactions, American Chemical Society National Meeting.
- 9/00 Plenary Lecture, PULS Conference, Poland.
- 9/00 Plenary Lecture, GdR Meeting on Ice, Porquerolles, France.
- 9/00 Invited Lecture, Symposium on Modeling and Catalysis, SFC 2000, French Chemical Society, Rennes, France.
- 10/00 Invited Lecture, International Meeting on Ultrafast Dynamics, Paris, France.
- 11/00 Two Invited Lectures, Frederick Kaufman Lecturer, University of Pittsburgh, PA.
- 1/01 Merck Frosst Lecturer, Chemistry Department, Concordia University, Montreal, Quebec, CA.
- 1/01 Seminar, Theoretical Chemistry Department, University of P. et M. Curie, Paris, FR.
- 1/01 Plenary Lecture, Inauguration of Center for Molecular Reactivity Modeling, Concordia University, Montreal, Quebec, CA.
- 1/01 Invited Seminar, CECAM, Ecole Normal Superieure, Lyon, FR.
- 3/01 Invited Lecture, Symposium on Dynamics in Ionic Solutions, Amer. Physical Society National meeting, Seattle, WA.
- 3/01 Seminar, Chemistry Department, University of Washington, Seattle, WA.
- 4/01 van Marum Lecture, Gorlaeus Labs, University of Leiden, Leiden, Netherlands.
- 4/01 Invited Seminar, Centre de Recherche en Chimie Moléculaire, Univ. of Bordeaux, Bordeaux, FR.
- 4/01 Plenary Lecture, 12<sup>th</sup> Congress, Argentinian PhysicoChemical Society, Buenos Aires, Argentina.
- 4/01 Invited Lecture, Nanophyschem 2001, San Martin de Los Andes, Argentina.
- 6/01 Invited Lecture, Summer School on Ultrafast Vibrational Spectroscopy, Berlin, DE.
- 7/01 Plenary Lecture, French Physical Society Meeting, Strasbourg, FR
- 9/01 Plenary Lecture, Femtochemistry V International Symposium, Toledo, Spain.
- 9/01 Plenary Lecture, International Symposium on Electronic Structure and Chemical

Reactivity, Barcelona, Spain.

- 10/01 Invited Seminar, Department of Chemistry, University of Texas, Austin, TX.
- 11/01 CU Wizards Show, Univ. of Colorado, Boulder, CO
- 1/02 Invited Lecture, Gordon Conference on Clusters, Ventura, CA.
- 3/02 Plenary Lecture, Ringberg Conference on Hydrogen Transfer and Transport, Tegernsee, DE
- 3/02 Seminar, Chemistry Dept., Penn. State Univ., University Park, PA
- 4/02 Invited Lecture, Symposium on Modeling Kinetics, Mechanism and Catalysis, ACS National Meeting, Orlando, FL.
- 4/02 Invited Lecture, CECAM Meeting on Nonadiabatic Transitions, Lyon, FR
- 5/02 Three lectures, Teacher Education Program "Reaction Mechanisms", ENS, Paris
- 5/02 Invited Lecture, Journées des Ecoles Doctorales Carnot (Bourgogne) et Pasteur (Franche-Comté), Besancon, FR
- 5/02 Invited Lecture, Société Vaudoise Sciences Naturelles, Lausanne, CH
- 5/02 Invited Lecture, French Group on Kinetics and Photochemistry in the Gas Phase, Paris, FR
- 6/02 Invited Lecture, Hydrogen Bonding and Transfer Program, Free University of Berlin, Berlin, DE.
- 6/02 Invited Lecture, European Science Foundation Summer School on "Theory and Experiment in Ultrafast Processes", Algarve, Portugal.
- 7/02 Invited Lecture, Gordon Research Conference on Vibrational Spectroscopy and Molecular Dynamics, Rhode Island.
- 7/02 Keynote Lecture, IV International Conference, International Society for Theoretical Chemical Physics, Paris, FR.
- 7/02 Invited Lecture, IUPAC International Meeting on Photochemistry, Budapest, Hungary.
- 9/02 Invited Lecture, Conference in Honor of M. El-Sayed and J. Jortner, Paris, FR.
- 11/02 Invited Lecture, Workshop on "The Molecular Basis of Catalysis", Academy Committee for Chemistry, Science Division, Netherlands Academy of Arts and Sciences, Amsterdam, Netherlands.
- 1/03 Invited Lecture, Institut de Recherche sur les Systemes Atomiques et Moleculaires

Complexes, Toulouse, FR.

- 1/03 Invited Lecture, Groupe de Recherche "Ice", Les Houches, FR.
- 3/03 Invited Seminar, Chemistry Department, Princeton Univ., Princeton, NJ.
- 3/03 Invited Lecture, Symposium on Analysis and Control of Ultrafast Photoinduced Reactions, Berlin, GE.
- 6/03 Invited Lecture, Symposium Honoring Joshua Jortner, Tel Aviv, IS
- 6/03 Invited Lecture, International Summer School of Femtochemistry, Algarve, Portugal.
- 6/03 Invited Seminar, Theoretical Chemistry, Oxford University, Oxford, UK
- 7/03 Invited Lecture, Symposium Honoring Jean-Louis Rivail, Nancy, FR.
- 9/03 Invited Lecture, CECAM Workshop on Multi-Scale Modeling of Chemical Reactivity, Lyon, FR
- 10/03 Invited Lecture, Mike Weaver Symposium, Electrochemical Society Meeting, Orlando, FL
- 11/03 CU Wizards Show, Univ. Colorado, Boulder CO
- 2/04 Plenary Lecture, International Symposium on "Theory and Application in Computational Chemistry", Korea
- 3/04 Invited Lecture, 7<sup>th</sup> Symposium on Molecular Reaction Dynamics in Condensed Matter, Laguna Beach, CA.
- 3/04 Invited Lecture, Symposium on H Transfer in Biological Systems, American Physical Society Mtng, Montreal, CA
- 3/04 2 Lectures, Symposium on Physics and Chemistry of the Atmosphere, American Physical Society Mtng, Montreal, CA.
- 3/04 Invited Lecture, 4<sup>th</sup> Symposium, Center for Research in Molecular Modelling, Concordia Univ., Montreal, CA
- 3/04 Invited Lecture, Symposium on Vibrational Analyses of Dry and Wet Surfaces, American Chemical Society Mtng, Anaheim, CA.
- 3/04 Invited Lecture, Symposium on Computations for Environmental Chemistry, American Chemical Society Mtng, Anaheim, CA.
- 5/04 Invited Lecture, Symposium on Classical and Quantum Approaches to Rare Events, Canadian Chemistry Conference, London, Ont., CA

- 6/04 Invited Seminar, Chemistry Dept., Univ. of Paris VII, Paris, FR
- 7/04 Invited Lecture, French Summer School on Ultrafast Processes, FR.
- 7/04 Invited Lecture, Gordon Research Conference on Computational Chemistry, New Hampshire
- 7/04 Oral Presentation, IUPAC Photochemistry Congress, Granada, SP
- 8/04 Invited Lecture, Symposium on Quantum/Classical Calculations in Chemistry and Biophysics, American Chemical Society Meeting, Philadelphia, PA.
- 8/04 Plenary Lecture, International Symposium "Modelling and Understanding in Theoretical Chemistry", Lucca, IT
- 9/04 Invited Lecture, CECAM Meeting on Energy Localization: From Small Polyatomic Molecules to Large Biomolecules, Lyon, FR
- 10/04 Plenary Lecture, Symposium on Computational Chemical Dynamics: from Gas-Phase to Condensed-Phase Systems, Univ. of Minnesota, Minneapolis, MN
- 10/04 Three Invited Hirschfelder Prize in Theoretical Chemistry Lectures, Chem. Dept., Univ. of Wisconsin, Madison, WI
- 10/04 Plenary Lecture, NSF Mathematical and Physical Sciences Workshop, Arlington, VA
- 12/04 Invited Lecture, Physical Chemistry/Chemical Physics, Univ. of Colorado, Boulder, CO
- 3/05 Invited Lecture, Symposium on Hydrogen Bonds, Amer. Chem. Soc. Mtng, San Diego, CA
- 3/05 Invited, Lecture, ACS Award Symposium, Amer. Chem. Soc. Mtng, San Diego, CA
- 6/05 Seminar, Theoretical Chemistry Dept., Bochum DE
- 6/05 Invited Lecture, IMS/NAREGI International Nanoscience Conference, Nara, JP
- 7/05 Plenary Lecture, Isotopes 2005, Bath, UK.
- 7/05 Plenary Lecture, International Conference on Photochemistry, Cairns, Australia
- 7/05 Plenary Lecture, Femtochemistry VII, Washington, DC

8/05 Invited Lecture, Symposium "Ions in Complex Physical, Chemical, and Biological Systems." Amer. Chem. Soc. Meeting, Washington, DC

9/05 Invited Lecture, International Bunsen-Discussion Meeting on "Time-resolved transformations in complex molecular environments », Gottingen, DE

11/05 Lecture, « CU Wizard » Popular Science series, Univ. CO, Bldr.

12/05 Invited Lecture, Symposium on Quantum and Classical Theory of Solvation, ACS Pacific Meeting, Honolulu

1/06 Frontier Lecture, Indian Inst. Of Science and Nehru Center for Advanced And Scientific Research, Bangalore, IN

2/06 Invited Lecture, Gordon Conference on Isotope Effects, Ventura, CA

3/06 Lecture, Davidson Chem. Dept., Univ of Kansas, Lawrence, KS

3/06 Lecture, Chem. Dept., Univ of Kansas, Lawrence, KS

3/06 Invited Lecture, EPFL, Lausanne, CH

3/06 Invited Lecture, Symposium on atmospheric chemistry, Amer. Chem. Soc. Meeting, Atlanta, GA

5/06 Invited Lecture, Workshop on Reactions in Solution and Biosystems, Kyoto, JP

5/06 Plenary Lecture, ESF Summer School on Ultrafast Dynamics, Algarve, Portugal

7/06 Invited Lecture, Gordon conf on vibrational dynamics, Maine

7/06 Invited Lecture, CIM International Workshop on Mathematics in Chemistry, Lisbon, Portugal

8/06 Invited Lecture Gordon Conference on Water, Holderness, NH

9/06 Invited Lecture, Symposium on 50 Years of Electron Transfer and RRKM Theory, ACS Meeting, San Francisco

10/06. Invited Seminar, Chem Dept, Yale Univ.

2/07 Welch Lecture, Chem. Dept., Southern Methodist Univ., Dallas, TX

2/07 Welch Lecture, Chem. Dept., Texas A&M, Commerce, TX

3/07 Welch Lecture, Chem. Dept., Tarleton State Univ., Stephenville, TX

3/07 Invited Lecture, Symposium on Electron and Ion Solvation in Clusters and the Condensed Phase, American Physical Soc. Natl Mtng, Denver, CO

3/07 Invited Lecture, Emily Carter Symposium, ACS Meeting, Chicago, IL

4/07 3 Invited Lectures, Spring College:Water in Physics, Chemistry and Biology, International Centre for Theoretical Physics, Trieste, IT

5/07 Invited Lecture, International Conference on Isotopes, Spain

5/07 Invited Lecture, Kapral/Whittington Conference, Toronto, Ontario, CA

8/07 Invited Lecture, Symposium on Quantum Effects, ACS Meeting, Boston, MA

9/07 Invited Lecture, International Meeting on Proton Conduction, Banff, Canada

10/07 Invited Lecture, International Meeting on Energy Transfer in Biological Systems, Paris, FR

11/07 Popular Science Lecture, 'CU Wizards', CU, Boulder

1/08 Invited Lecture, International Meeting on Proton Transfer, Eliat, Israel

1/08 Invited Lecture, UCI Workshop on Interfacial Processes Relevant for the Atmosphere, Newport Beach, CA.

6/08 Invited Lecture, 11<sup>ème</sup> Rencontre des Chimistes Théoriciens Francophones, Dinard, FR

6/08 Invited Lecture, COST D35 - ESF DYNA Workshop on Electronic Excited States in Condensed Phases, Sicily

7/08 Plenary Lecture, PAMO (French Physical Society) Meeting on Molecular Spectroscopy, Lille, FR

7/08 Invited Lecture, American Theoretical Chemistry Conference, Chicago, IL.

7/08 Invited Lecture, Gordon Conference on Water and Aqueous Solutions, NH

8/08 Invited Lecture, Symposium on Water Mediated Interaction, ACS Meeting, Philadelphia

10/08 Invited Lecture, International Workshop on Ultrafast Chemical Physics, Glasgow, UK.

3/09 Invited Lecture, Symposium on Functional Motions in Enzyme Catalysis, ACS Meeting, Salt Lake City, UT, USA.

3/09 Invited Lecture, Greater Boston Area Theoretical Lecture Series, Boston, MA

5/09 Invited Lecture, Isotopes 2009, Romania

7/09 Invited Lecture, Gordon Conference on Electronic Spectroscopy and Dynamics, Waterville, Maine.

7/09 Invited Plenary Lecture, International Conference on Photochemistry, Toledo, Spain

8/09 Invited Lecture, Femtochemistry IX, Beijing, China

9/09 Invited Lecture, Physical Chemistry/Chemical Physics Colloquium, U. Colorado, Boulder, CO

10/09 Invited Lecture, Dept. Chemistry, Colorado State Univ., Fort Collins, CO

11/09 Invited Lecture, CU Wizards Popular Science Lectures, Boulder, CO

2/10 Invited Lecture, Gentner Symposium, Proton Mobility in Chemical and Biological Systems, Lake Gallilee, Israel

3/10 Invited Lecture, Astrobiology Program, Univ. Colorado, Boulder, CO

5/10 Invited Lecture, PRG Chemistry Lecture, Univ. Paris VII, Paris, FR

5/10 Invited Lecture, CECAM Workshop, Quantum Coherence, Dublin, IR COMPLETE

7/10 Invited Seminar, Chemistry Dept, Univ. of Valencia, SP

7/10 Invited Lecture, Gordon Conference on Atomic and Molecular Interactions, New Hampshire

8/10 Invited Lecture, Gordon Conference on Vibrational Spectroscopy and Energy Transfer, New Hampshire

12/10 Invited Lecture, Symposium on Recent Advances in Molecular Processes at Liquid Interfaces, Pacificchem, Honolulu

4/11 Invited Session Chair, Faraday Discussion 150, Frontiers of Spectroscopy, Basel, CH

5/11 Invited Lecture, CECAM Workshop, Vibrational Spectroscopy of Complex Systems, Paris, FR

6/11 Invited Lecture, Time-Resolved Vibrational Spectroscopy XV, Ascona, Switzerland

7/11 Invited Lecture, Femtochemistry 10, Madrid, SP

7/11 Invited Lecture, 9<sup>th</sup> Congress, World Association of Theoretical and Computational Chemists, Santiago de Compostela, SP

7/11 Invited Lecture, Telluride Workshop "IR and far-IR spectroscopy: Studying hydration of ions and biomolecules---in clusters, at surfaces, and in the bulk", Telluride, CO

8/11 Invited Lecture, Symposium on Solar Photocatalysis, ACS National Meeting, Denver,

CO

9/11 Invited Plenary Lecture, 7<sup>th</sup> Congress International Society for Theoretical Chemical Physics, Tokyo, JP

9/11 Invited Lecture, Harvard-MIT Seminar, Cambridge, MA

9/11 Invited Lecture, Workshop on Temporally and Spatially Resolved Dynamical Phenomena , DRESSY, Hamburg, DE

10/11 Invited Lecture, Proton Coupled Electron Transfer 2011 'From biology to catalysis', Loire Valley, FR

10/11 2 Invited Lectures, Dept. Chemistry, Univ. of Bristol, UK

11/11 Invited Lecture, Mischa Bonn Symposium, AMOLF, Amsterdam, NE

1/12 CU Wizards Popular Science Show

3/12 Invited Lecture, Symposium on Water Mediated Assembly, ACS National Meeting, San Diego, CA

5/12 Invited Seminar, Physical and Theoretical Chemistry, Oxford Univ., UK

6/12 Invited Lecture, International Congress on Quantum Chemistry, Boulder, CO  
CANCELLED DUE TO ILLNESS

8/12 Invited Lecture, Gordon Conference on Water and Aqueous Solutions, Holderness, NH  
CANCELLED DUE TO ILLNESS

8/12 Invited Lecture, Symposium on Electron Transfer, ACS National Meeting, Philadelphia, PA. CANCELLED DUE TO ILLNESS

8/12 Invited Lecture, Symposium on Recent advances in studies of molecular processes at liquid interfaces, ACS National Meeting, Philadelphia, PA. CANCELLED DUE TO ILLNESS

7/13 Invited Lecture and Session Chair, Femto11, Copenhagen, DK

10/13 3<sup>rd</sup> Pople Lecture, Dept. of Chemistry, Carnegie-Mellon Univ., Pittsburgh, PA

12/13 CU Wizards Popular Science Lecture

2/14 Plenary Lecture, Bagchi Festschrift , Kanpur, IN

4/14 Invited Lecture, ICCMSE Congress, Electron and Proton Transfer Symposium, Athens, GR

5/14 Invited Lecture, CECAM meeting on Quantum Effects in Biological Systems, Paris, FR

6/14 Invited Lecture, PCET 2014, Stockholm, Sweden

7/14, Invited Lecture, Gordon Conference on Water, New Hampshire

8/14 Invited Lecture, Gordon Conference on Vibrations, Maine

8/14 **3** Invited Lectures, Amer Chem Soc Natl Mtng, San Francisco

9/14 Invited Seminar, Physical Chemistry/Chemical Physics, Univ. Colorado, Boulder, CO

9/14 Oscar K. Rice Lecture, Chemistry Dept., Univ. North Carolina, Chapel Hill, NC

3/15 Invited Seminar, Computational Chemistry and Materials Science Series, NREL, Golden, CO.

3/15 Invited Lecture, Symposium on Molecular Catalysts for Solar Fuels, ACS Natl. Mtng, Denver, CO

5/15 Invited Seminar, Precision Spectroscopy Laboratory, East China Normal Univ., Shanghai, China

5/15 Invited Seminar, Chemistry Dept., Fudan Univ. Shanghai, China

5/15 Invited Seminar, Computational Chemistry, ECNU-NYU, Shanghai, China

6/15 Invited Seminar, Theoretical Chemistry, Univ. Jaume 1, Castellon, Spain

6/15 Invited Seminar, Theoretical Chemistry, Univ. of Valencia, Valencia, Spain

10/15 Invited Lecture, International Conference on “Water at the Interface between Biology, Chemistry, Physics and Materials Science”, Int’l. Center for Theoretical Physics, Trieste, IT

3/16 Invited Lecture. “Status and Prognosis of Future Generation Photoconversion to Photovoltaics and Solar Fuels”, Arthur J. Nozik Fest, Boulder, CO.

4/16. Invited Seminar, Chemistry Dept. Univ. Texas, San Antonio, TX

5/16. Invited Lecture, International Meeting, Singapore cancelled

6/16 Three (3) Heinemann Hall Named Lectures, Chemistry, Bowling Green Univ. Ohio,

6/16. Invited Lecture, CECAM meeting on Prebiotic Chemistry, Paris, FR

6,7/16 Invited Plenary Lecture, 10<sup>th</sup> Congress on Electronic Structure: Principles and Applications, Castellon, SP

7/16 Invited Seminar, East China Normal University, Shanghai, China

9/16 Invited Lecture, GDR Ultrafast Phenomena Meeting, Paris, FR

4/17 Invited Lecture, American Chemical Society National Meeting, San Francisco, CA

8/17 Invited Lecture, Femto 13, Cancun, Mexico

9/17 invited Plenary Lecture, Annual Meeting of Japan Society for Molecular Science, Sendai, Japan

11/17 Invited Seminar, Theoretical Chemistry, Cambridge Univ., Cambridge UK

### **Commitments**

2/18 Invited Lecture, Recent Advances in Molecular Simulations, Indian Institute of Science, Bangalore IN (Cancelled due to illness)

10/18 Invited Lecture, Welch Foundation Conf. on Chemical Research: "Water: Science & Technology", Houston, TX

### **Conferences & Symposia Organized**

"Chemical Reactions in Solution", Dallas APS Meeting, Mar. 1982.

"Reactions in Solution", Gordon Conference on Physics and Chemistry of Liquids, Aug. 1983.

"Tunneling in Chemical Reactions", ACS Chicago Meeting, Sept. 1985.

"The Role of the Solvent in Charge Transfer Reactions", ACS New York Meeting, April 1986.

"ACS Pure Chemistry Award to P. G. Wolynes," ACS New York Meeting, April 1986.

"Molecular Dynamics Computer Simulation of Reactions in Solution," CECAM Workshop, Orsay, France, Sept. 1986.

"Chemical Reactions in Solution," French Physical Society, Paris, France, Sept. 1987 (member, organizing committee).

"Computer Simulation and Theory of Chemical Reactions in Solution" CECAM Workshop, Orsay, France, Aug. 1987.

"Nonlinear Processes in Chemistry", Toronto ACS Meeting, June 1988 (w/R. Kapral).

"Computer Simulation and Theory of Chemical Reactions in Solution" CECAM Workshop, Orsay, France, Aug. 1988.

"Molecular Dynamics Simulation of Proton Transfer Reactions in Solution", CECAM Discussion Meeting, Paris, France, July 1989 (w/D. Borgis).

"Quantum Chemistry and Chemical Reactions in Solution", CECAM Workshop, Paris,

France, October 1990 (w/D. Borgis).

"Ultrafast Processes in Solution", Paris, France, May 1993 (member, organizing committee).

"Ultrafast Phenomena in Liquids and Glasses", Zakopane, Poland, Sept. 1994 (member, scientific committee).

"Proton Transfer Reactions", (w/M. Kreevoy) Chicago, ACS, Aug. 1995.

"Femtochemistry VI", (w/M. Martin), Paris, FR July 2003.

Theoretical and Computational Conference (TACC), Shanghai, China Sept. 2008

### **Students and Postdoctoral Researchers**

#### Undergraduate Students

Charles C. Gubser - (5/92-5/93) - UROP Undergraduate Research Fellow, Hughes Foundation Trainee. (Subsequently Churchill Fellow at Cambridge University. Currently D. Phil. student, Cambridge University).

#### Graduate Students

Scott H. Northrup - Ph.D. 1979 - Chemical Reactions in Liquids. (Subsequently NIH Fellow w/J. A. McCammon, Houston. Currently Prof. Chem., Tennessee Tech. Univ.

David J. Nesbitt - Ph.D. 1981 - (Joint w/S. Leone) - Vibrational Relaxation in Solution. (Subsequently NRC Fellow with J. Hall, Boulder, Miller Fellow with C. B. Moore, Berkeley. Currently Adj. Prof. Chem., JILA Fellow, CU Boulder).

Richard F. Grote - Ph.D. 1981 - Chemical Reactions in Liquids. (Subsequently Postdoctoral fellow w/ A. DePristo, Iowa State). Currently, Industrial Pollution Prevention Specialist, Univ. of Wisconsin Solid and Hazardous Waste Prevention Center, Madison, WI.

Edwin L. Sibert, III - Ph.D. 1983 - Intramolecular Energy Flow. (Joint w/W. P. Reinhardt). (Subsequently NATO Postdoctoral Fellow w/M. Child, Oxford, Miller Fellow with W. H. Miller, Berkeley. Currently Professor, Dept. Chem., University of Wisconsin).

Jeffery Mathis - Ph.D. 1994 - Unimolecular Ionization in Solution. 1994 Procter and Gamble Award, (Currently NIH. Postdoctoral Fellow w/D. Poulter, University of Utah). Currently, Financial Analyst, The Prediction Company, Sante Fe, NM.

Benedetta Menucci, joint with University of Pisa (9/94-2/95) - Electronic Structure in Solution. Ph.D. Student, University of Pisa. Currently, Associate Professor, Univ. of Pisa.

Kenneth Geisshirt - (3/96-9/96) - visiting graduate student on Roskilde University (Denmark) fellowship.

Damien Laage - (9/98-12/01) - Département de Chimie, Ecole Normale Supérieure, Paris, ENS Doctoral Fellowship. Joint advisor with Dr. M. Martin, Laboratoire de Photophysique Moleculaire, Université Paris-Sud, Orsay, France. Subsequently Postdoctoral Fellow w/M. Parrinello, IBM Switzerland. Currently, CNRS Directeur de Recherche 2, Dept. de Chimie, ENS, Paris.

Ayman Al-Halabi, Institute of Chemistry, Leiden University, The Netherlands, Ph.D. student of Dr. G.J. Kroes. Leiden University Fellowship Visitor 2/99-5/99.

Hagop Demirdjian, (9/2000-9/2004) Département de Chimie, Ecole Normale Supérieure, Paris.

Wenlong Tian - (6/2002-) Biophysical Training Grant, 7/02-6/03.

Shuzhi Wang-(2/2003-10/2008). Subsequently, postdoctoral fellow, Lawrence Berkeley Lab, Berkeley, CA. Currently, Software Research Engineer, Google, Calif.

Yu-Ching Kuo (1/2014-). Joint with C. Musgrave, Chem. and Bio. Eng.

Joao Malhado (10/2004-09) , Portuguese Gov't Fellow, Department de Chimie, Ecole Normale Superieure, Currently Postdoctoral Fellow, Univ. Sao Paolo, Brazil. In Fall 2012, Marie Curie Postdoctoral Fellow, Imperial College , London.

Jean Boisson (10/2004-12/08). Dept. de Chimie, Ecole Normale Superieure. Currently, Research Associate, CEA, Saclay, FR

Francois-Xavier Coudert, (5/2002) 'Stage' ENS Chimie, Paris. Currently CNRS Charge de Recherche, ENSCP, Paris, FR

Luca Frediani, (1/03-3/03), visiting graduate student from University of Parma, Italy

Yu Zhou. 1/2016-, grad student. UC Boulder.

### Postdoctorals

J. O. Eaves - 1980 - (joint w/W. P. Reinhardt) - (Ph.D. w/J. O. Hirschfelder, Wisconsin) Currently Research Scientist, Bell Labs.

G. van der Zwan - (1980-83) - (Ph.D. 1980 with P. Mazur and D. Beadeaux, Leiden). Subsequently Postdoc w/R. Mazo, Oregon. Currently Assoc. Professor of Chemistry, Free University of Amsterdam.

J. S. Hutchinson - (1981-83) - (joint w/W. P. Reinhardt) (Ph.D. w/R. Wyatt, Texas). Currently Assoc. Professor of Chemistry, Rice Univ.

A. Zawadzki - (8/83-8/85) - (Ph.D. 1983 with R. Gordon, Harvard). Currently Research Scientist, Bell Labs.

- D. Ali - (9/83-6/87) - (Ph.D., 1983 with W. H. Miller, Berkeley).
- A. T. Uzer - (8/83-8/85) - (Ph.D. w/A. Dalgarno, Harvard). Currently. Professor of Physics, Georgia Tech.
- S. Y. Lee - (11/85-7/88) - (Ph.D. w/M. Karplus, Harvard) Currently Professor of Chemistry, National University, Seoul, Korea.
- D. Zichi - (1/86-2/89) - (Ph.D. w/P. Rossky, Austin). Subsequently Research Scientist Agouron Pharmaceuticals, San Diego, Cal. Currently, Research Scientist, SomaLogic, Boulder, Colo.
- E. Carter - (8/87-6/88) - (Ph.D. w/W. Goddard, Cal. Tech.). Professor of Chemistry, UCLA. Currently, Prof of Energy and the Environment, Princeton Univ. NJ.
- D. Borgis - (10/87-10/88) - (Ph.D. w/M. Moreau, Lab. de Physique Théorique des Liquides, University of Paris VI.) CNRS/NSF Postdoctoral Fellow. Directeur de Recherche, Paris VI, France. Currently, Dir. Recherche, ENS, Paris, FR
- S. Klippenstein - (9/88-8/89) - (Ph.D. w/R. Marcus. Cal. Tech.). Subs. Professor of Chemistry, Case Western University. Currently Senior Scientist, Chem. & Engin., Argonne National Lab, IL
- H. Kim - (9/88-8/92) - (Ph.D. w/H. Friedman, Stony Brook.). Currently, Professor of Chemistry, Carnegie-Mellon University.
- J. Timoneda - (9/89-3/92) - (Ph.D. w/K. Hunt, Michigan State, Postdoc w/T. Haymet, Berkeley and Utah). Currently, Patent Lawyer, Johnson and Johnson.
- S.H. Jung - (1/90-8/91) - (Ph.D. w/ M. Karplus, Harvard). Subsequently Postdoc, NIH. Currently, Research Scientist, Korea Inst. Science and Technology, Seoul.
- B. Smith - (1/90-12/91) - (Ph.D., C. Koval, Colorado). Subsequently, Postdoc w/W. Halley, Minnesota. currently Research Scientist, NREL, Golden, Colorado.
- M. Bruehl - (1/90-2/92) - (Ph.D. w/ G. Schatz, Northwestern) NSF Postdoctoral Fellow. Manager, Information Technology, Sun Microsystems, Broomfield, Colorado.
- B. Gertner - (8/90-2/95) - (Ph.D. w/K. Lindenberg and K.R. Wilson, UCSD). Subsequently, CIRES Visiting Fellow, Boulder, Colorado. Currently, Chief Software Specialist, Interactive Software Systems, Denver, CO.
- R. Bianco - (2/91- ) - (Joint D.Sc., Univ. of Pisa, w/J. Tomasi and J.T. Hynes) (8/99-; Senior Research Associate).
- A. Staib - (2/92-2/94) - (Ph.D., w/E. Schlag, Munich) Heisenberg Postdoctoral Fellow. Subsequently, "Poste Rouge", Paris VI. Currently, Habilitation, Univ. Düsseldorf.
- K. Ando - (10/92-3/95) - (Ph.D., S. Kato, Kyoto) Japanese Government Postdoctoral Fellow. Currently Assoc. Professor, University of Kyoto, Japan

- R. Rey - (10/92-10/93) - (Ph.D., E. Guardia, Barcelona) Spanish Government Postdoctoral Fellow. Currently, Associate Professor, Polytechnic University of Barcelona, Spain.
- J. Zhu - (9/94-12/95) - (Ph.D. w/J. Rasaih, Maine). Currently, Software Engineer, Computer Associates, NYC.
- G. Peslherbe - (10/95-8/98) - (Ph.D., W. Hase, Wayne State) currently Associate Professor, Concordia University, Montreal, Canada.
- W. Thompson - (3/97-12/00) - (Ph.D., W. Miller, UC Berkeley). Currently, Assoc. Professor of Chemistry, University of Kansas.
- T. Schroeder - (2/97-8/98) - (Ph.D., Reinhardt Schinke, Gottingen), (German Government Postdoctoral Fellow).
- P. Kiefer - (12/96- ) - (Ph.D., J. Onuchic, UC San Diego), (joint with S. Copley) NIH Postdoctoral Fellow, 4/98 - 3/00.
- G. Granucci - (5/97-9/99) - (Ph.D., M. Persico, Pisa). (European Community Postdoctoral Fellow, joint with Ph. Milli , Saclay, France.) Currently, Scientific Staff., Univ. of Pisa, IT.
- A. Morita - (3/99-8/00) - (Ph.D. S. Kato, Kyoto). Currently, Professor of Chemistry, University of Tohoku, Japan.
- K. Moller - (1/01-7/02) - (Ph.D, Danish Technical Univ. Postdoc, A. Zewail, CalTech) EC Postdoc at ENS, Paris. Currently, Assoc. Prof., Technical Univ. Denmark, Lyngby, DN
- M. Dolores Elola –(2/02-4/02) Postdoctoral Visitor, ENS. (Ph. D. , D. Laria and D. Estrin, Univ. of Buenos Aires, Argentina).
- S. Xu (11/02-10/03)) (Ph.D., Chinese Academy of Sciences, University of Beijing, China). K.C. Wong Postdoctoral Fellow at ENS, Paris.
- B. Nigro (2/03-8/04) (Ph.D. University of Padova, 1/03), EC Postdoc at ENS, Paris
- R. Spezia (1/04-1/05) (Ph.D. Univ. Roma I, 12/03), CNRS-DFG Postdoc at ENS, Paris. Currently CNRS Charge de recherch , Univ. Evry, FR
- S. Re (4/05-12/07) Japanese Physical Society Fellowship at ENS, Paris. Currently, Contract Researcher, Theoretical Biochem. Lab, RIKEN, Japan
- A. Mukherjee (5/05-5/07) (Ph.D. '05, Ind. Inst. Sci). Currently Asst. Prof. Indian Institute of Science Education and Research, Pune , IN
- D. Koch (12/05-11/06). (Ph.D Concordia Univ. 12/05). Chateaubriand Fellow at ENS, Paris. Currently, Scientific Staff, Dept. Chem, Concordia Univ, Montreal, CA

F. Ingrosso (1/06-08) (Ph. D. Univ. of Pisa) Marie Curie Postdoctoral Fellow at ENS (4/07-) Currently, Maitre de Conference, Chemistry, Univ. Nancy, France

S. Ramesh (10/06-07 (Ph. D. Univ. of Wisconsin). Subsequently, postdoctoral fellow Tech. Univ. Munich, presently Assistant Professor, Indian Institute of Science, Bangalore, IN

P. Marquetand (4/08-) (Ph.D. Univ. Wurzburg). German Government Postdoctoral Fellow at ENS. Currently, Habilitation, Inst. Theor. Chem., Univ. of Vienna, Austria

F. Sterpone (12/08-9/10) de Gennes Postdoctoral Fellow, at ENS, Paris. Currently, CNRS, Lab. De Biochimie Theorique, Institut de Biologie Physico-Chimie, Paris, FR

Y. Li (7/10-7/11) (Ph.D. State Key Lab., Jilin Univ), at ENS, Paris. Currently, postdoc, Theor. Chem., Univ. Cologne, DE

G. Stirnemann (6/11-12/11) (Ph. D. ENS), at ENS, Paris. Subsequently postdoc, Columbia Univ., currently CNRS CR2, Lab. De Biochimie Theorique, Institut de Biologie Physico-Chimie, Paris, FR.

T. Joutsuka (4/12-) (Ph.D. Univ of Kyoto) At ENS. Currently, Postdoc, Chemistry, Tohoku Univ. JP

S. Daschakraborty (10/13-12/16) (Ph. D., IIT, Kanpur). Currently, Asst Prof. IIT Patna, IN

### Faculty Visitors

Prof. M. Child, (9/87-4/88) - Theoretical Chemistry Dept., University of Oxford.

Prof. G. Ciccotti, (9/87-12/87), (9/88-12/88) - Physics Dept., University of Rome.

Prof. J. Simon, (6/89-8/90) - Chemistry Dept., UCSD., San Diego, CA

Prof. W. Hase (1/91-5/91) - Chemistry Dept., Wayne State, Detroit, MI

Prof. S.-Y. Lee (2/93-2/94) - Chemistry Dept., Seoul National University.

Prof. M. Maroncelli (9/94-12/94) - Chemistry Dept., Pennsylvania State

Prof. R. Rey (7/01 at ENS)-Physics Dept., Univ. Politecnica Catalunya, Spain

Prof. A. Morita (9/01) - Chemistry Dept., University of Kyoto, Japan

Prof. H. Kim (9/01-12/01) - Chemistry Dept., Carnegie-Mellon University, Pittsburgh, PA

Prof. D. Laria (7/02 at ENS) - Chemistry Dept., University of Buenos Aires, Argentina

Prof. B. Bagchi (7/02 at ENS) - Indian Institute of Sciences, Bangalore, India

Prof. G. van der Zwan (7/03 at ENS)-Chemistry Dept., Free University Amsterdam,  
Holland

Prof. T. Elsaesser (6/04 at ENS)- Physics Dept., MPI, Berlin, Germany

Prof. A. Stolow (6/04 at ENS)-National Research Council, Ottawa, Canada

Prof. B. Bagchi (3/05 at ENS)-Indian Institute of Sciences, Bangalore, India

Prof. B. Gerber (4/05 at ENS)-Chemistry Dept., Hebrew Univ., Jerusalem, Israel

Prof. H. Bakker (4/05 at ENS)- AMOLF, Amsterdam, Netherlands

Prof. B. Cabral (summer 06 at ENS)-Univ. Lisboa, Lisbon, Portugal

Prof. T. Martinez (5/06 at ENS)-Univ. Illinois, Urbana, Illinois

Prof. B. Bagchi (7/06 at ENS)-Indian Institute of Science, Bangalore, India

Prof. E. Pines (8-10/06)-Chemistry Dept., Ben Gurion Univ. of Negev, Beer Sheva, Israel  
Prof. I. Tunon (7/07 at ENS)- Univ. Valencia, Spain  
Prof. P. Rossky (6/08 at ENS)- Univ. of Texas, Austin, USA  
Prof. R. Rey (8/08-7/09)- Physics Dept., Univ. Politecnica Catalunya, Spain  
Dr. Jeffrey Hay (9/08-). Retired from Los Alamos National Lab  
Prof. B. Roux (5,6/09 at ENS). Biophysics, Univ. Chicago, USA  
Prof. E. Pines (3/2010)- Chemistry Dept. Ben-Gurion Univ. of Negev, Beer Sheva, Israel  
Prof. E. Pines (1/2012)- Chemistry Dept. Ben-Gurion Univ. of Negev, Beer Sheva, Israel

## Committee Service

### Department

Chemistry - Chem. Eng. Committee (73-76); Seminar Chairman (73-75); Scholastic Committee, Chr (73-76), (83-); Graduate Admissions Committee (77-78, Chr 81-82); Chemical Physics Seminar Chairman (77-78); Executive Committee (80-83;85-88); Departmental Newsletter Committee (83); Various Faculty Search Committees (81,82, Chair, 83, 84, 85, 94, 95); Colloquium Chair (83,84); General Chemistry Committee (85); Scholastic and Honors Committee Chair (87-90); Instructional Improvement Chair (96-97); Library Committee (98-); Computer Committee (97-); Cochair, SuperGroup on Clusters and Aerosols (98-01); Member, Biophysical Program (98-). Theoretical Search Committee Chair (08,09); Curriculum Committee (08-), Member, Awards Committee (9x-10). Chair, PhysChemPropRvw Committee, 2014-, Member, Theoretical Search Committee (15-16)

### University

Committee on Academic Planning and Practices (77-78), Public Information Committee (80-81), Boulder Faculty Assembly (80-81), A&S Deans Search Committee (80), Chemical Physics Committee (73-75, 82-) Graduate Foundation Award Committee (83), Physics Dept. Internal Review Committee (80), A&S Committee on Courses (85-89), Chemical Physics Chair (87-90), Chemical Physics Seminar Chair(89-90). Program Review Panel (94-96), Mr. Wizard: The Next Generation (94-); CU Science Connect (94-97); Area Teacher-Scholar Coordinator, Natural Sciences (96-97); New Science Library Committee (98-99); Member, JILA Physical Chemistry Search Committee (02-03); Associate, Astrobiology Program (03-); Member, JILA Physical Chemistry Search Committee (04).; Affiliate, CU Renewable and Sustainable Energy Initiative.(08-09), Affiliate, Renewable and Sustainable Energy Institute (1/10-). Member, Commission of Specialists, ENS (99-08)); Member, Committee 'Plateforme Environnement', ENS ('02-'08)).

### National, International

ACS Physical Chemistry Graduate Examination Committee (75-78); ACS Theoretical Chemistry Division Nomination Committee (82); Pimentel NAS Report on Chemistry - Condensed Phase Dynamics Section, (82); ACS Speakers Bureau (83-87); ACS Examination Committee (Phys. Chem.), (83-90); ACS Theoretical Division, Vice-Chair (84), Chair-Elect (85), Chair (86); ACS Hildebrand Award Nomination Committee, Chair (87-88); ACS Physical Chemistry Division Executive Committee (89-91); Journal of Physical Chemistry, Advisory Board (90-98); Editorial Board, Journal of Molecular Liquids (91- ); Advisory Editorial Board, International Journal of Quantum Chemistry (93-98); NSF Postdoctoral Fellowship Committee (93); TRIUMF Scientific Review Committee, Vancouver, BC, Canada (93-96 ); ACS Debye Award Canvassing Committee (98-01); Coeditor, Chem.Phys.Chem. (99-10); American Editor, Progress in Reaction Kinetics and Mechanism (99-05); Member, Editorial Board, Chemical Physics Letters (03-08); Member, Editorial Board, Journal of Chemical Physics (03-05); Review Committee, Pacific Northwest National Lab ('04). APS Division of Chemical Physics Nominating Committee ('04); ACS Award Committees (06-10); NSF Major Research Instrumentation Review Panel (08); APS Broida Prize Selection

Committee (08-10); Gordon Research Conference (Vibr. Spectroscopy) Monitor ('10). Member, International Advisory Board, Chemical Society Reviews (05-07):Member, Editorial Board, Interdisciplinary Sciences: Computational Life Sciences (09-). ; Selection Committee NAS Award for Chemistry in Service to Society ('12-), Designated Editor, PNAS ('12, '13) ; Member Editorial Board, Journal of Chemical Physics (14-16).. Member, International Advisory Committee, Femto 13: Frontiers of Ultrafast Phenomena in Physics, Chemistry, and Biology ('15-). Panel Member, Future of Chemical Physics Meeting, (JCP, APS) Oxford.UK'16.

French Council on Physical Chemistry (99-08); Member, Commission of Specialists, Sec. 31-63, French University System (99-06).

### **Courses Taught**

General Chemistry, Honors General Chemistry, Chemical Thermodynamics, Quantum Chemistry, Transport and Kinetics, Thermochemistry & Statistical Thermodynamics, Statistical Mechanics, Physical Chemistry of Macromolecules, Quantum Chemistry, Advanced Quantum Chemistry, Mathematical Methods, Chemical Kinetics, Theory of Reactions in Solution, Advanced Physical Chemistry, Physical Organic Chemistry (Magistere program, +Mechanique Statistique, ENS, Paris).

### Grants Received

U. of Colo. Summer Research Initiation Grant	6/71 - 8/71	\$ 2,000
PRF Starter Grant "Statistical Mechanics of Molecular Motion in Liquids"	10/71 - 10/74	\$ 7,500
NSF Grant "Non-Linear Effects and Boundary Effects in Molecular Relaxation Theory"	11/1/74 for 3 yrs.	\$19,000/yr
Alfred P. Sloan Foundation Fellowship	9/75 - 9/77	\$18,600
NATO Grant (with R. Kapral and M. Weinberg) "Nonlinear and Hydrodynamic Effects in Relaxation Processes"	10/75 - 10/78	\$ 7,000
U. of Colo. Faculty Fellowship	12/77	\$10,000
John Simon Guggenheim Fellowship	3/78	\$16,000
NSF Grant "Theoretical Studies of Molecular Dynamics in Dense Fluids"	7/1/78 for 2.67 yrs.	\$40,000/yr
NSF Grant "Theoretical Studies of Chemical Reactions in Liquids"	7/1/81 for 3 yrs.	\$60,000/yr
U. of Colo. CRCW Award "Curve Crossing Dynamics in Solution"	1/82 - 12/82	\$ 500
NOAA Grant "Theoretical Investigation of Atmospheric Reactions"	6/82 - 12/82	\$ 5,000
PRF Grant (w/W.P. Reinhardt) "Intramolecular Energy Flow in Straight Chain and Cyclic Hydrocarbons"	9/1/82 for 3 yrs.	\$15,000/yr
NSF Grant (w/G.B. Ellison, T. Cech, D. Walba, D. McKay and C. DePuy, for purchase of a VAX 11/750 Computer)	7/84	\$42,200 and \$90,000 in VAX



PRF Grant "Molecular Dynamics Computer Simulation of Atom Transfer and S N 2 Reactions in Solution."	1/85 - 8/88	\$52,500
National Center for Atmospheric Research (w/S.V. O'Neil) "Reaction Dynamics in Proton Hydrate Systems."	12/84 - 12/85	13 CRAY 720 hrs
SERC Fellowship (w/M.S. Child) "Theory of Heavy Atom Blocking of Energy Flow in Chemical Reactions."	6/85 - 8/85	3,000
NSF Grant "Theoretical Studies of Chemical Reactions in Solution."	5/85 - 4/88	\$76,000/yr
CECAM - for Workshop on "Molecular Dynamics Simulation of Chemical Reactions in Solution."	9/86	\$7,000
NATO (w/Ray Kapral, G. Ciccotti) "MD Simulation of Ionic Association Reactions."	5/87 - 4/88 (unfunded extension to 8/92)	\$5,000
NSF Supercomputer Program "Simulation of Ionic Reactions in Solution"	6/87 - 5/88	30 hrs CRAY XMP time
CECAM - for Workshop on "Computer Simulation and Theory for Chemical Reactions in Solution"	8/87	\$7,000
NSF US-UK Cooperative Research Grant. "Theoretical Studies of Highly Vibrationally Excited and Reactive Molecules"	1/88 - 12/90	\$10,534
CECAM - for Workshop on "Computer Simulation and Theory for Chemical Reactions in Solution"	8/88	\$5,500
NSF Grant "Theoretical Studies of Chemical Reactions in Solution."	6/88 - 5/91	\$80,000/yr
(Creativity Award Extension 1/91 - 12/93; additional \$10,000/yr.+ \$30,000 instrumentation)		
U. of CO. CRCW Award:	5/88	\$2000

"Proton Transfer Reactions"

NIH Grant "Theory of Proton and Hydride Transfer Reaction Rates"	12/88 - 11/91	\$159,210/yr
Pittsburgh Supercomputer Center	8/88 - 5/90	132 Hrs. of CRAY XMP, YMP time
CECAM - for Discussion Meeting on "Molecular Dynamics Simulation of Proton Transfer Reactions in Solution"	3/88	\$10,000
University of Colorado CRCW Award: "Electron Transfers at Electrodes"	11/89 - 10/90	\$2,000
CECAM - for workshop on "Quantum Chemistry and Chemical Reactions in Solution"	10/90	\$17,000
NSF- US-France Cooperative Research Grant "Simulation of Proton Transfer Reactions in Solution"	5/90 - 4/93	\$ 7,500
Pittsburgh Supercomputer Center	10/90 - 9/91	99 hrs. of CRAY YMP time
CU UROP Summer undergraduate Fellowship to Charles Gubser, for undergraduate research of Proton Transfer Reactions	5/92 - 8/92	\$ 2,000
NIH Shannon Award	10/92 - 9/94	\$ 50,000/yr
NCAR, "HCl Acid Ionization on PSC Ice"	6/93 - 5/97	\$52,560 (7200 hrs IBM/RS 6000 Model 590 = 360 GAU @ \$146/GAU)
NSF, "Chemical Reactions in Solution"	12/93 - 6/97	\$133,000/yr
Petroleum Research Fund, "Acid Ionization at Air-Ice and Air-Water Interfaces"	1/94 - 8/96	\$50,000
Pittsburgh Supercomputer Center	3/94 - 12/94	99 hrs. of CRAY YMP time
CU CRCW "Theory of Proton and Hydride Transfer Rates"	2/93 - 2/94	\$4,500

NCAR "HBr Acid Ionization on Ice"	3/96 - 6/97	\$36,500 (5000 hrs IBM/RS 600 Model 590 = 250 GAU @ \$146/GAU)
NCAR "Ab initio Study of the Reaction of Chlorine Nitrate with Water on Ice"	6/95 - 12/96	\$14,600 (2000 hrs IBM/RS 6000 Model 590 = 100 GAU @ \$146/GAU)
NSF (Atmospheric Chemistry) "Theoretical Studies of Heterogeneous Halogen Chemistry on Stratospheric and Tropospheric Ice"	1/97 - 12/99	\$120,000/yr
NSF (International Programs), "Photo-Induced Acid-Base Chemistry in Solution: Excited State Hydroxy-Arene Reaction Dynamics in Water"	3/97 - 2/02	\$17,200
NSF (Theoretical and Computational Chemistry), "Theory of Chemical Reactions in Solution in Clusters and at Surfaces"	5/97 - 6/01	\$110,000/year
"Purchase of a Departmental Parallel Processing Computer", NSF (Chemistry Research Instrumentation and Facilities), (joint proposal with five other faculty members, with 50% of computer access to members of Professor Hynes' group)	7/97 - 8/00	\$220,000
Molecular Science Computing Facility DOE/Environmental Molecular Sciences Lab., Pacific Northwest National Lab. "A Computational Approach to Understanding Oxidant Chemistry and Aerosol Formation in the Troposphere" (with Bruce Garrett, team leader, and five other senior team members)	1/98 - 12/01	Computational Time: 900,000 Node Hours Over a 3 year Period PNNL, IBM-SP2 Machine
National Renewable Energy Laboratory (NREL)	10/98 - 9/01	\$280,260/3yrs.
Subcontract to CU "Research and Development of New Theoretical Models to Describe Electron Transfer at Semiconductor-Molecule Interfaces"		Primarily to support Dr. B. Smith in his independent NREL research 3 wks. of summer. Salary/yr. for JTH
European Community Scientific Network Grant	3/00 - 2/03	Approximately \$160,000 total for three years to JTH

"Solvation Dynamics" together with  
five other scientists

NSF Atmospheric Chemistry "Heterogeneous Chemistry on Stratospheric and Tropospheric Sulfate Aerosols"	9/00-8/03	\$120,000/yr.
NSF (Theoretical and Computational Chemistry), "Theory of Chemical Reactions in Solution and at Surfaces	6/01-5/04	\$ 118,000/year
ECOS -Sud (France-South America). International Collaboration Grant. Travel grant for collaboration of JTH with Dr. Daniel Laria, Univ. of Buenos Aires, Argentina on HNO <sub>3</sub> on Ice in the Upper Troposphere.	3/02-2/05	\$10,000
Molecular Science Computing Facility DOE/Environmental Molecular Sciences Lab., Pacific Northwest National Lab. "A Computational Approach to Understanding Oxidant Chemistry and Aerosol Formation in the Troposphere" (with Bruce Garrett, team leader, and five other senior team members)	1/02-1/05	Computational Time: 900,000 Node Hours Over a 3 year Period PNNL, IBM-SP2 Machine
CNRS-DGR French-German Collaboration Grant "Theoretical Study of Excited State Dynamics in the Yellow Protein" JTH (PI) w/M. Martin (ENS), L. Cederbaum (Heidelberg)	11/02-10/05	to JTH 50,000 euros
France-India Institute for Fundamental Research, "Theory of Intercalation of Drug Molecules into DNA" JTH = co-PI, with B. Bagchi, Bangalore, IN	4/04-3/07	total to JTH =€100,000
NSF (Theoretical and Computational Chemistry), "Theory of Chemical Reactions in Solution and at Surfaces	8/04-7/07	\$ 130,000/year
CNRS-Sciences de l'Univers "Etudes Theoriques de Reactions Heterogenese Produisant de la Glycine Dans le Milieu Interstellaire	9/04-8/05	3000 euros

Keck Foundation "Peptide Bond Formation in Vivo"	1/05-7/05	\$15,000
ANR (FRANCE).. ' Réactions en solution et aux surfaces transfert de proton contrôlé et transfert d'électron important pour l'environnement.'	12/06-12/09	210,000 euros
NSF (Organic and Macromolecular Chemistry), "Peptide Bond Formation in the Peptidyl Transferase Center"	8/06-7/09	\$128,000/year
CU/NREL Renewable Energy Seed Grant "Theory of Catalysis of Water Splitting"	6/07-5/08	\$38,000
BSF (Israel) " Solute-solvent interactions and proton transfer reactions of physiologically protonatable groups" (with E. Pines (Ben-Gurion U.) and V. Batista (Yale)	10/07-9/11	\$15,000/yr to JTH
NSF (Theoretical and Computational Chemistry), "Theory of Chemical Reactions in Solution and at Surfaces	6/08-5/11	\$ 124,000/year
ANR (France) JTH ALADDIN ("Drug Intercalation into and Protein Association with DNA" (with R. Lavery ( Lyon) and P. Plaza (ENS).	12/08-5/12	224.000 euros to JTH
NSF (Theoretical and Computational Chemistry), "Theory of Chemical Reactions in Solution and at Surfaces"	8/11-7/14 (+ to 7/'17)	\$ 140,000/year
NIH Costs "The Physiological Role of Carbonic Acid and Lactic Acid as Protonating Agents of Amine and Nitrogen Bases in Model Biological Environments" (w/E. Pines, Ben Gurion Univ. Israel)	4/12-3/17	\$ 988,097 Direct

CNRS/Ministère recherche	150 k€
Programme Sésame Ile-de-France	60 k€
Bourse CNRS – K.C. Wong	20 k€