Publications of Donald G. Truhlar

Chapters

C1. "Electron-Impact Spectroscopy: Vibrational−Rotational Excitation," S. Trajmar, J. K. Rice, A. Kuppermann, and D. G. Truhlar, in *Advances in Chemical Physics*, Vol. 18, edited by I. Prigogine and S. A. Rice (John Wiley and Sons, New York, 1970), pp 70−83.

C2. "Algebraic Variational Methods in Scattering Theory," D. G. Truhlar, J. Abdallah, Jr., and R. L. Smith, in *Advances in Chemical Physics*, Vol. 25, edited by I. Prigogine and S. A. Rice (John Wiley and Sons, New York, 1974), pp 211−293.

C3. "Time-Reversal Invariance, Representations for Scattering Wave Functions, Symmetry of the Scattering Matrix, and Differential Cross Sections," D. G. Truhlar, C. A. Mead, and M. A. Brandt, in *Advances in Chemical Physics*, Vol. 33, edited by I. Prigogine and S. A. Rice (John Wiley and Sons, New York, 1975), pp 296−344.

C4. "Electron Scattering," D. G. Truhlar, in *Semiempirical Methods of Electronic Structure Calculations, Part B*: Applications, edited by G. A. Segal (Plenum Press, New York, 1977), pp 247−288. [*Mod. Theor. Chem.* **8**, 247−288 (1977).]

C5. "History of H_3 Kinetics," D. G. Truhlar and R. E. Wyatt, in *Annual Review of Physical Chemistry*, Vol. 27, edited by B. S. Rabinovitch (Annual Reviews, Inc., Palo Alto, CA, 1976), pp 1−43.

C6. "H + H_2: Potential Energy Surfaces and Elastic and Inelastic Scattering," D. G. Truhlar and R. E. Wyatt, in *Advances in Chemical Physics*, Vol. 36, edited by I. Prigogine and S. A. Rice (John Wiley and Sons, New York, 1977), pp 141−204.

C7. "Monte Carlo Trajectory Study of Ar + H_2 Collisions. Translation to Vibration Energy Transfer from Different Initial States," N. C. Blais and D. G. Truhlar, in *State-to-State Chemistry*, edited by P. R. Brooks and E. F. Hayes (*ACS Symp. Ser.* Volume 56, Washington, D.C., 1977), pp 243−246.

C8. "Reactive Scattering Cross Sections: Quasiclassical and Semiclassical Methods," D. G. Truhlar and J. T. Muckerman, in *Atom-Molecule Collision Theory*: *A Guide for the Experimentalist*, edited by R. B. Bernstein (Plenum Press, New York, 1979), pp 505−566.

C9. "Direct-Mode Chemical Reactions: Classical Theories," D. G. Truhlar and D. A. Dixon, in *Atom-Molecule Collision Theory: A Guide for the Experimentalist*, edited by R. B. Bernstein (Plenum Press, New York, 1979), pp 595−646.

C10. "Polarization Potentials for Electron Scattering," D. G. Truhlar, D. A. Dixon, R. A. Eades, F. A. Van-Catledge, and K. Onda, in *Electron−Molecule and Photon-Molecule Collisions*, edited by T. N. Rescigno, V. McKoy, and B. I. Schneider (Plenum Press, New York, 1979), pp 151−165.

C11. "Applications of Close Coupling Algorithms to Electron-Atom, Electron−Molecule, and Atom-Molecule Scattering," D. G. Truhlar, N. M. Harvey, K. Onda, and M. A. Brandt, in *Algorithms and Computer Codes for Atomic and Molecular Quantum Scattering Theory*, Vol. 1, edited by L. Thomas (National Resource for Computation in Chemistry, Lawrence Berkeley Laboratory, Berkeley, CA, 1979), pp 220−289.

C12. "The Coupling of Electronically Adiabatic States in Atomic and Molecular Collisions," B. C. Garrett and D. G. Truhlar, in *Theoretical Chemistry: Advances and Perspectives*, Vol. 6A, edited by D. Henderson (Academic Press, New York, 1981), pp 215−289. [*Theor. Chem.* (New York) **6A** ("Theory of Scattering: Papers in Honor of Henry Eyring"), 215−289 (1981).]

C13. "Introduction," P. Politzer and D. G. Truhlar, in *Chemical Applications of Atomic and Molecular Electrostatic Potentials*, edited by P. Politzer and D. G. Truhlar (Plenum Press, New York, 1981), pp 1−6.

C14. "Some Relationships Between Different Uses of the Electrostatic Potential," D. G. Truhlar, *ibid.*, pp 85−91.

C15. "Effective Potentials for Intermediate-Energy Electron Scattering: Testing Theoretical Models," D. G. Truhlar, *ibid.*, pp 123−172.

C16. "Adiabatic Polarization Potentials for the Water and Nitrogen Molecules. A Comparison of Large and Small Basis Sets," C. H. Douglass, Jr., D. A. Weil, P. A. Charlier, R. A. Eades, D. G. Truhlar, and D. A. Dixon, *ibid.*, pp 173−213.

C17. "Reaction, Dissociation, and Energy Transfer as a Function of Initial State for H + H_2 on an Accurate Ab Initio Potential Energy Surface," N. C. Blais and D. G. Truhlar, in *Potential Energy Surfaces and Dynamics Calculations*, edited by D. G. Truhlar (Plenum Press, New York, 1981), pp 431−473.

C18. "Determination of the Bottleneck Regions of Potential Energy Surfaces for Atom Transfer Reactions by Variational Transition State Theory," B. C. Garrett, D. G. Truhlar, and R. S. Grev, *ibid.*, pp 587−637.

C19. "Derivative Coupling Elements in Electronically Adiabatic Representations and Their Use in Scattering Calculations," B. C. Garrett, D. G. Truhlar, and C. F. Melius, in *Energy Storage and Redistribution in Molecules*, edited by J. Hinze (Plenum Press, New York, 1983), pp 375−395.

C20. "Generalized Transition State Theory," D. G. Truhlar, A. D. Isaacson, and B. C. Garrett, in *Theory of Chemical Reaction Dynamics*, edited by M. Baer (CRC Press, Boca Raton, FL, 1985), Vol. 4, pp 65−137.

C21. "Variational Transition State Theory," D. G. Truhlar and B. C. Garrett, in *Annual Review of Physical Chemistry*, Vol. 35, edited by B. S. Rabinovitch, J. M. Schurr, and H. L. Strauss (Annual Reviews, Inc., Palo Alto, CA, 1984), pp 159−189.

C22. "Variational Transition State Theory and Tunneling Calculations of Potential Energy Surface Effects on the Reaction of $O(^3P)$ with H_2," D. G. Truhlar, K. Runge, and B. C. Garrett, in *Twentieth Symposium (International) on Combustion* (Combustion Institute, Pittsburgh, PA, 1984), pp 585−593.

C23. "Adiabatic and Nonadiabatic Methods for Energies, Lifetimes, and Branching Probabilities of Bimolecular Reactive Collisions," B. C. Garrett, D. W. Schwenke, R. T. Skodje, D. Thirumalai, T. C. Thompson, and D. G. Truhlar, in *Resonances in Electron−Molecule Scattering, van der Waals Complexes, and Reactive Chemical Dynamics*, edited by D. G. Truhlar (*ACS Symp. Ser.* Volume 263, Washington, D.C., 1984), pp 375−400.

C24. "Transition State Theory," M. M. Kreevoy and D. G. Truhlar, in *Investigation of Rates and Mechanisms of Reactions*, fourth ed., edited by C. F. Bernasconi (John Wiley and Sons, New York, 1986), Part 1, pp 13−95. [*Tech. Chem.* (New York), fourth ed., **6**/Pt. 1, 13−95 (1986).]

10.1021/jp058267d CCC: $33.50
Published on Web 01/12/2006

C25. "Dynamics Calculations Based on Ab Initio Potential Energy Surfaces," D. G. Truhlar, F. B. Brown, D. W. Schwenke, R. Steckler, and B. C. Garrett, in *Comparison of Ab Initio Quantum Chemistry with Experiment for Small Molecules*, edited by R. J. Bartlett (Reidel, Dordrecht, Holland, 1985), pp 95−139.

C26. "Large-Scale Quantum Mechanical Scattering Calculations on Vector Computers," D. W. Schwenke and D. G. Truhlar, in *Supercomputer Applications*, edited by R. W. Numrich (Plenum Press, New York, 1985), pp 215−254.

C27. "Potential Energy Surfaces," D. G. Truhlar, in *The Encyclopedia of Physical Science and Technology*, edited by R. A. Meyers (Academic Press, New York, 1987), Vol. 11, pp 206−214. Updates: second ed. (1992), Vol. 13, pp 385−393; third ed. (2001), Vol. 13, pp 9−17.

C28. "Converged Calculations of Rotational Excitation and V−V Energy Transfer in the Collision of Two Molecules," D. W. Schwenke and D. G. Truhlar, in *Supercomputer Simulations in Chemistry*, edited by M. Dupuis (Springer-Verlag, Berlin, 1986), pp 165−197. [*Lect. Notes Chem.* **44**, 165−197 (1986).]

C29. "The Representation and Use of Potential Energy Surfaces in the Wide Vicinity of a Reaction Path for Dynamics Calculations on Polyatomic Reactions," D. G. Truhlar, F. B. Brown, R. Steckler, and A. D. Isaacson, in *The Theory of Chemical Reaction Dynamics*, edited by D. C. Clary (D. Reidel, Dordrecht, Holland, 1986), pp 285−329. [*NATO ASI Ser., Ser. C* **170**, 285−329 (1986).]

C30. "Supercomputer Research in Chemistry and Chemical Engineering: An Introduction," K. F. Jensen and D. G. Truhlar, in *Supercomputer Research in Chemistry and Chemical Engineering*, edited by K. F. Jensen and D. G. Truhlar (*ACS Symp. Ser.* Volume 353, Washington, D.C., 1987), pp 1−14.

C31. "Large-Scale Quantum Mechanical Calculations of the Sensitivity of Vibrational and Rotational Energy Transfer to the Potential Energy Surface in the Collision of Two Molecules," D. W. Schwenke and D. G. Truhlar, *ibid.*, pp 176−199.

C32. "Chemical Reaction Rate Calculations Using a Cray-2 Computer and Their Use to Test Approximate Theories," K. Haug, D. W. Schwenke, Y. Shima, D. G. Truhlar, J. Z. H. Zhang, Y. Zhang, Y. Sun, D. J. Kouri, and B. C. Garrett, in *Science and Engineering on Cray Supercomputers* (Proceedings of the Third International Symposium, Minneapolis, MN, Sept. 1987; Cray Research, Minneapolis, MN, 1987), pp 427−447.

C33. "New Time-Dependent and Time-Independent Computational Methods for Molecular Collisions," D. J. Kouri, Y. Sun, R. C. Mowrey, J. Z. H. Zhang, D. G. Truhlar, K. Haug, and D. W. Schwenke, in *Mathematical Frontiers in Computational Chemical Physics*, edited by D. G. Truhlar (Springer-Verlag, New York, 1988), pp 207−244.

C34. "Dynamical Formulation of Transition State Theory: Variational Transition States and Semiclassical Tunneling," S. C. Tucker and D. G. Truhlar, in *New Theoretical Concepts for Understanding Organic Reactions*, edited by J. Bertrán and I. G. Csizmadia (Kluwer, Dordrecht, The Netherlands, 1989), pp 291−346. [*NATO ASI Ser., Ser. C* **267**, 291−346 (1989).]

C35. "Computational Strategies and Improvements in the Linear Algebraic Variational Approach to Rearrangement Scattering," D. W. Schwenke, M. Mladenovic, M. Zhao, D. G. Truhlar, Y. Sun, and D. J. Kouri, in *Supercomputer Algorithms for Reactivity, Dynamics, and Kinetics of Small Molecules*, edited by A. Laganà (Kluwer, Dordrecht, The Netherlands, 1989), pp 131−168. [*NATO ASI Ser., Ser. C* **277**, 131−168 (1989).]

C36. "The HF Dimer: Potential Energy Surface and Dynamical Processes," D. G. Truhlar, in *Dynamics of Polyatomic van der Waals Complexes*, edited by N. Halberstadt and K. C. Janda (Plenum, New York, 1990), pp 159−185. [*NATO ASI Ser., Ser. B* **227**, 159−185 (1990).]

C37. "Localized Basis Functions and Other Computational Improvements in Variational Nonorthogonal Basis Function Methods for Quantum Mechanical Scattering Problems Involving Chemical Reactions," D. W. Schwenke and D. G. Truhlar, in *Computing Methods in Applied Sciences and Engineering*, edited by R. Glowinski and A. Lichnewsky (Society for Industrial and Applied Mathematics, Philadelphia, PA, 1990), pp 291−310.

C38. "RMPROP: A Computer Program for Quantum Mechanical Close Coupling Calculations for Inelastic Collisions," M. J. Unekis, D. W. Schwenke, N. M. Harvey, and D. G. Truhlar, in *Modern Techniques in Computational Chemistry*: MOTECC-91, edited by E. Clementi (ESCOM, Leiden, 1991), pp 749−772. [*Mod. Tech. Comput. Chem.*: MOTECC-91, 749−72 (1991).]

C39. "Variational Transition State Theory with Multidimensional Semiclassical Ground-State Transmission Coefficients: Applications to Secondary Deuterium Kinetic Isotope Effects in Reactions Involving Methane and Chloromethane," D. G. Truhlar, D.-h. Lu, S. C. Tucker, X. G. Zhao, A. Gonzàlez-Lafont, T. N. Truong, D. Maurice, Y.-P. Liu, and G. C. Lynch, in *Isotope Effects in Chemical Reactions and Photodissociation Processes*, by J. A. Kaye (*ACS Symp. Ser.* 502, Washington, D.C., 1992), pp 16−36.

C40. "Linear Algebraic Formulation of Reactive Scattering with General Basis Functions," G. J. Tawa, S. L. Mielke, D. G. Truhlar, and D. W. Schwenke, in *Advances in Molecular Vibrations and Collision Dynamics*, Vol. 2B, edited by J. M. Bowman (JAI Press, Greenwich, CT, 1994), pp 45−116. [*Adv. Mol. Vib. Collision Dyn.* **2B**, 45−116 (1994).]

C41. "RMPROP−Version 2: A Computer Program for Quantum Mechanical Close Coupling Calculations for Inelastic Collisions," M. J. Unekis, D. W. Schwenke, N. M. Harvey, and D. G. Truhlar, in *Methods and Techniques in Computational Chemistry*: METECC-94, edited by E. Clementi (STEF, Cagliari, Italy, 1993), Vol. C, pp 1−46.

C42. "Continuum Solvation Models: Classical and Quantum Mechanical Implementations," C. J. Cramer and D. G. Truhlar, in *Reviews in Computational Chemistry*, Vol. 6, edited by K. B. Lipkowitz and D. B. Boyd (VCH Publishers, New York, 1995), pp 1−72.

C43. "Development and Biological Applications of Quantum Mechanical Continuum Solvation Models," C. J. Cramer and D. G. Truhlar, in *Quantitative Treatments of Solute/Solvent Interactions*, edited by P. Politzer and J. S. Murray (Elsevier, Amsterdam, 1994), pp 9−54. [*Theor. Comp. Chem.* **2**, 9−54 (1994).]

C44. "Large-Scale Calculations of the Quantum Dynamics of Molecular Collisions and Reactions," D. G. Truhlar, D. W. Schwenke, S. L. Mielke, M. S. Reeves, R. W. Numrich, D. H. Briesemeister, D. C. Chatfield, R. S. Friedman, M. Kalke, G. J. Tawa, and M. J. Unekis, in *Toward Teraflop Computing and New Grand Challenge Applications*, edited by R. K. Kalia and P. Vashishta (Nova Science Publishers, Commack, NY, 1995), pp 151−171.

C45. "Theoretical Approaches to the Reaction Dynamics of Clusters," A. Gonzàlez-Lafont and D. G. Truhlar, in *Chemical Reactions in Clusters*, edited by E. R. Bernstein (Oxford University Press, New York, 1996), pp 1−39.

C46. "Reaction Path Approach to Dynamics at a Gas−Solid Interface: Quantum Tunneling Effects for an Adatom on a Non-Rigid Metallic Surface," S. E. Wonchoba, W.-P. Hu, and D. G. Truhlar, in *Theoretical and Computational Approaches to Interface Phenomena*, edited by H. L. Sellers and J. T. Golab (Plenum, New York, 1994), pp 1−33.

C47. "Structure and Reactivity in Aqueous Solutions: An Overview," C. J. Cramer and D. G. Truhlar, in *Structure and Reactivity in Aqueous Solution: Characterization of Chemical and Biological Systems*, edited by C. J. Cramer and D. G. Truhlar (*ACS Symp. Ser.* 568, Washington, D.C., 1994), pp 1−9.

C48. "Solvation Modeling in Aqueous and Nonaqueous Solvents: New Techniques and a Re-examination of the Claisen Rearrangement," J. W. Storer, D. J. Giesen, G. D. Hawkins, G. C. Lynch, C. J. Cramer, D. G. Truhlar, and D. A. Liotard, *ibid.*, pp 24−49.

C49. "Think Globally, Act Locally: An Introduction to Domain-Based Parallelism and Problem Decomposition Methods," D. E. Keyes, Y. Saad, and D. G. Truhlar, in *Domain-Based Parallelism and Problem Decomposition Methods in Computational Science and Engineering*, edited by D. Keyes, Y. Saad, and D. G. Truhlar (Society for Industrial and Applied Mathematics, Philadelphia, PA, 1995), pp vii−xiv.

C50. "Problem Decomposition Techniques in Quantum Mechanical Reactive Scattering," D. W. Schwenke and D. G. Truhlar, *ibid.*, pp 303−323.

C51. "Direct Dynamics Method for the Calculation of Reaction Rates," D. G. Truhlar, in *The Reaction Path in Chemistry: Current Approaches and Perspectives*, edited by D. Heidrich (Kluwer, Dordrecht, The Netherlands, 1995), pp 229−255. [*Understanding Chem. React.* **16**, 229−255 (1995).]

C52. "Continuum Solvation Models," C. J. Cramer and D. G. Truhlar, in *Solvent Effects and Chemical Reactivity*, edited by O. Tapia and J. Bertrán (Kluwer, Dordrecht, The Netherlands, 1996), pp 1−80. [*Understanding Chem. React.* **17**, 1−80 (1996).]

C53. "Computational Spectroscopy of the Transition State," D. C. Chatfield, R. S. Friedman, S. L. Mielke, G. C. Lynch, T. C. Allison, D. G. Truhlar, and D. W. Schwenke, in *Dynamics of Molecules and Chemical Reactions*, edited by R. E. Wyatt and J. Z. H. Zhang (Marcel Dekker, New York, 1996), pp 323−386.

C54. "Die Photochemischen Bildung des Chlorwasserstoffs. Dynamics of $Cl + H_2 \leftrightarrow HCl + H$ on a New Potential Energy Surface: The Photosynthesis of Hydrogen Chloride Revisited 100 Years after Max Bodenstein," T. C. Allison, S. L. Mielke, D. W. Schwenke, G. C. Lynch, M. S. Gordon, and D. G. Truhlar, in *Gas-Phase Chemical Reaction Systems: Experiments and Models 100 Years after Max Bodenstein*, edited by J. Wolfrum, H.-R. Volpp, R. Rannacher, J. Warnatz (Springer, Berlin, 1996), pp 111−124. [*Springer Ser. Chem. Phys.* **61**, 111−124 (1996), Volume Date 1995.]

C55. "Barrier Resonances and Chemical Reactivity," R. S. Friedman and D. G. Truhlar, in *Multiparticle Quantum Scattering with Applications to Nuclear, Atomic, and Molecular Physics*, edited by D. G. Truhlar and B. Simon (Springer, New York, 1997), pp 243−281. [*IMA Vol. Math. Its Appl.* **89**, 243−281 (1997).]

C56. "Modeling Free Energies of Solvation and Transfer," D. J. Giesen, C. C. Chambers, G. D. Hawkins, C. J. Cramer, and D. G. Truhlar, in *Computational Thermochemistry*, edited by K. Irikura and D. J. Frurip (*ACS Symp. Ser.* Volume 677, Washington, D.C., 1998), pp 285−300 (1998).

C57. "Theoretical Chemistry," D. G. Truhlar, in *Macmillan Encyclopedia of Chemistry*, edited by J. J. Lagowski (Simon & Schuster Macmillan, New York, 1997), pp 1432−1433 (in Vol. 4). New edition: updated version, 2002.

C58. "Transition State Theory," B. C. Garrett and D. G. Truhlar, in *Encyclopedia of Computational Chemistry*, edited by P. v. R. Schleyer, N. L. Allinger, T. Clark, J. Gasteiger, P. A. Kollman, and H. F. Schaefer III (John Wiley & Sons, Chichester, U.K., 1998), Volume 5, pp 3094−3104.

C59. "Testing the Accuracy of Practical Semiclassical Methods: Variational Transition State Theory with Optimized Multidimensional Tunneling," T. C. Allison and D. G. Truhlar, in *Modern Methods for Multidimensional Dynamics Computations in Chemistry*, edited by D. L. Thompson (World Scientific, Singapore, 1998), pp 618−712.

C60. "Modeling the Effect of Solvation on Structure, Reactivity, and Partitioning of Organic Solutes: Utility in Drug Design," C. C. Chambers, D. J. Giesen, G. D. Hawkins, W. H. J. Vaes, C. J. Cramer, and D. G. Truhlar, in *Rational Drug Design*, edited by D. G. Truhlar, W. J. Howe, A. J. Hopfinger, J. M. Blaney, and R. A. Dammkoehler (Springer, New York, 1999), pp 51−72. [*IMA Vol. Math. Its Appl.* **108**, 51−72 (1999).]

C61. "New Tools for Rational Drug Design," G. D. Hawkins, J. Li, T. Zhu, C. C. Chambers, D. J. Giesen, D. A. Liotard, C. J. Cramer, and D. G. Truhlar, in *Rational Drug Design: Novel Methodology and Practical Applications*, edited by A. L. Parrill and M. R. Reddy (*ACS Symp. Ser.* Volume 719, Washington, D.C., 1999), pp 121−140.

C62. "Universal Solvation Models," G. D. Hawkins, T. Zhu, J. Li, C. C. Chambers, D. J. Giesen, D. A. Liotard, C. J. Cramer, and D. G. Truhlar, in *Combined Quantum Mechanical and Molecular Mechanical Methods*, edited by J. Gao and M. A. Thompson (*ACS Symp. Ser.* Volume 712, Washington, D.C., 1998), pp 201−219.

C63. "Dual-Level Methods for Electronic Structure Calculations of Potential Energy Functions that Use Quantum Mechanics as the Lower Level," J. C. Corchado and D. G. Truhlar, *ibid.*, pp 106−127.

C64. "Quantum Catalysis: The Modeling of Catalytic Transition States," M. B. Hall, P. Margl, G. Náray-Szabó, V. L. Schramm, D. G. Truhlar, R. A. van Santen, A. Warshel, and J. L. Whitten, in *Transition State Modeling for Catalysis*, edited by D. G. Truhlar and K. Morokuma (*ACS Symp. Ser.* Volume 721, Washington, D.C., 1999), pp 2−17.

C65. "Ethylene Polymerization by Zirconocene Catalysis," P. K. Das, D. W. Dockter, D. R. Fahey, D. E. Lauffer, G. D. Hawkins, J. Li, T. Zhu, C. J. Cramer, D. G. Truhlar, S. Dapprich, R. D. J. Froese, M. C. Holthausen, Z. Liu, K. Mogi, S. Vyboishchikov, D. G. Musaev, and K. Morokuma, *ibid.*, pp 208−224.

C66. "Solvation Thermodynamics and the Treatment of Equilibrium and Nonequilibrium Solvation Effects by Models Based on Collective Solvent Coordinates," C. J. Cramer and D. G. Truhlar, in *Free Energy Calculations in Rational Drug Design*, edited by M. R. Reddy and M. D. Erion (Kluwer Academic/Plenum, New York, 2001), pp 63−95.

C67. "Molecular-Scale Modeling of Reactions and Solvation," D. G. Truhlar, in *First International Conference on Foundations of Molecular Modeling and Simulation*; edited by P. T. Cummings. P. R. Westmoreland, and B. Carnahan (*AIChE Symp. Ser.* Vol. 97, New York, 2001), pp 71−83. [*AIChE Symp. Ser.* (2001), 325 (Foundations of Molecular Modeling and Simulation), pp 71−83.]

C68. "Quantum Mechanical Methods for Enzyme Kinetics," J. Gao and D. G. Truhlar, in *Annual Review of Physical Chemistry*, Vol. 53, edited by S. R. Leone, P. Alivisatos, and A. E. McDermott (Annual Reviews, Inc., Palo Alto, CA, 2002), pp 467−505.

C69. "Non-Born−Oppenheimer Chemistry: Potential Surfaces, Couplings, and Dynamics," A. W. Jasper, B. K. Kendrick, C. A. Mead, and D. G. Truhlar, in *Modern Trends in Chemical Reaction Dynamics: Experiment and Theory (Part 1)*, edited by X. Yang and K. Liu (World Scientific, Singapore, 2004), pp 329−391. [*Adv. Ser. Phys. Chem.* **14**, 329−391 (2004).]

C70. "Multilevel Methods for Thermochemistry and Thermochemical Kinetics," B. J. Lynch and D. G. Truhlar, in *Recent Advances in Electron Correlation Methodology*, edited by A. K. Wilson and K. A. Peterson (*ACS Symp. Ser.*, Oxford University Press, Washington, D.C., 2005), in press.

C71. "Variational Transition State Theory and Multidimensional Tunneling for Simple and Complex Reactions in the Gas Phase, Solids, Liquids, and Enzymes," D. G. Truhlar, in *Isotope Effects in Chemistry and Biology*, edited by A. Kohen and H. H. Limbach (Taylor & Francis, CRC Press: New York, 2005), pp 579−620.

C72. "Hydrogen Atom Transfers in B_{12} Enzymes," R. Banerjee, D. G. Truhlar, A. Dybala-Defratyka, P. Paneth, in *Biological Aspects of Hydrogen Transfer*, edited by R. Schowen and J. Klinman; Vol. 2 of *Handbook of Hydrogen Transfer*, edited by R. L. Schowen (Wiley-VCH, Weinheim, Germany, 2005), in press.

C73. "Variational Transition State Theory in the Treatment of Hydrogen Transfer Reactions," B. C. Garrett and D. G. Truhlar, in *Physical and Chemical Aspects of Hydrogen Transfer*, edited by J. T. Hynes and H. H. Limbach; Vol. 1 of *Handbook of Hydrogen Transfer*, edited by R. L. Schowen (Wiley-VCH, Weinheim, Germany, 2005), in press.

C74. "Decoherence in Combined Quantum Mechanical and Classical Mechanical Methods for Dynamics as Illustrated for Non-Born−Oppenheimer Trajectories," D. G. Truhlar, in *Quantum Dynamics of Complex Molecular Systems*, edited by D. A. Micha and I. Burghardt (Chemical Physics Series of Springer-Verlag), in press.

Chemical Reaction Dynamics and Photochemistry

2. "Application of the Statistical Phase-Space Theory to Reactions of Atomic Hydrogen with Deuterium Halides," D. G. Truhlar and A. Kuppermann, *J. Phys. Chem.* **73**, 1722−1734 (1969).

3. "Statistical Phase-Space Theory of the Reaction $C^+ + D_2$, Including Threshold Behavior," D. G. Truhlar, J. Chem. Phys. **51**, 4617−4623 (1969).

5. "Quantum Mechanics of the H + H_2 Reaction: Exact Scattering Probabilities for Collinear Collisions," D. G. Truhlar and A. Kuppermann, *J. Chem. Phys.* **52**, 3841−3843 (1970).

9. "The Adiabatic Theory of Chemical Reactions," D. G. Truhlar, *J. Chem. Phys.* **53**, 2041−2044 (1970).

10. "Application of the Statistical Phase Space Theory to the Reaction K + HCl → KCl + H and to Inelastic Scattering," D. G. Truhlar, *J. Chem. Phys.* **54**, 2635−2641 (1971).

11. "Exact Tunneling Calculations," D. G. Truhlar and A. Kuppermann, *J. Am. Chem. Soc.* **93**, 1840−1851 (1971).

13. "A Test of Transition State Theory Against Exact Quantum Mechanical Calculations," D. G. Truhlar and A. Kuppermann, *Chem. Phys. Lett.* **9**, 269−272 (1971).

15. "Potential Energy Surfaces for Atom Transfer Reactions Involving Hydrogens and Halogens," C. A. Parr and D. G. Truhlar, *J. Phys. Chem.* **75**, 1844−1860 (1971).

18. "Enhancement of the Reaction Cross Section of He + $H_2^+ \rightarrow HeH^+ + H$ by Vibrational Excitation of H_2^+ According to the Statistical Phase-Space Theory," D. G. Truhlar, *J. Chem. Phys.* **56**, 1481−1486 (1972).

20. "Exact and Approximate Quantum Mechanical Reaction Probabilities and Rate Constants for the Collinear H + H_2 Reaction," D. G. Truhlar and A. Kuppermann, *J. Chem. Phys.* **56**, 2232−2252 (1972).

21. "Multiple Potential Energy Surfaces for Reactions of Species in Degenerate Electronic States," D. G. Truhlar, *J. Chem. Phys.* **56**, 3189−3190 (1972), **61**, 440(E) (1974).

22. "Comparison of Boundary-Value and Initial-Value Methods for the Accurate Quantum-Mechanical Solution of the Collinear Reactive Scattering Problem," D. J. Diestler, D. G. Truhlar, and A. Kuppermann, *Chem. Phys. Lett.* **13**, 1−5 (1972).

31. "Comment on Enhancement of the Reaction Cross Section of He + $H_2^+ \rightarrow HeH^+ + H$ by Vibrational Excitation of H_2^+ and the Treatment of Nuclear Spin by the Statistical Phase-Space Theory," A. F. Wagner and D. G. Truhlar, *J. Chem. Phys.* **57**, 4063−4064 (1972).

32. "Test of Bond-Order Methods for Predicting the Position of the Minimum-Energy-Path for Hydrogen Atom Transfer Reactions," D. G. Truhlar, *J. Am. Chem. Soc.* **94**, 7584−7586 (1972).

36. "Monte Carlo Trajectories: Dynamics of the Reaction F + D_2 on a Semiempirical Valence-Bond Potential Energy Surface," N. C. Blais and D. G. Truhlar, *J. Chem. Phys.* **58**, 1090−1108 (1973).

41. "A Direct Test of the Vibrationally Adiabatic Theory of Chemical Reactions," J. M. Bowman, A. Kuppermann, J. T. Adams, and D. G. Truhlar, *Chem. Phys. Lett.* **20**, 229−232 (1973).

42. "Exact Quantum Mechanical Reaction Probabilities and Rate Constants for the Isotopic Collinear H + H_2 Reactions," D. G. Truhlar, A. Kuppermann, and J. T. Adams, *J. Chem. Phys.* **59**, 395−402 (1973).

48. "Exact Quantum Mechanical Reaction Probabilities for the Collinear H + H_2 Reaction on a Porter-Karplus Potential Energy Surface," J. W. Duff and D. G. Truhlar, *Chem. Phys. Lett.* **23**, 327−330 (1973).

51. "Classical S Matrix: Numerical Applications to Classically Allowed Chemical Reactions," J. W. Duff and D. G. Truhlar, *Chem. Phys.* **4**, 1−23 (1974).

57. "Monte Carlo Trajectories: The Reaction H + $Br_2 \rightarrow$ HBr + Br," N. C. Blais and D. G. Truhlar, *J. Chem. Phys.* **61**, 4186−4203 (1974). Erratum: **65**, 3803−3804 (1976).

59. "Effect of Curvature of the Reaction Path on Dynamic Effects in Endothermic Reactions and Product Energies in Exothermic Reactions," J. W. Duff and D. G. Truhlar, *J. Chem. Phys.* **62**, 2477−2491 (1975).

63. "Intermediate-Coupling Probability Matrix Approach to Chemical Reactions: Dependence of the Reaction Cross Section for K + HCl → KCl + H on Initial Translational and Vibrational Energy," D. G. Truhlar, *J. Am. Chem. Soc.* **97**, 6310−6317 (1975).

71. "Classical S. Matrix: Application of the Bessel Uniform Approximation to a Chemical Reaction," J. W. Duff and D. G. Truhlar, *Chem. Phys. Lett.* **40**, 251−256 (1976).

74. "Comparison of Trajectory Calculations, Transition State Theory, and Quantum Mechanical Reaction Probabilities and Rate Constants for the Collinear Reaction H + $Cl_2 \rightarrow$ HCl + Cl," D. G. Truhlar, J. A. Merrick, and J. W. Duff, *J. Am. Chem. Soc.* **98**, 6771−6783 (1976).

75. "Quasiclassical Predictions of Final Vibrational State Distributions in Reactive and Nonreactive Collisions," D. G. Truhlar, *Int. J. Quantum Chem., Symp.* **10**, 239−250 (1976).

78. "Interpretation of Ortho-Para Hydrogen Conversion," D. G. Truhlar, *J. Chem. Phys.* **65**, 1008−1010 (1976).

84. "Monte Carlo Trajectory Study of Ar + H_2 Collisions. I. Potential Energy Surface and Cross Sections for Dissociation, Recombination, and Inelastic Scattering," N. C. Blais, and D. G. Truhlar, *J. Chem. Phys.* **65**, 5335−5356 (1976).

85. "Monte Carlo Trajectory Study of Ar + H_2 Collisions. II. Vibrational and Rotational Enhancement of Cross Sections for Dissociation," N. C. Blais and D. G. Truhlar, *J. Chem. Phys.* **66**, 772−778 (1977).

86. "The Importance of Isotope-Dependent Transmission Coefficients in Calculating Low-Temperature Isotope Effects," D. G. Truhlar, A. Kuppermann, and J. Dwyer, *Mol. Phys.* **33**, 683−688 (1977).

87. "Legendre Moment Method for Calculating Differential Scattering Cross Sections from Classical Trajectories with Monte Carlo Initial Conditions," D. G. Truhlar and N. C. Blais, *J. Chem. Phys.* **67**, 1532−1539 (1977).

88. "Monte Carlo Trajectories: Alignment of HBr Rotational Angular Momentum as a Function of Scattering Angle for the Reaction H + Br_2 → HBr + Br," N. C. Blais and D. G. Truhlar, *J. Chem. Phys.* **67**, 1540−1546 (1977).

89. "Interpretation of Activation Energy," D. G. Truhlar, *J. Chem. Educ.* **55**, 309−311 (1978).

90. "Direct Calculation of the Equilibrium Value of the Energy of Activation for Dissociation of H_2 by Ar and Evidence for the Important Contribution of Collisional Dissociation from Low Vibrational Quantum Numbers at Shock-Tube Temperatures," D. G. Truhlar and N. C. Blais, *J. Am. Chem. Soc.* **99**, 8108−8109 (1977).

93. "Functional Representation of Liu and Siegbahn's Accurate ab initio Potential Energy Calculations for H + H_2," D. G. Truhlar and C. J. Horowitz, *J. Chem. Phys.* **68**, 2466−2476 (1978). Erratum: **71**, 1514 (1979).

94. "Generalized Valence-Bond Investigation of the Reaction H + Br_2 → HBr + Br," P. Baybutt, F. W. Bobrowicz, L. R. Kahn, and D. G. Truhlar, *J. Chem. Phys.* **69**, 4809−4822 (1978). Erratum: **70**, 2050 (1979).

95. "Quasiclassical Trajectory Calculations Compared to Quantum Mechanical Reaction Probabilities, Rate Constants, and Activation Energies for Two Different Potential Surfaces for the Collinear Reaction H_2 + I → H+ HI, Including Dependence on Initial Vibrational State," J. C. Gray, D. G. Truhlar, L. Clemens, J. W. Duff, F. M. Chapman, Jr., G. O. Morrell, and E. F. Hayes, *J. Chem. Phys.* **69**, 240−252 (1978).

96. "Interpretation and Temperature Dependence of the Energy of Activation for the Reactions H + Cl_2, H_2 + I, H + H_2, and Isotopic Analogues," D. G. Truhlar and J. C. Gray, *Chem. Phys. Lett.* **57**, 93−99 (1978).

99. "Monte Carlo Trajectory Study of Ar + H_2: Vibrational Selectivity of Dissociative Collisions at 4500 K and the Characteristics of Dissociation under Equilibrium Conditions," N. C. Blais and D. G. Truhlar, *J. Chem. Phys.* **70**, 2962−2978 (1979).

103. "Accuracy of Trajectory Calculations and Transition State Theory for Thermal Rate Constants of Atom Transfer Reactions," D. G. Truhlar, *J. Phys. Chem.* **83**, 188−198 (1979). (Symp. on Current Status of Kinetics of Elementary Gas Reactions.)

104. "Accuracy of Tunneling Corrections to Transition State Theory for Thermal Rate Constants of Atom Transfer Reactions," B. C. Garrett and D. G. Truhlar, *J. Phys. Chem.* **83**, 200−203, 3058(E) (1979). (Symp. on Current Status of Kinetics of Elementary Gas Reactions.)

105. "Criterion of Minimum State Density in the Transition State Theory of Bimolecular Reactions," B. C. Garrett and D. G. Truhlar, *J. Chem. Phys.* **70**, 1593−1598 (1979).

106. "Test of Trajectory Calculations Against Quantum Mechanical State-to-State and Thermal Collinear Reaction Rates for H + Cl_2 → HCl + Cl," J. C. Gray, D. G. Truhlar, and M. Baer, *J. Phys. Chem.* **83**, 1045−1052 (1979). (Don Louis Bunker Memorial Issue.)

107. "Generalized Transition State Theory. Classical Mechanical Theory and Applications to Collinear Reactions of Hydrogen Molecules," B. C. Garrett and D. G. Truhlar, *J. Phys. Chem.* **83**, 1052−1079, 3058(E) (1979), **87**, 4553(E) (1983). (Don Louis Bunker Memorial Issue.)

110. "Monte Carlo Trajectory Study of Ar + H_2 Collisions: Master-Equation Simulation of a 4500 K Shock Wave Experiment with Thermal Rotation," D. G. Truhlar, N. C. Blais, J.-C. J. Hajduk, and J. H. Kiefer, *Chem. Phys. Lett.* **63**, 337−343 (1979).

112. "Generalized Transition State Theory. Quantum Effects for Collinear Reactions of Hydrogen Molecules," B. C. Garrett and D. G. Truhlar, *J. Phys. Chem.* **83**, 1079−1112 (1979), **84**, 682−686(E) (1980); **87**, 4553−4554(E) (1983). (Don Louis Bunker Memorial Issue.)

120. "Generalized Transition State Theory. Bond Energy-Bond Order Method for Canonical Variational Calculations with Applications to Hydrogen Atom Transfer Reactions," B. C. Garrett and D. G. Truhlar, *J. Am. Chem. Soc.* **101**, 4534−4548 (1979).

121. "Generalized Transition State Theory. Canonical Variational Calculations using the Bond Energy-Bond Order Method for Bimolecular Reactions of Combustion Products," B. C. Garrett and D. G. Truhlar, *J. Am. Chem. Soc.* **101**, 5207−5217 (1979).

122. "Detailed Balance in Quasiclassical Trajectory Calculations of Thermal Rate Constants for Chemical Reactions," J. C. Gray, B. C. Garrett, and D. G. Truhlar, *J. Chem. Phys.* **70**, 5921−5922 (1979).

126. "Reliable Ab Initio Calculation of a Chemical Reaction Rate and a Kinetic Isotope Effect: H + H_2 and D + D_2," B. C. Garrett and D. G. Truhlar, *Proc. Natl. Acad. Sci. U.S.A.* **76**, 4755−4759 (1979).

127. "Monte Carlo Trajectory Study of Ar + H_2 Collisions: Thermally Averaged Vibrational Transition Rates at 4500 K," J. W. Duff, N. C. Blais, and D. G. Truhlar, *J. Chem. Phys.* **71**, 4304−4320 (1979).

128. "Semiclassical Tunneling Calculations," B. C. Garrett and D. G. Truhlar, *J. Phys. Chem.* **83**, 2921−2926 (1979).

130. "Variational Transition State Theory. Primary Kinetic Isotope Effects for Atom Transfer Reactions," B. C. Garrett and D. G. Truhlar, *J. Am. Chem. Soc.* **102**, 2559−2570 (1980).

131. "Quasiclassical Trajectory Studies of Vibrational Enhancement of Collision-Induced Dissociation in Collinear Collisions," J. C. Gray, G. A. Fraser, and D. G. Truhlar, *Chem. Phys. Lett.* **68**, 359−364 (1979).

133. "Generalized Transition State Theory Calculations for the Reactions D + H_2 and H + D_2 using an Accurate Potential Energy Surface: Explanation of the Kinetic Isotope Effect," B. C. Garrett and D. G. Truhlar, *J. Chem. Phys.* **72**, 3460−3471 (1980).

135. "Improved Canonical Variational Theory for Chemical Reaction Rates. Classical Mechanical Theory and Applications

to Collinear Reactions," B. C. Garrett and D. G. Truhlar, *J. Phys. Chem.* **84**, 805−812 (1980).

140. "Improved Treatment of Threshold Contributions in Variational Transition State Theory," B. C. Garrett, D. G. Truhlar, R. S. Grev, and A. W. Magnuson, *J. Phys. Chem.* **84**, 1730−1748 (1980), **87**, 4554(E) (1983).

141. "Application of Variational Transition State Theory and the Unified Statistical Model to H + Cl_2 → HCl + Cl," B. C. Garrett, D. G. Truhlar, and R. S. Grev, *J. Phys. Chem.* **84**, 1749−1752 (1980).

142. "Comparison of Variational Transition State Theory and the Unified Statistical Model with Vibrationally Adiabatic Transmission Coefficients to Accurate Collinear Rate Constants for T + HD → TH + D," B. C. Garrett, D. G. Truhlar, R. S. Grev, and R. B. Walker, *J. Chem. Phys.* **73**, 235−240 (1980).

145. "Variational Transition State Theory, Vibrationally Adiabatic Transmission Coefficients, and the Unified Statistical Model Tested Against Accurate Quantal Rate Constants for Collinear F + H_2, H + F_2, and Isotopic Analogues," B. C. Garrett, D. G. Truhlar, R. S. Grev, A. W. Magnuson, and J. N. L. Connor, *J. Chem. Phys.* **73**, 1721−1728 (1980).

148. "Variational Transition State Theory and Vibrationally Adiabatic Transmission Coefficients for Kinetic Isotope Effects in the Cl−H−H Reaction System," B. C. Garrett, D. G. Truhlar, and A. W. Magnuson, *J. Chem. Phys.* **74**, 1029−1043 (1981).

152. "Variational Transition-State Theory," D. G. Truhlar and B. C. Garrett, *Acc. Chem. Res.* **13**, 440−448 (1980).

156. "Parabolic Tunneling Calculations," R. T. Skodje and D. G. Truhlar, *J. Phys. Chem.* **85**, 624−628 (1981).

157. "Dynamical Calculation of the Temperature Dependence of the Activation Energy for a Chemical Reaction from 444 to 2400 K," N. C. Blais, D. G. Truhlar, and B. C. Garrett, *J. Phys. Chem.* **85**, 1094−1096 (1981).

158. "Monte Carlo Trajectory Calculations of the Energy of Activation for Collision-Induced Dissociation of H_2 by Ar as Functions of Rotational Energy," N. C. Blais and D. G. Truhlar, *J. Chem. Phys.* **74**, 6709−6712 (1981).

159. "Classical Generalized Transition State Theory. Application to a Collinear Reaction with Two Saddle Points," B. C. Garrett, D. G. Truhlar, and R. S. Grev, *J. Phys. Chem.* **85**, 1569−1572 (1981).

160. "Reaction Probabilities, Resonances, and Thermal Rate Constants for the Collinear Reactions H + FH and D + FD on a Low-Barrier Surface: Close Coupling and Tunneling Calculations, Variational Transition State Theory, and the Unified Statistical Model," B. C. Garrett, D. G. Truhlar, R. S. Grev, G. C. Schatz, and R. B. Walker, *J. Phys. Chem.* **85**, 3806−3817 (1981).

165. "New Semiempirical Method of Modeling Potential Energy Surfaces for Generalized TST and Application to Kinetic Isotope Effects in the Cl−H−H System," B. C. Garrett, D. G. Truhlar, and A. W. Magnuson, *J. Chem. Phys.* **76**, 2321−2331 (1982).

168. "A General Small-Curvature Approximation for Transition-State-Theory Transmission Coefficients," R. T. Skodje, D. G. Truhlar, and B. C. Garrett, *J. Phys. Chem.* **85**, 3019−3023 (1981).

169. "Semiclassical Vibrationally Adiabatic Model for Resonances in Reactive Collisions," B. C. Garrett and D. G. Truhlar, *J. Phys. Chem.* **86**, 1136−1141 (1982). (Joseph O. Hirschfelder Commemorative Issue.) Erratum: **87**, 4554 (1983).

170. "The Incorporation of Quantum Effects in Generalized Transition State Theory," D. G. Truhlar, A. D. Isaacson, R. T. Skodje, and B. C. Garrett, *J. Phys. Chem.* **86**, 2252−2261 (1982), **87**, 4554(E) (1983). (*Proc. Am. Conf. Theor. Chem.*, 1981)

173. "Polyatomic Canonical Variational Theory for Chemical Reaction Rates. Separable-Mode Formalism with Application to OH + H_2 → H_2O + H," A. D. Isaacson and D. G. Truhlar, *J. Chem. Phys.* **76**, 1380−1391 (1982).

175. "Kinetic Isotope Effects in the Mu + H_2 and Mu + D_2 Reactions: Accurate Quantum Calculations for the Collinear Reactions and Variational Transition State Theory Predictions for One and Three Dimensions," D. K. Bondi, D. C. Clary, J. N. L. Connor, B. C. Garrett, and D. G. Truhlar, *J. Chem. Phys.* **76**, 4986−4995 (1982).

176. "Temperature Dependence of the Activation Energy: D + H_2," N. C. Blais, D. G. Truhlar, and B. C. Garrett, *J. Chem. Phys.* **76**, 2768−2770 (1982).

177. "Canonical Unified Statistical Model. Classical Mechanical Theory and Applications to Collinear Reactions," B. C. Garrett and D. G. Truhlar, *J. Chem. Phys.* **76**, 1853−1858 (1982).

178. "Stabilization Calculations of Resonance Energies for Chemical Reactions," T. C. Thompson and D. G. Truhlar, *J. Chem. Phys.* **76**, 1790−1794 (1982). Erratum: **77**, 3777−3778 (1982).

179. "Quasiclassical Trajectory Calculation of the State-Specified Differential Cross Sections and Opacity Functions for F + H_2 → HF(v') + H," N. C. Blais and D. G. Truhlar, *J. Chem. Phys.* **76**, 4490−4492 (1982).

182. "Wigner-Distribution Trajectory Method for Collision-Induced Dissociation," J. C. Gray and D. G. Truhlar, *J. Chem. Phys.* **76**, 5350−5355 (1982).

189. "High-Energy Collision-Induced Dissociation of H_2 by H," N. C. Blais and D. G. Truhlar, *Ap. J.* **258**, L79−L81 (1982).

192. "Statistical-Diabatic Model for State-Selected Reaction Rates. Theory and Application of Vibrational-Mode Correlation Analysis to OH(n_{OH}) + H_2(n_{HH}) → H_2O + H," D. G. Truhlar and A. D. Isaacson, *J. Chem. Phys.* **77**, 3516−3522 (1982).

193. "Semiclassical Self-Consistent-Field Method for Reactive Resonances," B. C. Garrett and D. G. Truhlar, *Chem. Phys. Lett.* **92**, 64−70 (1982).

195. "Vibrationally Adiabatic Models for Reactive Tunneling," R. T. Skodje, D. G. Truhlar, and B. C. Garrett, *J. Chem. Phys.* **77**, 5955−5976 (1982).

197. "New Method for Estimating Widths of Scattering Resonances from Real Stabilization Graphs," T. C. Thompson and D. G. Truhlar, *Chem. Phys. Lett.* **92**, 71−75 (1982).

198. "Third Body Efficiencies for Collision-Induced Dissociation of Diatomics. Rate Coefficients for H + H_2 → 3H," N. C. Blais and D. G. Truhlar, *J. Chem. Phys.* **78**, 2388−2393 (1983).

201. "Comparison of Variational Transition State Theory and Quantum Sudden Calculation of Three-Dimensional Rate Coefficients for the Reactions D(H) + BrH → DBr(HBr) + H," D. C. Clary, B. C. Garrett, and D. G. Truhlar, *J. Chem. Phys.* **78**, 777−782 (1983).

202. "Quasiclassical Trajectory (and Variational Transition State Theory) Study of the Rates and Temperature-Dependent Activation Energies of the Reactions Mu + H_2 (Completely Thermal) and H, D, and Mu + H_2($v = 0, j = 2$)," N. C. Blais, D. G. Truhlar, and B. C. Garrett, *J. Chem. Phys.* **78**, 2363−2367 (1983).

204. "Reaction-Path Interpolation Models for Variational Transition-State Theory," D. G. Truhlar, N. J. Kilpatrick, and B. C. Garrett, *J. Chem. Phys.* **78**, 2438−2442 (1983).

207. "Variational Transition State Theory and Tunneling for a Heavy-Light-Heavy Reaction using an Ab Initio Potential Energy Surface. $^{37}Cl + H(D)^{35}Cl \rightarrow H(D)^{37}Cl + {}^{35}Cl$," B. C. Garrett, D. G. Truhlar, A. F. Wagner, and T. H. Dunning, Jr., *J. Chem. Phys.* **78**, 4400−4413 (1983).

208. "Test of Variational Transition State Theory with a Large-Curvature Tunneling Approximation Against Accurate Quantal Reaction Probabilities and Rate Coefficients for Three Collinear Reactions with Large Reaction-Path Curvature: Cl + HCl, Cl + DCl, and Cl + MuCl," D. K. Bondi, J. N. L. Connor, B. C. Garrett, and D. G. Truhlar, *J. Chem. Phys.* **78**, 5981−5989 (1983).

209. "Accurate Calculations of the Rate Constants and Kinetic Isotope Effects for Tritium-Substituted Analogues of the H + H_2 Reaction," D. G. Truhlar, R. S. Grev, and B. C. Garrett, *J. Phys. Chem.* **87**, 3415−3419 (1983).

210. "Nonequilibrium Effects in Chemical Kinetics. Straight-Line Paths for Homonuclear Diatomic Dissociation-Recombination," C. Lim and D. G. Truhlar, *J. Phys. Chem.* **87**, 2683−2699 (1983).

219. "The Current Status of Transition State Theory," D. G. Truhlar, W. L. Hase, and J. T. Hynes, *J. Phys. Chem.* **87**, 2664−2682, 5523(E) (1983). (Henry Erying Dedicative Issue.)

220. "The Existence of Straight-Line Paths, Invariant Vectors, and Invariant Tensors Characterizing Nonequilibrium State Distributions During Chemical Reactions," C. Lim and D. G. Truhlar, *J. Chem. Phys.* **79**, 3296−3306 (1983).

221. "Reaction-Path Hamiltonian Model of Partial Widths for Vibrationally Elastic and Inelastic Decay of Adiabatically Trapped Reactive Resonances," R. T. Skodje, D. W. Schwenke, D. G. Truhlar, and B. C. Garrett, *J. Phys. Chem.* **88**, 628−636 (1984). (Bryce Crawford, Jr. Commemorative Issue.)

222. "Probability Densities for Quantum Mechanical Collision Resonances in Reactive Scattering," T. C. Thompson and D. G. Truhlar, *Chem. Phys. Lett.* **101**, 235−241 (1983).

224. "Small-Curvature Adiabatic Approximation for Reaction-Path Reduced-Dimensionality Effective Hamiltonian," R. T. Skodje and D. G. Truhlar, *J. Chem. Phys.* **79**, 4882−4888 (1983).

225. "Variational Transition State Theory Calculations for an Atom-Radical Reaction with No Saddle Point: O + OH," S. N. Rai and D. G. Truhlar, *J. Chem. Phys.* **79**, 6046−6059 (1983).

226. "A Least-Action Variational Method for Calculating Multidimensional Tunneling Probabilities for Chemical Reactions," B. C. Garrett and D. G. Truhlar, *J. Chem. Phys.* **79**, 4931−4938 (1983).

227. "Stabilization Calculations and Probability Densities for the Well Studied Collisional Resonances in Collinear F + H_2, F + HD, and F + D_2," T. C. Thompson and D. G. Truhlar, *J. Phys. Chem.* **88**, 210−214 (1984).

228. "Two New Potential Energy Surfaces for the F + H_2 Reaction," D. G. Truhlar, B. C. Garrett, and N. C. Blais, *J. Chem. Phys.* **80**, 232−240 (1984).

229. "Dependence of Reaction Attributes, Including Differential Cross Sections and Resonance Features, on Changes in the Potential Energy Surface for the F + D_2 Reaction," R. B. Walker, N. C. Blais, and D. G. Truhlar, *J. Chem. Phys.* **80**, 246−254 (1984).

230. "Calculated Product-State Distributions for the Reaction H + $D_2 \rightarrow$ HD + D at Relative Translational Energies 0.55 and 1.30 eV," N. C. Blais and D. G. Truhlar, *Chem. Phys. Lett.* **102**, 120−125 (1983).

232. "Study of Mixture Effects in the Nonequilibrium Kinetics of Homonuclear Diatomic Dissociation and Recombination," C. Lim and D. G. Truhlar, *J. Phys. Chem.* **88**, 778−792 (1984).

234. "Nearly Encounter-Controlled Reactions: The Equivalence of the Steady-State and Diffusional Viewpoints," D. G. Truhlar, *J. Chem. Educ.* **62**, 104−106 (1985).

235. "Calculation of Partial Widths and Isotope Effects for Reactive Resonances by a Reaction-Path Hamiltonian Model: Test Against Accurate Quantal Results for a Twin-Saddlepoint System," R. T. Skodje, D. W. Schwenke, D. G. Truhlar, and B. C. Garrett, *J. Chem. Phys.* **80**, 3569−3573 (1984).

236. "Rational Fraction Analytic Continuation Method for Complex Resonance Energies in Multi-dimensional Systems," D. Thirumalai, T. C. Thompson, and D. G. Truhlar, *J. Chem. Phys.* **80**, 5864−5865 (1984).

240. "WKB Approximation for the Reaction-Path Hamiltonian: Application to Variational Transition State Theory, Vibrationally Adiabatic Excited-State Barrier Heights, and Resonance Calculations," B. C. Garrett and D. G. Truhlar, *J. Chem. Phys.* **81**, 309−317 (1984).

242. "Test of Variational Transition State Theory against Accurate Quantal Results for a Reaction with Very Large Reaction-Path Curvature and a Low Barrier," D. G. Truhlar, B. C. Garrett, P. G. Hipes, and A. Kuppermann, *J. Chem. Phys.* **81**, 3542−3545 (1984).

245. "Characterization of Exit-Channel Barriers for Chemical Reactions Producing Specific Vibrational States," R. Steckler, D. G. Truhlar, B. C. Garrett, N. C. Blais, and R. B. Walker, *J. Chem. Phys.* **81**, 5700−5708 (1984).

247. "Improved Canonical and Microcanonical Variational Transition State Theory Calculations for a Polyatomic System: OH + $H_2 \rightarrow H_2O$ + H," A. D. Isaacson, M. T. Sund, S. N. Rai, and D. G. Truhlar, *J. Chem. Phys.* **82**, 1338−1340 (1985).

248. "Dissociation Potential for Breaking a C−H Bond in Methane," F. B. Brown and D. G. Truhlar, *Chem. Phys. Lett.* **113**, 441−446 (1985).

249. "An Improved Potential Energy Surface for F + $H_2 \rightarrow$ HF + H and H + H′F → HF + H′," F. B. Brown, R. Steckler, D. W. Schwenke, D. G. Truhlar, and B. C. Garrett, *J. Chem. Phys.* **82**, 188−201 (1985).

250. "Variational Transition State Theory with Least-Action Tunneling Calculations for the Kinetic Isotope Effects in the Cl + H_2 Reaction: Tests of Extended-LEPS, Information-Theoretic, and Diatomics-in-Molecules Potential Energy Surfaces," S. C. Tucker, D. G. Truhlar, B. C. Garrett, and A. D. Isaacson, *J. Chem. Phys.* **82**, 4102−4119 (1985).

251. "Generalized Transition State Theory and Least-Action Tunneling Calculations for the Reaction Rates of H(D) + H_2(n = 1) → H_2(HD) + H," B. C. Garrett and D. G. Truhlar, *J. Phys. Chem.* **89**, 2204−2208 (1985). (*Proc. Am. Conf. Theor. Chem.*, 1984.)

253. "Internal-State Nonequilibrium Effects for a Fast, Second-Order Reaction," C. Lim and D. G. Truhlar, *J. Phys. Chem.* **89**, 5−7 (1985).

254. "Variational Transition States for Ion−Molecule Reactions," D. G. Truhlar, *J. Chem. Phys.* **82**, 2166−2167 (1985).

255. "Effect of Bending Potential on Calculated Product-State Distributions for the Reaction H + $D_2 \rightarrow$ HD + D," N. C. Blais, D. G. Truhlar, and B. C. Garrett, *J. Chem. Phys.* **82**, 2300−2304 (1985).

257. "New Techniques for the Study of Nonequilibrium Effects in Non-First-Order Systems," C. Lim and D. G. Truhlar, *Chem. Phys. Lett.* **114**, 253−257 (1985).

258. "Variational Transition State Theory Calculations for the Reaction Rates of F with H_2, D_2, and HD and the Intermolecular and Intramolecular Kinetic Isotope Effects," R. Steckler, D. G. Truhlar, and B. C. Garrett, *J. Chem. Phys.* **82**, 5499−5505 (1985).

260. "Nuclear-Motion Corrections to Born−Oppenheimer Barrier Heights for Chemical Reactions," B. C. Garrett and D. G. Truhlar, *J. Chem. Phys.* **82**, 4543−4547 (1985). Erratum: **84**, 7057 (1986).

262. "Test of Variational Transition State Theory and the Least-Action Approximation for Multidimensional Tunneling Probabilities Against Accurate Quantal Rate Constants for a Collinear Reaction Involving Tunneling in an Excited State," B. C. Garrett, N. Abusalbi, D. J. Kouri, and D. G. Truhlar, *J. Chem. Phys.* **83**, 2252−2258 (1985).

265. "Effect of Transition-State Bond Angle on the Vibrational Energy Release in Chemical Reactions," N. C. Blais and D. G. Truhlar, *Chem. Phys. Lett.* **118**, 379−383 (1985).

266. "Product State Distributions for Inelastic and Reactive H + D_2 Collisions as Functions of Collision Energy," N. C. Blais and D. G. Truhlar, *J. Chem. Phys.* **83**, 2201−2206 (1985).

268. "A High-Barrier Potential Energy Surface for F + H_2 → HF + H," R. Steckler, D. G. Truhlar, and B. C. Garrett, *J. Chem. Phys.* **83**, 2870−2877 (1985).

271. "A Multi-Property Empirical Potential Energy Surface for the Reaction H + Br_2 → HBr + Br," N. C. Blais and D. G. Truhlar, *J. Chem. Phys.* **83**, 5546−5558 (1985).

273. "Thermal and State-Selected Rate Constant Calculations for $O(^3P)$ + H_2 → OH + H and Isotopic Analogues," B. C. Garrett and D. G. Truhlar, *Int. J. Quantum Chem.* **29**, 1463−1482 (1986). (*Proc. Int. Congress Quantum Chem., 4th.*)

275. "An Improved Calculation of the Transition State for the F + H_2 Reaction," R. Steckler, D. W. Schwenke, F. B. Brown, and D. G. Truhlar, *Chem. Phys. Lett.* **121**, 475−478 (1985).

277. "The 1985 Conference on the Dynamics of Molecular Collisions," D. G. Truhlar and P. J. Dagdigian, *Comments At. Mol. Phys.* **17**, 335−342 (1986).

278. "Stabilization Calculations of Resonance Energies for the Coplanar Reactions H + FH and H + H_2," J. G. Lauderdale and D. G. Truhlar, *J. Chem. Phys.* **84**, 192−196 (1986).

280. "The Effect of Vibrational−Rotational Disequilibrium on the Rate Constant for an Atom-Transfer Reaction," C. Lim and D. G. Truhlar, *J. Phys. Chem.* **90**, 2616−2634 (1986).

281. "Test of Variational Transition State Theory and Multidimensional Semiclassical Transmission Coefficient Methods Against Accurate Quantal Rate Constants for H + H_2/HD, D + H_2, and O + H_2/D_2/HD, Including Intra- and Intermolecular Kinetic Isotope Effects," B. C. Garrett, D. G. Truhlar, and G. C. Schatz, *J. Am. Chem. Soc.* **108**, 2876−2881 (1986).

284. "Ab Initio Predictions and Experimental Confirmation of Large Tunneling Contributions to Rate Constants and Kinetic Isotope Effects for Hydrogen-Atom Transfer Reactions," B. C. Garrett, D. G. Truhlar, J. M. Bowman, A. F. Wagner, D. Robie, S. Arepalli, N. Presser, and R. J. Gordon, *J. Am. Chem. Soc.* **108**, 3515−3516 (1986).

285. "Tests of the Extension of Variational Transition State Theory to Calculate Reaction Rates for Molecules in Selected Excited Vibrational States," R. Steckler, D. G. Truhlar, and B. C. Garrett, *J. Chem. Phys.* **84**, 6712−6718 (1986).

287. "The Potential Energy Surface for the F + H_2 Reaction as a Function of Bond Angle in the Saddle Point Vicinity," D. W. Schwenke, R. Steckler, F. B. Brown, and D. G. Truhlar, *J. Chem. Phys.* **84**, 5706−5710 (1986).

288. "Semiclassical Variational Transition State Calculations for the Reactions of H and D with Thermal and Vibrationally Excited H_2," B. C. Garrett, D. G. Truhlar, A. J. C. Varandas, and N. C. Blais, *Int. J. Chem. Kinet.* **18**, 1065−1077 (1986).

289. "Evaluation of Dynamical Approximations for Calculating the Effects of Vibrational Excitation on Reaction Rates. O + H_2(n = 0, 1) ↔ OH(n = 0, 1) + H," B. C. Garrett, D. G. Truhlar, J. M. Bowman, and A. F. Wagner, *J. Phys. Chem.* **90**, 4305−4311 (1986).

290. "Phenomenological Manifestations of Large-Curvature Tunneling in Hydride Transfer Reactions," M. M. Kreevoy, D. Ostovic, D. G. Truhlar, and B. C. Garrett, *J. Phys. Chem.* **90**, 3766−3774 (1986).

292. "Scaling All Correlation Energy in Perturbation Theory Calculations of Bond Energies and Barrier Heights," M. S. Gordon and D. G. Truhlar, *J. Am. Chem. Soc.* **108**, 5412−5419 (1986).

293. "Dynamics Calculations of Kinetic Isotope Effects for the Reactions of Muonium Atoms with F_2 and Cl_2," R. Steckler, D. G. Truhlar, and B. C. Garrett, Int. *J. Quantum Chem., Symp.* **20**, 495−506 (1986).

294. "Reaction Rates of O + HD → OH + D and O + HD → OH + H," B. C. Garrett and D. G. Truhlar, *Int. J. Quantum Chem.* **31**, 17−31 (1987).

297. "Monte Carlo Trajectory and Master Equation Study of the Nonequilibrium Dissociation Rate Coefficient for Ar + H_2 → Ar + 2H at 4500 K," K. Haug, D. G. Truhlar, and N. C. Blais, *J. Chem. Phys.* **86**, 2697−2716 (1987), **96**, 5556−5557-(E) (1992).

300. "Dynamics of Gas-Phase Reactions of Muonium," B. C. Garrett, R. Steckler, and D. G. Truhlar, *Hyperfine Interact.* **32**, 779−793 (1986).

301. "Potential Energy Surfaces for Polyatomic Reaction Dynamics," D. G. Truhlar, R. Steckler, and M. S. Gordon, *Chem. Rev.* **87**, 217−236 (1987).

303. "Dynamical Bottlenecks and Semiclassical Tunneling Paths for Chemical Reactions," D. G. Truhlar and B. C. Garrett, *J. Chim. Phys.* **84**, 365−369 (1987).

304. "Propagation Method for the Solution of the Arrangement-Channel Coupling Equations for Reactive Scattering in Three Dimensions," D. W. Schwenke, D. G. Truhlar, and D. J. Kouri, *J. Chem. Phys.* **86**, 2772−2786 (1987).

306. "L^2 Solution of the Quantum Mechanical Reactive Scattering Problem. The Threshold Energy for D + H_2(v = 1) → HD + H," K. Haug, D. W. Schwenke, Y. Shima, D. G. Truhlar, J. Zhang, and D. J. Kouri, *J. Phys. Chem.* **90**, 6757−6759 (1986).

307. "Estimation of Higher-Order Correlation Effects on the Potential Energy Surface for the F + H_2 Reaction in the Saddle Point Vicinity," D. W. Schwenke, R. Steckler, F. B. Brown, and D. G. Truhlar, *J. Chem. Phys.* **86**, 2443−2444 (1987).

311. "Accurate Partial Resonance Widths for Collinear Reactive Collisions," D. W. Schwenke and D. G. Truhlar, *J. Chem. Phys.* **87**, 1095−1106 (1987).

314. "A Double Many-Body Expansion of the Two Lowest-Energy Potential Surfaces and Nonadiabatic Coupling for H_3," A. J. C. Varandas, F. B. Brown, C. A. Mead, D. G. Truhlar, and N. C. Blais, *J. Chem. Phys.* **86**, 6258−6269 (1987).

317. "L^2 Amplitude Density Method for Multichannel Inelastic and Rearrangement Collisions," J. Z. H. Zhang, D. J.

Kouri, K. Haug, D. W. Schwenke, Y. Shima, and D. G. Truhlar, *J. Chem. Phys.* **88**, 2492−2512 (1988).

318. "Accurate Quantum Mechanical Reaction Probabilities for the Reaction O + H_2 → OH + H," K. Haug, D. W. Schwenke, D. G. Truhlar, Y. Zhang, J. Z. H. Zhang, and D. J. Kouri, *J. Chem. Phys.* **87**, 1892−1894 (1987).

319. "L^2 Calculations of Accurate Quantal Dynamical Reactive Scattering Transition Probabilities and Their Use to Test Semiclassical Applications," J. Z. H. Zhang, Y. Zhang, D. J. Kouri, B. C. Garrett, K. Haug, D. W. Schwenke, and D. G. Truhlar, *Faraday Discuss. Chem. Soc.* **84**, 371−386 (1987).

321. "POLYRATE: A General Computer Program for Variational Transition State Theory and Semiclassical Tunneling Calculations of Chemical Reaction Rates," A. D. Isaacson, D. G. Truhlar, S. N. Rai, R. Steckler, G. C. Hancock, B. C. Garrett, and M. J. Redmon, *Comput. Phys. Commun.* **47**, 91−102 (1987).

323. "A Comparative Study of Potential Energy Surfaces for CH_3 + H_2 ↔ CH_4 + H," R. Steckler, K. J. Dykema, F. B. Brown, G. C. Hancock, D. G. Truhlar, and T. Valencich, *J. Chem. Phys.* **87**, 7024−7035 (1987).

324. "A New Potential Energy Surface for the CH_3 + H_2 ↔ CH_4 + H Reaction: Calibration, Rate Constants, and Kinetic Isotope Effects by Variational Transition State Theory and Semiclassical Tunneling Calculations," T. Joseph, R. Steckler, and D. G. Truhlar, *J. Chem. Phys.* **87**, 7036−7049 (1987).

325. "Algorithms and Accuracy Requirements for Computing Reaction Paths by the Method of Steepest Descent," B. C. Garrett, M. J. Redmon, R. Steckler, D. G. Truhlar, K. K. Baldridge, D. Bartol, M. W. Schmidt, and M. S. Gordon, *J. Phys. Chem.* **92**, 1476−1488 (1988).

326. "Variational Basis-Set Calculations of Accurate Quantum Mechanical Reaction Probabilities," D. W. Schwenke, K. Haug, D. G. Truhlar, Y. Sun, J. Z. H. Zhang, and D. J. Kouri, *J. Phys. Chem.* **91**, 6080−6082 (1987).

327. "Quantum Mechanical Algebraic Variational Methods for Inelastic and Reactive Molecular Collisions," D. W. Schwenke, K. Haug, M. Zhao, D. G. Truhlar, Y. Sun, J. Z. H. Zhang, and D. J. Kouri, *J. Phys. Chem.* **92**, 3202−3216 (1988). (*Proc. Am. Conf. Theor. Chem.*, 1987.)

331. "The Final State and Velocity Distribution of the Reaction D + H_2 → HD + H as a Function of Scattering Angle," N. C. Blais and D. G. Truhlar, *J. Chem. Phys.* **88**, 5457−5464 (1988).

332. "Quantum Mechanical Calculations of Vibrational Population Inversion in Chemical Reactions," Y. C. Zhang, J. Z. H. Zhang, D. J. Kouri, K. Haug, D. W. Schwenke, and D. G. Truhlar, *Phys. Rev. Lett.* **60**, 2367−2370 (1988).

335. "Improved Potential Energy Surfaces for the Reaction $O(^3P)$ + H_2 → OH + H," T. Joseph, D. G. Truhlar, and B. C. Garrett, *J. Chem. Phys.* **88**, 6982−6990 (1988).

337. "Effect of Orbital and Rotational Angular Momentum Averaging on Branching Ratios of Dynamical Resonances in the Reaction H + *p*-H_2 → *o*-H_2 + H," M. Mladenovic, M. Zhao, D. G. Truhlar, D. W. Schwenke, Y. Sun, and D. J. Kouri, *Chem. Phys. Lett.* **146**, 358−363 (1988).

338. "Thermochemical Kinetic Analysis of Tunneling and the Incorporation of Tunneling Contributions in Thermochemical Kinetics," D. G. Truhlar and B. C. Garrett, *J. Am. Chem. Soc.* **111**, 1232−1236 (1989).

339. "Comparison of Classical Simulations of the H + H_2 Reaction to Accurate Quantum Mechanical State-to-State Partial Cross Sections with Total Angular Momentum $J = 0-4$ and to Experiment for All *J*," M. Zhao, M. Mladenovic, D. G. Truhlar, D. W. Schwenke, Y. Sun, D. J. Kouri, and N. C. Blais, *J. Am. Chem. Soc.* **111**, 852−859 (1989).

340. "Supercomputer Chemistry: Structure, Dynamics, and Biochemical Applications," J. Almlöf, D. G. Truhlar, and T. P. Lybrand, *Interdiscip. Sci. Rev.* **15**, 252−263 (1990).

341. "The Effect of a Conical Intersection on Cross Sections for Collision-Induced Dissociation," N. C. Blais, D. G. Truhlar, and C. A. Mead, *J. Chem. Phys.* **89**, 6204−6208 (1988).

342. "Iterative Methods for Solving the Non-Sparse Equations of Quantum Mechanical Reactive Scattering," C. Duneczky, R. E. Wyatt, D. Chatfield, K. Haug, D. W. Schwenke, D. G. Truhlar, Y. Sun, and D. J. Kouri, *Comput. Phys. Commun.* **53**, 357−380 (1989).

343. "Calculation of Reaction Rates and Kinetic Isotope Effects for Dissociative Chemisorption of H_2 and D_2 on Ni-(100), Ni(110), and Ni(111) Surfaces," T. N. Truong, G. Hancock, and D. G. Truhlar, *Surf. Sci.* **214**, 523−559 (1989).

344. "Converged Quantum Mechanical Calculation of the Product Vibration−Rotation State Distribution of the H + *p*-H_2 Reaction," M. Mladenovic, M. Zhao, D. G. Truhlar, D. W. Schwenke, Y. Sun, and D. J. Kouri, *J. Phys. Chem.* **92**, 7035−7038 (1988).

346. "Reaction Rates of H(H_2), D(H_2), and H(D_2) van der Waals Molecules and the Threshold Behavior of the Bimolecular Gas-Phase Rate Coefficient," G. C. Hancock, C. A. Mead, D. G. Truhlar, and A. J. C. Varandas, *J. Chem. Phys.* **91**, 3492−3503 (1989).

347. "Test of the Accuracy of Small-Curvature and Minimum-Energy Reference Paths for Parametrizing the Search for Least-Action Tunneling Paths: (H,D) + H′Br → (H,D)Br + H′," G. C. Lynch, D. G. Truhlar, and B. C. Garrett, *J. Chem. Phys.* **90**, 3102−3109 (1989), **91**, 3280(E) (1989).

348. "Global Potential Energy Surfaces for H_2Cl," D. W. Schwenke, S. C. Tucker, R. Steckler, F. B. Brown, G. C. Lynch, D. G. Truhlar, and B. C. Garrett, *J. Chem. Phys.* **90**, 3110−3120 (1989).

349. "Ab Initio Reaction Paths and Direct Dynamics Calculations," K. K. Baldridge, M. S. Gordon, R. Steckler, and D. G. Truhlar, *J. Phys. Chem.* **93**, 5107−5119 (1989).

350. "Converged Quantum Dynamics Calculations for the F + H_2 Reaction on the Well Studied M5 Potential Energy Surface," C.-h. Yu, Y. Sun, D. J. Kouri, P. Halvick, D. G. Truhlar, and D. W. Schwenke, *J. Chem. Phys.* **90**, 7608−7609 (1989).

351. "Quantum Mechanical Interference Effects on Vibrational Excitation in the Reaction D + H_2 → HD + H: Delay Times and Dependence of Vibrational Enhancement on Angular Momentum," M. Zhao, D. G. Truhlar, D. J. Kouri, Y. Sun, and D. W. Schwenke, *Chem. Phys. Lett.* **156**, 281−288 (1989).

352. "Direct Calculation of the Reactive Transition Matrix by L^2 Quantum Mechanical Variational Methods with Complex Boundary Conditions," Y. Sun, C.-h. Yu, D. J. Kouri, D. W. Schwenke, P. Halvick, M. Mladenovic, and D. G. Truhlar, *J. Chem. Phys.* **91**, 1643−1657 (1989).

353. "Comparison of Quasiclassical Trajectory Calculations to Accurate Quantum Mechanics for State-to-State Partial Cross Sections at Low Total Angular Momentum for the Reaction D + H_2 → HD + H," N. C. Blais, M. Zhao, M. Mladenovic, D. G. Truhlar, D. W. Schwenke, Y. Sun, and D. J. Kouri, *J. Chem. Phys.* **91**, 1038−1042 (1989).

354. "Semiclassical and Quantum Mechanical Calculations of Isotopic Kinetic Branching Ratios for the Reaction of $O(^3P)$ with HD," G. C. Lynch, P. Halvick, D. G. Truhlar, B. C. Garrett,

D. W. Schwenke, and D. J. Kouri, *Z. Naturforsch.* **44a**, 427−434 (1989). (Festschrift für Jacob Bigeleisen.)

355. "Transition State Structure, Barrier Height, and Vibrational Frequencies for the Reaction $Cl + CH_4 \rightarrow CH_3 + HCl$," T. N. Truong, D. G. Truhlar, K. K. Baldridge, M. S. Gordon, and R. Steckler, *J. Chem. Phys.* **90**, 7137−7142 (1989).

356. "Generalized Born Fragment Charge Model for Solvation Effects as a Function of Reaction Coordinate," S. C. Tucker and D. G. Truhlar, *Chem. Phys. Lett.* **157**, 164−170 (1989).

357. "Converged Three-Dimensional Quantum Mechanical Reaction Probabilities and Delay Times for the $F + H_2$ Reaction on a Potential Energy Surface with a Realistic Exit Valley," C.-h. Yu, D. J. Kouri, M. Zhao, D. G. Truhlar, and D. W. Schwenke, *Chem. Phys. Lett.* **157**, 491−495 (1989).

358. "Parameters for Scaling the Correlation Energy of the Bonds Si−H, P−H, S−H, and Cl−H and Application to the Reaction of Silyl Radical with Silane," M. S. Gordon, K. A. Nguyen, and D. G. Truhlar, *J. Phys. Chem.* **93**, 7356−7358 (1989).

359. "Ab Initio Calculations of the Transition State Geometry and Vibrational Frequencies of the S_N2 Reaction of Cl^- with CH_3Cl," S. C. Tucker and D. G. Truhlar, *J. Phys. Chem.* **93**, 8138−8142 (1989).

360. "Application of the Large-Curvature Tunneling Approximation to Polyatomic Molecules: Abstraction of H or D by Methyl Radical," B. C. Garrett, T. Joseph, T. N. Truong, and D. G. Truhlar, *Chem. Phys.* **136**, 271−284 (1989), **140**, 207(E) (1990). (Special issue: Spectroscopy and Dynamics of Elementary Proton Transfer in Polyatomic Systems.)

361. "Embedded Diatomics-in-Molecules (EDIM): A Method to Include Delocalized Electronic Interactions in the Treatment of Covalent Chemical Reactions at Metal Surfaces," T. N. Truong, D. G. Truhlar, and B. C. Garrett, *J. Phys. Chem.* **93**, 8227−8239 (1989).

362. "Spectroscopic Analysis of Transition State Energy Levels: Bending-Rotational Spectrum and Lifetime Analysis of H_3 Quasibound States," M. Zhao, M. Mladenovic, D. G. Truhlar, D. W. Schwenke, O. Sharafeddin, Y. Sun, and D. J. Kouri, *J. Chem. Phys.* **91**, 5302−5309 (1989).

363. "Generalized Newton Variational Principle − L^2 Amplitude Density Treatment of the 3-Dimensional Quantal Reaction $F + H_2 \rightarrow HF(v_f) + H$: Comparison of Reaction Probabilities and State-to-State Collisional Delay Times for Zero and Nonzero Total Angular Momentum," C.-h. Yu, D. J. Kouri, M. Zhao, D. G. Truhlar, and D. W. Schwenke, *Int. J. Quantum Chem., Symp.* **23**, 45−58 (1989).

365. "New Variational Principles for Photodissociation: L^2 Amplitude Density and Scattered Wave Methods," D. J. Kouri and D. G. Truhlar, *J. Chem. Phys.* **91**, 6919−6925 (1989).

366. "The $H + D_2$ Reaction: Quasiclassical Simulation of Nascent HD Rovibrational State Distributions Under Experimentally Probed High-Energy Conditions," N. C. Blais and D. G. Truhlar, *Chem. Phys. Lett.* **162**, 503−510 (1989).

367. "A Comparative Analysis of Variational Methods for Inelastic and Reactive Scattering," Y. Sun, D. J. Kouri, and D. G. Truhlar, *Nucl. Phys. A* **508**, 41c−62c (1990).

369. "A Six-Body Potential Energy Surface for the S_N2 Reaction $Cl^-(g) + CH_3Cl(g)$ and a Variational Transition State Theory Calculation of the Rate Constant," S. C. Tucker and D. G. Truhlar, *J. Am. Chem. Soc.* **112**, 3338−3347 (1990).

370. "The Effect of Nonequilibrium Solvation on Chemical Reaction Rates. Variational Transition State Theory Studies of the Microsolvated Reaction $Cl^-(H_2O)_n + CH_3Cl$," S. C. Tucker and D. G. Truhlar, *J. Am. Chem. Soc.* **112**, 3347−3361 (1990).

371. "Rapid Convergence of Basis Set Expansions for Quantum Mechanical Reactive Amplitude Densities: Channel-Dependent Expansion Lengths," P. Halvick, D. G. Truhlar, D. W. Schwenke, Y. Sun, and D. J. Kouri, *J. Phys. Chem.* **94**, 3231−3236 (1990).

372. "Exact Quantum Dynamics Tests of the Distorted Wave Approximation for the $O(^3P) + HD$ Reaction," P. Halvick, M. Zhao, D. G. Truhlar, D. W. Schwenke, and D. J. Kouri, *J. Chem. Soc., Faraday Trans.* **86**, 1705−1719 (1990). (Special issue on New Theoretical Methods for Reactive and Inelastic Scattering.)

373. "Effect of Rotational Excitation on State-to-State Differential Cross Sections: $D + H_2 \rightarrow HD + H$," M. Zhao, D. G. Truhlar, D. W. Schwenke, and D. J. Kouri, *J. Phys. Chem.* **94**, 7074−7090 (1990).

374. "Quantum Mechanical Dynamics and Quasiclassical Trajectories for Comparison to Stimulated Raman Pumping Measurements of the High-Energy State-to-State Reaction Dynamics of $D + H_2(v = j = 1) \rightarrow HD(v' = 1, j') + H$," N. C. Blais, M. Zhao, D. G. Truhlar, D. W. Schwenke, and D. J. Kouri, *Chem. Phys. Lett.* **166**, 11−19 (1990), **188**, 368(E) (1992).

375. "Contracted Basis Functions for Variational Solutions of Quantum Mechanical Reactive Scattering Problems," M. Zhao, D. G. Truhlar, D. W. Schwenke, C.-h. Yu, and D. J. Kouri, *J. Phys. Chem.* **94**, 7062−7069 (1990).

377. "Quantum Dynamics of Chemical Reactions by Converged Algebraic Variational Calculations," D. G. Truhlar, D. W. Schwenke, and D. J. Kouri, *J. Phys. Chem.* **94**, 7346−7352 (1990). (Feature Article.)

378. "Are Classical Molecular Dynamics Calculations Accurate for State-to-State Transition Probabilities in the $H + D_2$ Reactions?" M. Zhao, D. G. Truhlar, N. C. Blais, D. W. Schwenke, and D. J. Kouri, *J. Phys. Chem.* **94**, 6696−6706 (1990).

380. "Effect of Steps and Surface Coverage on Rates and Kinetic Isotope Effects for Reactions Catalyzed by Metallic Surfaces: Chemisorption of Hydrogen on Ni," T. N. Truong and D. G. Truhlar, *J. Phys. Chem.* **94**, 8262−8279 (1990).

381. "Ab Initio Transition State Theory Calculations of the Reaction Rate for $OH + CH_4 \rightarrow H_2O + CH_3$," T. N. Truong and D. G. Truhlar, *J. Chem. Phys.* **93**, 1761−1769 (1990). Erratum: **97**, 8820 (1992).

383. "What is the Effect of Variational Optimization of the Transition State on α-Deuterium Secondary Kinetic Isotope Effects? A Prototype: $CD_3H + H \leftrightarrow CD_3 + H_2$," D.-h. Lu, D. Maurice, and D. G. Truhlar, *J. Am. Chem. Soc.* **112**, 6206−6214 (1990).

384. "From Force Fields to Dynamics: Classical and Quantal Paths," D. G. Truhlar, and M. S. Gordon, *Science* **249**, 491−498 (1990).

387. "Global Control of Suprathreshold Reactivity by Quantized Transition States," D. C. Chatfield, R. S. Friedman, D. G. Truhlar, B. C. Garrett, and D. W. Schwenke, *J. Am. Chem. Soc.* **113**, 486−494 (1991).

389. "Solvent and Secondary Kinetic Isotope Effects for the Microhydrated S_N2 Reaction of $Cl^-(H_2O)_n$ with CH_3Cl," X. G. Zhao, S. C. Tucker, and D. G. Truhlar, *J. Am. Chem. Soc.* **113**, 826−832 (1991).

392. "Benchmark Calculations of Thermal Reaction Rates. I. Quantal Scattering Theory," D. C. Chatfield, D. G. Truhlar, and D. W. Schwenke, *J. Chem. Phys.* **94**, 2040−2044 (1991).

393. "Benchmark Calculations of Thermal Reaction Rates. II. Direct Calculation of the Flux Autocorrelation Function for a Canonical Ensemble," P. N. Day and D. G. Truhlar, *J. Chem. Phys.* **94**, 2045−2056 (1991).

394. "The Effect of Hydration and Dimerization on the Formamidine Rearrangement," K. A. Nguyen, M. S. Gordon, and D. G. Truhlar, *J. Am. Chem. Soc.* **113**, 1596−1600 (1991).

395. "Variational Reactive Scattering Calculations: Computational Optimization Strategies," D. W. Schwenke, S. L. Mielke, and D. G. Truhlar, *Theor. Chim. Acta* **79**, 241−269 (1991).

396. "Direct Dynamics Calculations with Neglect of Diatomic Differential Overlap Molecular Orbital Theory with Specific Reaction Parameters," A. Gonzàlez-Lafont, T. N. Truong, and D. G. Truhlar, *J. Phys. Chem.* **95**, 4618−4627 (1991).

398. "The Definition of Reaction Coordinates for Reaction-Path Dynamics," G. A. Natanson, B. C. Garrett, T. N. Truong, T. Joseph, and D. G. Truhlar, *J. Chem. Phys.* **94**, 7875−7892 (1991).

399. "Use of Scaled External Correlation, a Double Many-Body Expansion, and Variational Transition State Theory to Calibrate a Potential Energy Surface for FH_2," G. C. Lynch, R. Steckler, D. W. Schwenke, A. J. C. Varandas, D. G. Truhlar, and B. C. Garrett, *J. Chem. Phys.* **94**, 7136−7149 (1991).

400. "Converged Three-Dimensional Quantum Mechanical Reaction Probabilities for the F + H_2 Reaction on a Potential Energy Surface with Realistic Entrance and Exit Channels and Comparisons to Results for Three Other Surfaces," G. C. Lynch, P. Halvick, M. Zhao, D. G. Truhlar, C.-h. Yu, D. J. Kouri, and D. W. Schwenke, *J. Chem. Phys.* **94**, 7150−7158 (1991).

401. "Quantum-Dynamical Characterization of Reactive Transition States," D. C. Chatfield, R. S. Friedman, D. G. Truhlar, and D. W. Schwenke, *Faraday Discuss. Chem. Soc.* **91**, 289−304 (1991).

402. "An Experimentally Based Family of Potential Surfaces for Hydride Transfer Between NAD^+ Analogues," Y. Kim, D. G. Truhlar, and M. M. Kreevoy, *J. Am. Chem. Soc.* **113**, 7837−7847 (1991).

403. "Critical Tests of Variational Transition State Theory and Semiclassical Tunneling Methods for Hydrogen and Deuterium Atom Transfer Reactions and Use of the Semiclassical Calculations to Interpret the Overbarrier and Tunneling Dynamics," B. C. Garrett and D. G. Truhlar, *J. Phys. Chem.* **95**, 10374−10379 (1991). (Michael Kasha Festschrift.)

404. "Improved Techniques for Outgoing Wave Variational Principle Calculations of Converged State-to-State Transition Probabilities for Chemical Reactions," S. L. Mielke, D. G. Truhlar, and D. W. Schwenke, *J. Chem. Phys.* **95**, 5930−5939 (1991).

405. "Calculation of Thermal Rate Coefficients from the Quantum Flux Autocorrelation Function: Converged Results and Variational Quantum Transition State Theory for O + HD ↔ OD + H and O + HD ↔ OH + D," P. N. Day and D. G. Truhlar, *J. Chem. Phys.* **95**, 5097−5112 (1991).

406. "Chemical Reaction Thresholds are Resonances," R. S. Friedman and D. G. Truhlar, *Chem. Phys. Lett.* **183**, 539−546 (1991).

407. "General Parameterized SCF Model for Free Energies of Solvation in Aqueous Solution," C. J. Cramer and D. G. Truhlar, *J. Am. Chem. Soc.* **113**, 8305−8311, 9901(E) (1991).

410. "Quantized Transition State Structure in the Cumulative Reaction Probabilities for the Cl + HCl, I + HI, and I + DI Reactions," D. C. Chatfield, R. S. Friedman, G. C. Lynch, and D. G. Truhlar, *J. Phys. Chem.* **96**, 57−63 (1992).

411. "Interpolated Variational Transition State Theory: Practical Methods for Estimating Variational Transition State Properties and Tunneling Contributions to Chemical Reaction Rates from Electronic Structure Calculations," A. Gonzàlez-Lafont, T. N. Truong, and D. G. Truhlar, *J. Chem. Phys.* **95**, 8875−8894 (1991).

412. "Temperature Dependence of the Kinetic Isotope Effect for a Gas-Phase S_N2 Reaction: Cl^- + CH_3Br," A. A. Viggiano, J. Paschkewitz, R. A. Morris, J. F. Paulson, A. Gonzàlez-Lafont, and D. G. Truhlar, *J. Am. Chem. Soc.* **113**, 9404−9405 (1991).

413. "High-Energy State-to-State Quantum Dynamics for D + $H_2(v = j = 1)$ → $HD(v' = 1, j')$ + H," S. L. Mielke, R. S. Friedman, D. G. Truhlar, and D. W. Schwenke, *Chem. Phys. Lett.* **188**, 359−367 (1992).

414. "Control of Chemical Reactivity by Quantized Transition States," D. C. Chatfield, R. S. Friedman, D. W. Schwenke, and D. G. Truhlar, *J. Phys. Chem.* **96**, 2414−2421 (1992). (Feature Article.)

415. "State-Selected Chemical Reaction Dynamics at the S Matrix Level: Final-State Specificities of Near Threshold Processes at Low and High Energy," D. C. Chatfield, D. G. Truhlar, and D. W. Schwenke, *J. Chem. Phys.* **96**, 4313−4323 (1992).

416. "A New Diabatic Representation of the Coupled Potential Energy Surfaces for $Na(3p\ ^2P)$ + H_2 → $Na(3s\ ^2S)$ + H_2 or NaH + H," P. Halvick and D. G. Truhlar, *J. Chem. Phys.* **96**, 2895−2909 (1992), **100**, 4718(E) (1994).

417. "Optimized Calculations of Reaction Paths and Reaction-Path Functions for Chemical Reactions," V. S. Melissas, D. G. Truhlar, and B. C. Garrett, *J. Chem. Phys.* **96**, 5758−5772 (1992).

419. "POLYRATE 4: A New Version of a Computer Program for the Calculation of Chemical Reaction Rates for Polyatomics," D.-h. Lu, T. N. Truong, V. S. Melissas, G. C. Lynch, Y.-P. Liu, B. C. Garrett, R. Steckler, A. D. Isaacson, S. N. Rai, G. C. Hancock, J. G. Lauderdale, T. Joseph, and D. G. Truhlar, *Comput. Phys. Commun.* **71**, 235−262 (1992).

421. "Trajectory Calculations and Converged Quantum Cross Sections for D + $H_2(v = 1, j = 1, E_{rel} = 1.02$ eV) → $HD(v' = 1, j')$ + H on a New Potential Energy Surface," W. J. Keogh, A. I. Boothroyd, P. G. Martin, S. L. Mielke, D. G. Truhlar, and D. W. Schwenke, *Chem. Phys. Lett.* **195**, 144−152 (1992).

422. "MORATE: A Program for Direct Dynamics Calculations of Chemical Reaction Rates by Semiempirical Molecular Orbital Theory," T. N. Truong, D.-h. Lu, G. C. Lynch, Y.-P. Liu, V. S. Melissas, J. J. P. Stewart, R. Steckler, B. C. Garrett, A. D. Isaacson, A. Gonzàlez-Lafont, S. N. Rai, G. C. Hancock, T. Joseph, and D. G. Truhlar, *Comput. Phys. Commun.* **75**, 143−159 (1993).

426. "Resonance State Approach to Quantum Mechanical Variational Transition State Theory," D. G. Truhlar and B. C. Garrett, *J. Phys. Chem.* **96**, 6515−6518 (1992).

427. "Use of an Improved Ion−Solvent Potential Energy Function to Calculate the Reaction Rate and α-Deuterium and Microsolvation Kinetic Isotope Effects for the Gas-Phase S_N2 Reaction of $Cl^-(H_2O)$ with CH_3Cl," X. G. Zhao, D.-h. Lu, Y.-P. Liu, G. C. Lynch, and D. G. Truhlar, *J. Chem. Phys.* **97**, 6369−6383 (1992).

429. "Complex Generalized Minimal Residual Algorithm for Iterative Solution of Quantum Mechanical Reactive Scattering Equations," D. C. Chatfield, M. S. Reeves, D. G. Truhlar, C. Duneczky, and D. W. Schwenke, *J. Chem. Phys.* **97**, 8322−8333 (1992).

430. "What Causes Aqueous Acceleration of the Claisen Rearrangement?" C. J. Cramer and D. G. Truhlar, *J. Am. Chem. Soc.* **114**, 8794−8799 (1992).

431. "The Nature and Role of Quantized Transition States in the Accurate Quantum Dynamics of the Reaction O + H_2 →

OH + H," D. C. Chatfield, R. S. Friedman, G. C. Lynch, D. G. Truhlar, and D. W. Schwenke, *J. Chem. Phys.* **98**, 342−362 (1993).

435. "Inclusion of Nonequilibrium Continuum Solvation Effects in Variational Transition State Theory," D. G. Truhlar, G. K. Schenter, and B. C. Garrett, *J. Chem. Phys.* **98**, 5756−5770 (1993).

437. "Molecular Modeling of the Kinetic Isotope Effect for the [1,5]-Sigmatropic Rearrangement of *cis*-1,3-Pentadiene," Y.-P. Liu, G. C. Lynch, T. N. Truong, D.-h. Lu, D. G. Truhlar, and B. C. Garrett, *J. Am. Chem. Soc.* **115**, 2408−2415 (1993).

439. "Interpolated Variational Transition State Theory and Tunneling Calculations of the Rate Constant of the Reaction OH + CH_4 at 223−2400 K," V. S. Melissas and D. G. Truhlar, *J. Chem. Phys.* **99**, 1013−1027 (1993).

442. "Bond-Distance and Bond-Angle Constraints in Reaction-Path Dynamics Calculations," D.-h. Lu and D. G. Truhlar, *J. Chem. Phys.* **99**, 2723−2738 (1993).

443. "Preconditioned Complex Generalized Minimal Residual Algorithm for Dense Algebraic Variational Equations in Quantum Reactive Scattering," M. S. Reeves, D. C. Chatfield, and D. G. Truhlar, *J. Chem. Phys.* **99**, 2739−2751 (1993).

444. "Direct Dynamics Calculation of the Kinetic Isotope Effect for an Organic Hydrogen-Transfer Reaction, Including Corner-Cutting Tunneling in 21 Dimensions," Y.-P. Liu, D.-h. Lu, A. Gonzàlez-Lafont, D. G. Truhlar, and B. C. Garrett, *J. Am. Chem. Soc.* **115**, 7806−7817 (1993).

445. "Deuterium and Carbon-13 Kinetic Isotope Effects for the Reaction of OH with CH_4," V. S. Melissas and D. G. Truhlar, *J. Chem. Phys.* **99**, 3542−3552 (1993).

446. "Kinetic Isotope Studies of the Gas-Phase Reaction (H, D, Mu) + HBr → (H,D,Mu)H + Br," G. C. Lynch, D. G. Truhlar, F. B. Brown, and J.-g. Zhao, *Hyperfine Interact.* **87**, 885−898 (1994).

448. "A More Accurate Potential Energy Surface and Quantum Mechanical Cross Section Calculations for the F + H_2 Reaction," S. L. Mielke, G. C. Lynch, D. G. Truhlar, and D. W. Schwenke, *Chem. Phys. Lett.* **213**, 10−16 (1993), **217**, 173(E) (1994).

450. "Variational Transition State Theory and Semiclassical Tunneling Calculations with Interpolated Corrections: A New Approach to Interfacing Electronic Structure Theory and Dynamics for Organic Reactions," W.-P. Hu, Y.-P. Liu, and D. G. Truhlar, *J. Chem. Soc., Faraday Trans.* **90**, 1715−1725 (1994). (*Proc. Faraday Symp.* 29 on Potential-Energy Surfaces and Organic Reaction Paths.)

451. "A Separable Rotation Approximation for the Calculation of Chemical Reaction Rates," S. L. Mielke, G. C. Lynch, D. G. Truhlar, and D. W. Schwenke, *Chem. Phys. Lett.* **216**, 441−446 (1993).

452. "Interpolated Variational Transition State Theory and Semiclassical Tunneling Calculations of the Rate Constant of the Reaction OH + C_2H_6 at 200−3000 K," V. S. Melissas and D. G. Truhlar, *J. Phys. Chem.* **98**, 875−886 (1994).

453. "Comparison of Theoretical and Experimental Differential Cross Sections for the H + D_2 Reaction," S. L. Mielke, D. G. Truhlar, and D. W. Schwenke, *J. Phys. Chem.* **98**, 1053−1057 (1994).

458. "Modeling Transition State Solvation at the Single-Molecule Level: Test of Correlated Ab Initio Predictions Against Experiment for the Gas-Phase S_N2 Reaction of Microhydrated Fluoride with Methyl Chloride," W.-P. Hu and D. G. Truhlar, *J. Am. Chem. Soc.* **116**, 7797−7800 (1994).

460. "Ab Initio Chemical Kinetics: Converged Quantal Reaction Rate Constants for the D + H_2 System," S. L. Mielke, G. C. Lynch, D. G. Truhlar, and D. W. Schwenke, *J. Phys. Chem.* **98**, 8000−8008 (1994).

461. "Tunneling in the Presence of a Bath: A Generalized Transition State Theory Approach," D. G. Truhlar, Y.-P. Liu, G. K. Schenter, and B. C. Garrett, *J. Phys. Chem.* **98**, 8396−8405 (1994).

462. "A New Potential Energy Surface for H_2Br and its Use to Calculate Branching Ratios and Kinetic Isotope Effects for the H + HBr Reaction," G. C. Lynch, D. G. Truhlar, F. B. Brown, and J.-g. Zhao, *J. Phys. Chem.* **99**, 207−225 (1995).

464. "Long-Standing Themes in Computational Chemical Dynamics," D. G. Truhlar, *Comput. Phys. Commun.* **84**, 78−90 (1994). (25th Anniversary Issue.)

466. "Dual-Level Reaction-Path Dynamics (The///Approach to VTST with Semiclassical Tunneling). Application to OH + NH_3 → H_2O + NH_2" J. C. Corchado, J. Espinosa-Garcia, W.-P. Hu, I. Rossi, and D. G. Truhlar, *J. Phys. Chem.* **99**, 687−694 (1995).

468. "Reaction-Path Potential and Vibrational Frequencies in Terms of Curvilinear Internal Coordinates," C. F. Jackels, Z. Gu, and D. G. Truhlar, *J. Chem. Phys.* **102**, 3188−3201 (1995).

469. "Parameterization of NDDO Wavefunctions using Genetic Algorithms: An Evolutionary Approach to Parameterizing Potential Energy Surfaces and Direct Dynamics Calculations for Organic Reactions," I. Rossi and D. G. Truhlar, *Chem. Phys. Lett.* **233**, 231−236 (1995).

470. "Quantum Photochemistry. Accurate Quantum Scattering Calculations for an Electronically Nonadiabatic Reaction," S. L. Mielke, G. J. Tawa, D. G. Truhlar, and D. W. Schwenke, *Chem. Phys. Lett.* **234**, 57−63 (1995).

472. "Quantum Mechanical Threshold Resonances for Unsymmetric Potential Energy Barriers," R. S. Friedman, V. D. Hullinger, and D. G. Truhlar, *J. Phys. Chem.* **99**, 3184−3194 (1995).

478. "A Dual-Level Shepard Interpolation Method for Generating Potential Energy Surfaces for Dynamics Calculations," K. A. Nguyen, I. Rossi, and D. G. Truhlar, *J. Chem. Phys.* **103**, 5522−5530 (1995).

479. "Deuterium Kinetic Isotope Effects and their Temperature Dependence in the Gas-Phase S_N2 Reactions X^- + CH_3Y → CH_3X + Y^- (X, Y = Cl, Br, I)," W.-P. Hu and D. G. Truhlar, *J. Am. Chem. Soc.* **117**, 10726−10734 (1995).

480. "Quantum Photochemistry. The Competition Between Electronically Nonadiabatic Reaction and Electronic-to-Vibrational, Rotational, Translational Energy Transfer in Br* Collisions with H_2," S. L. Mielke, D. G. Truhlar, and D. W. Schwenke, *J. Phys. Chem.* **99**, 16210−16216 (1995).

483. "Factors Affecting Competitive Ion−Molecule Reactions: ClO^- + C_2H_5Cl and C_2D_5Cl via E2 and S_N2 Channels," W.-P. Hu and D. G. Truhlar, *J. Am. Chem. Soc.* **118**, 860−869 (1996).

484. "Current Status of Transition State Theory," D. G. Truhlar, B. C. Garrett, and S. J. Klippenstein, *J. Phys. Chem.* **100**, 12771−12800 (1996). (Centennial Issue.)

486. "Reaction-Path Dynamics in Curvilinear Internal Coordinates Including Torsions," K. A. Nguyen, C. F. Jackels, and D. G. Truhlar, *J. Chem. Phys.* **104**, 6491−6496 (1996).

489. "An Improved Potential Energy Surface for the H_2Cl System and its Use for Calculations of the Rate Constants and Kinetic Isotope Effects," T. Allison, G. C. Lynch, D. G. Truhlar, and M. S. Gordon, *J. Phys. Chem.* **100**, 13575−13587 (1996).

490. "Quantum Mechanical Rate Constants for the Cl + H_2 Reaction," S. L. Mielke, T. C. Allison, D. G. Truhlar, and D. W. Schwenke, *J. Phys. Chem.* **100**, 13588−13593 (1996).

491. "Factors Controlling Regioselectivity in the Reduction of Polynitroaromatics in Aqueous Solution," S. E. Barrows, C. J. Cramer, D. G. Truhlar, M. S. Elovitz, and E. J. Weber, *Environ. Sci. Technol.* **30**, 3028−3038 (1996).

494. "Dynamics of the Simplest Chlorine Atom Reaction: An Experimental and Theoretical Study," M. Alagia, N. Balucani, L. Cartechini, P. Casavecchia, E. H. van Kleef, G. G. Volpi, F. J. Aoiz, L. Bañares, D. W. Schwenke, T. C. Allison, S. L. Mielke, and D. G. Truhlar, *Science* **273**, 1519−1522 (1996).

498. "Funnel States as Mediators of Born−Oppenheimer Breakdown in Reactions at an Avoided Crossing," T. C. Allison, S. L. Mielke, D. W. Schwenke, and D. G. Truhlar, *J. Chem. Soc., Faraday Trans.* **93**, 825−832 (1997). (Special issue on Quantum Theory of Chemical Reactions.)

505. "Improved Dual-Level Direct Dynamics Method for Reaction Rate Calculations with Inclusion of Multidimensional Tunneling Effects and Validation for the Reaction of H with trans-N_2H_2," Y.-Y. Chuang and D. G. Truhlar, *J. Phys. Chem. A* **101**, 3808−3814 (1997). Erratum: **101**, 8741 (1997).

506. "Molecular Modeling of Combustion Kinetics. The Abstraction of Primary and Secondary Hydrogens by Hydroxyl Radical," W.-P. Hu, I. Rossi, J. C. Corchado, and D. G. Truhlar, *J. Phys. Chem. A* **101**, 6911−6921 (1997).

507. "Reaction-Path Dynamics with Harmonic Vibration Frequencies in Curvilinear Internal Coordinates: H + *trans*-$N_2H_2 \rightarrow NH_2 + H_2$," Y.-Y. Chuang and D. G. Truhlar, *J. Chem. Phys.* **107**, 83−89 (1997).

510. "Variational Transition State Theory Without the Minimum Energy Path," J. Villà and D. G. Truhlar, *Theor. Chem. Acc.* **97**, 317−323 (1997). (Jan Erik Almlöf Memorial Issue.)

511. "Statistical Model for Nonadiabatic Decay of an Exciplex Strongly Coupled to a Dissociative Continuum," M. S. Topaler and D. G. Truhlar, *J. Chem. Phys.* **107**, 392−401 (1997).

514. "Importance of Quantum Effects for C−H Bond Activation Reactions," J. Espinosa-García, J. C. Corchado, and D. G. Truhlar, *J. Am. Chem. Soc.* **119**, 9891−9896 (1997).

515. "Singlet−Triplet Splittings and 1,2-Hydrogen Shift Barriers for Methylphenylborenide, Methylphenylcarbene, and Methylphenylnitrenium in the Gas Phase and Solution. What a Difference a Charge Makes," C. J. Cramer, D. G. Truhlar, and D. E. Falvey, *J. Am. Chem. Soc.* **119**, 12338−12342 (1997).

516. "Reaction-Path Dynamics in Redundant Internal Coordinates," Y.-Y. Chuang and D. G. Truhlar, *J. Phys. Chem. A* **102**, 242−247 (1998).

519. "ABCRATE: A Program for the Calculation of Atom−Diatom Reaction Rates," B. C. Garrett, G. C. Lynch, T. C. Allison, and D. G. Truhlar, *Comput. Phys. Commun.* **109**, 47−54 (1998).

520. "Potential Energy Surfaces of NaFH," M. S. Topaler, D. G. Truhlar, X. Y. Chang, P. Piecuch, and J. C. Polanyi, *J. Chem. Phys.* **108**, 5349−5377 (1998).

521. "The Photoabsorption Spectrum of Na···FH van der Waals Molecule. Comparison of Theory and Experiment for a Harpooning Reaction Studied by Transition State Spectroscopy," M. S. Topaler, D. G. Truhlar, X. Y. Chang, P. Piecuch, and J. C. Polanyi, *J. Chem. Phys.* **108**, 5378−5390 (1998).

522. "Test of Trajectory Surface Hopping Against Accurate Quantum Dynamics for an Electronically Nonadiabatic Chemical Reaction," M. S. Topaler, T. C. Allison, D. W. Schwenke, and D. G. Truhlar, *J. Phys. Chem. A* **102**, 1666−1673 (1998).

524. "Interpolated Variational Transition State Theory by Mapping," J. C. Corchado, E. L. Coitiño, Y.-Y. Chuang, P. L. Fast, and D. G. Truhlar, *J. Phys. Chem. A* **102**, 2424−2438 (1998).

529. "Entropic Effects on the Dynamical Bottleneck Location and Tunneling Contributions for $C_2H_4 + H \rightarrow C_2H_5$. Variable Scaling of External Correlation Energy for Association Reactions," J. Villà, A. González-Lafont, J. M. Lluch, and D. G. Truhlar, *J. Am. Chem. Soc.* **120**, 5559−5567 (1998).

530. "Variational Transition State Theory and Tunneling Calculations with Reorientation of the Generalized Transition States for Methyl Cation Transfer," A. González-Lafont, J. Villà, J. M. Lluch, J. Bertrán, R. Steckler, and D. G. Truhlar, *J. Phys. Chem. A* **102**, 3420−3428 (1998).

531. "Variational Transition State Theory Calculations of Thermal Rate Coefficients for the $O(^3P)$ + HCl Reaction," T. C. Allison, B. Ramachandran, J. Senekowitsch, D. G. Truhlar, and R. E. Wyatt, *J. Mol. Struct.: THEOCHEM* **454**, 307−314 (1998).

532. "Dual-Level Direct Dynamics Calculations of Deuterium and Carbon-13 Kinetic Isotope Effects for the Reaction Cl + CH_4," by O. Roberto-Neto, E. L. Coitiño, and D. G. Truhlar, *J. Phys. Chem. A* **102**, 4568−4578 (1998).

534. "Dual-Level Direct Dynamics Calculations of the Reaction Rates for a Jahn−Teller Reaction: Hydrogen Abstraction from CH_4 or CD_4 by $O(^3P)$," by J. C. Corchado, J. Espinosa-Garcia, O. Roberto-Neto, Y.-Y. Chuang, and D. G. Truhlar, *J. Phys. Chem. A* **102**, 4899−4910 (1998).

536. "Interface of Electronic Structure and Dynamics for Reactions in Solution," Y.-Y. Chuang, C. J. Cramer, and D. G. Truhlar, *Int. J. Quantum Chem.* **70**, 887−896 (1998). (Sanibel issue.)

537. "What is the Best Semiclassical Method for Photochemical Dynamics in Systems with Conical Intersections?" M. S. Topaler, T. C. Allison, D. W. Schwenke, and D. G. Truhlar, *J. Chem. Phys.* **109**, 3321−3345 (1998), **110**, 687−688(E) (1999), **113**, 3928(E) (2000).

538. "An Embedded Diatomics-in-Molecules Potential Energy Function for Methyl Radical and Methane on Nickel Surfaces," S. E. Wonchoba and D. G. Truhlar, *J. Phys. Chem. B* **102**, 6842−6860 (1998).

539. "Variational Reaction Path Algorithm," P. L. Fast and D. G. Truhlar, *J. Chem. Phys.* **109**, 3721−3729 (1998).

540. "The Calculation of Kinetic Isotope Effects Based on a Single Reaction Path," P. L. Fast, J. C. Corchado, and D. G. Truhlar, *J. Chem. Phys.* **109**, 6237−6245 (1998).

543. "Chemical Reaction Theory: Summarizing Remarks," D. G. Truhlar, *Faraday Discuss. Chem. Soc.* **110**, 521−535 (1998).

544. "Explanation of Deuterium and Muonium Kinetic Isotope Effects for Hydrogen Atom Addition to an Olefin," J. Villà, J. C. Corchado, A. González-Lafont, J. M. Lluch, and D. G. Truhlar, *J. Am. Chem. Soc.* **120**, 12141−12142 (1998).

546. "Quantum Mechanism in the Photodissociation of NaFH Complex: A Challenge to Semiclassical Analysis," Y. Zeiri, G. Katz, R. Kosloff, M. S. Topaler, D. G. Truhlar, and J. C. Polanyi, *Chem. Phys. Lett.* **300**, 523−528 (1999).

547. "Quantum Mechanical Dynamical Effects in an Enzyme-Catalyzed Proton-Transfer Reaction," C. Alhambra, J. Gao, J. C. Corchado, J. Villà, and D. G. Truhlar, *J. Am. Chem. Soc.* **121**, 2253−2258 (1999).

551. "Analytic Potential Energy Surfaces and their Couplings for the Electronically Nonadiabatic Chemical Processes Na(3p) + H_2 → Na(3s) + H_2 and Na(3p) + H_2 → NaH + H," M. D. Hack and D. G. Truhlar, *J. Chem. Phys.* **110**, 4315−4337 (1999).

552. "Exciplex Funnel Resonances in Chemical Reaction Dynamics: The Nonadiabatic Tunneling Case Associated with an Avoided Crossing at a Saddle Point," R. S. Friedman, T. C. Allison, and D. G. Truhlar, *Phys. Chem. Chem. Phys.* **1**, 1237−1247 (1999). (Special issue on Chemical Reaction Theory.)

555. "Mapped Interpolation Scheme for Single-Point Energy Corrections in Reaction Rate Calculations and a Critical Evaluation of Dual-Level Reaction-Path Dynamics Methods," Y.-Y. Chuang, J. C. Corchado, and D. G. Truhlar, *J. Phys. Chem. A* **103**, 1140−1149 (1999).

556. "Transition State Resonances in the Reaction Cl + H_2 → HCl + H," J. Srinivasan, T. C. Allison, D. W. Schwenke, and D. G. Truhlar, *J. Phys. Chem. A* **103**, 1487−1503 (1999).

557. "Implicit Solvation Models: Equilibria, Structure, Spectra, and Dynamics," C. J. Cramer and D. G. Truhlar, *Chem. Rev.* **99**, 2161−2200 (1999).

562. "Are Semiclassical Methods Accurate for Electronically Nonadiabatic Transitions Between Weakly Coupled Potential Energy Surfaces?" Y. L. Volobuev, M. D. Hack, and D. G. Truhlar, *J. Phys. Chem. A* **103**, 6225−6233 (1999).

565. "Variational Transition State Theory with Optimized Orientation of the Dividing Surface and Semiclassical Tunneling Calculations for Deuterium and Muonium Kinetic Isotope Effects in the Free Radical Association Reaction H + C_2H_4 → C_2H_5," J. Villà, J. C. Corchado, A. González-Lafont, J. M. Lluch, and D. G. Truhlar, *J. Phys. Chem. A* **103**, 5061−5074 (1999).

566. "Direct Dynamics for Free Radical Kinetics in Solution: Solvent Effect on the Rate Constant for the Reaction of Methanol with Atomic Hydrogen," Y.-Y. Chuang, M. L. Radhakrishnan, P. L. Fast, C. J. Cramer, and D. G. Truhlar, *J. Phys. Chem. A* **103**, 4893−4909 (1999).

569. "Quantum Mechanical and Quasiclassical Trajectory Surface Hopping Studies of the Electronically Nonadiabatic Predissociation of the $\tilde{A}$ State of NaH_2," M. D. Hack, A. W. Jasper, Y. L. Volobuev, D. W. Schwenke, and D. G. Truhlar, *J. Phys. Chem. A* **103**, 6309−6326 (1999).

574. "Energetic and Structural Features of the CH_4 + O(^{3}P) → CH_3 + OH Abstraction Reaction: Does Perturbation Theory from a Multiconfiguration Reference State (Finally) Provide a Balanced Treatment of Transition States?" O. Roberto-Neto, F. B. C. Machado, and D. G. Truhlar, *J. Chem. Phys.* **111**, 10046−10052 (1999), **113**, 3929(E) (2000).

575. "Nonequilibrium Solvation Effects for a Polyatomic Reaction in Solution," Y.-Y. Chuang and D. G. Truhlar, *J. Am. Chem. Soc.* **121**, 10157−10167 (1999).

577. "Multidimensional Transition State Theory and the Validity of Grote−Hynes Theory," D. G. Truhlar and B. C. Garrett, *J. Phys. Chem. B* **104**, 1069−1072 (2000).

579. "Do Semiclassical Trajectory Theories Provide an Accurate Picture of Radiationless Decay for Systems with Accessible Surface Crossings?" M. D. Hack, A. W. Jasper, Y. L. Volobuev, D. W. Schwenke, and D. G. Truhlar, *J. Phys. Chem. A* **104**, 217−232 (2000).

581. "Comment on Rate Constants for Reactions of Tritium Atoms with H_2, D_2, and HD," J. Srinivasan and D. G. Truhlar, *J. Phys. Chem. A* **104**, 1965−1967 (2000).

582. "How Should We Calculate Transition State Geometries for Radical Reactions? The Effect of Spin Contamination on the Prediction of Geometries for Open-Shell Saddle Points," Y.-Y. Chuang, E. L. Coitiño, and D. G. Truhlar, *J. Phys. Chem. A* **104**, 446−450 (2000).

583. "An MIMD Strategy for Quantum Mechanical Reactive Scattering," Y. L. Volobuev and D. G. Truhlar, *Comput. Phys. Commun.* **128**, 465−476 (2000). (Special issue on Parallel Computing in Chem. Phys.)

587. "Potential Energy Surface, Thermal and State-Selected Rate Constants and Kinetic Isotope Effects for Cl + CH_4 → HCl + CH_3," J. C. Corchado, D. G. Truhlar, and J. Espinosa-Garcia, *J. Chem. Phys.* **112**, 9375−9389 (2000).

588. "Multiconfiguration Molecular Mechanics Algorithm for Potential Energy Surfaces of Chemical Reactions," Y. Kim, J. C. Corchado, J. Villà, J. Xing, and D. G. Truhlar, *J. Chem. Phys.* **112**, 2718−2735 (2000).

589. "Dynamics of the Cl+H_2/D_2 Reaction: A Comparison of Crossed Molecular Beam Experiments with Quasiclassical Trajectory and Quantum Mechanical Calculations," M. Alagia, N. Balucani, L. Cartechini, P. Casavecchia, G. G. Volpi, F. J. Aoiz, L. Bañares, T. C. Allison, S. L. Mielke, and D. G. Truhlar, *Phys. Chem. Chem. Phys.* **2**, 599−612 (2000).

590. "Quantized Dynamical Bottlenecks and Transition State Control of the Reaction of D with H_2. Effect of Varying the Total Angular Momentum," D. C. Chatfield, S. L. Mielke, T. C. Allison, and D. G. Truhlar, *J. Chem. Phys.* **112**, 8387−8408 (2000).

591. "Continuous Surface Switching: An Improved Time-Dependent Self-Consistent-Field Method for Nonadiabatic Dynamics," Y. L. Volobuev, M. D. Hack, M. S. Topaler, and D. G. Truhlar, *J. Chem. Phys.* **112**, 9716−9726 (2000).

596. "Adiabatic Connection for Kinetics," B. J. Lynch, P. L. Fast, M. Harris, and D. G. Truhlar, *J. Phys. Chem. A* **104**, 4811−4815 (2000).

597. "Quantum Dynamics of Hydride Transfer in Enzyme Catalysis," C. Alhambra, J. C. Corchado, M. L. Sanchez, J. Gao, and D. G. Truhlar, *J. Am. Chem. Soc.* **122**, 8197−8203 (2000).

598. "Nonadiabatic Trajectories at an Exhibition," M. D. Hack and D. G. Truhlar, *J. Phys. Chem. A* **104**, 7917−7926 (2000). (Feature Article.)

599. "Analysis of the Resonance in H + D_2 → HD($v' = 3$) + D," T. C. Allison, R. S. Friedman, D. J. Kaufman, and D. G. Truhlar, *Chem. Phys. Lett.* **327**, 439−445 (2000).

603. "Improved Algorithm for Corner Cutting Calculations," A. Fernandez-Ramos and D. G. Truhlar, *J. Chem. Phys.* **114**, 1491−1496 (2001).

604. "Quantum Mechanical Dynamics of Hydride Transfer in Polycyclic Hydoxy Ketones in the Condensed Phase," R. M. Nicoll, I. H. Hillier, and D. G. Truhlar, *J. Am. Chem. Soc.* **123**, 1459−1463 (2001).

605. "Electronically Nonadiabatic Trajectories: Continuous Surface Switching II," M. D. Hack and D. G. Truhlar, *J. Chem. Phys.* **114**, 2894−2902 (2001).

606. "Convex Arrhenius Plots and Their Interpretation," D. G. Truhlar and A. Kohen, *Proc. Natl. Acad. Sci. U.S.A.* **98**, 848−851 (2001).

607. "Reductive Dechlorination of Hexachloroethane in the Environment. Mechanistic Studies via Computational Electrochemistry," E. V. Patterson, C. J. Cramer, and D. G. Truhlar, *J. Am. Chem. Soc.* **123**, 2025−2031 (2001).

608. "Thermal and State-Selected Rate Coefficients for the O(^{3}P) + HCl Reaction and New Calculations of the Barrier Height and Width," S. Skokov, S. Zou, J. M. Bowman, T. C. Allison, D. G. Truhlar, Y. Lin, B. Ramachandran, B. C. Garrett,

and B. J. Lynch, *J. Phys. Chem. A* **105**, 2298−2307 (2001). (Aron Kuppermann Festschrift.)

609. "How Well Can Hybrid Density Functional Methods Predict Transition State Geometries and Barrier Heights?" B. J. Lynch and D. G. Truhlar, *J. Phys. Chem. A* **105**, 2936−2941 (2001).

611. "A Natural Decay of Mixing Algorithm for Non-Born Oppenheimer Trajectories," M. D. Hack and D. G. Truhlar, *J. Chem. Phys.* **114**, 9305−9314 (2001).

612. "Inclusion of Quantum Mechanical Vibrational Energy in Reactive Potentials of Mean Force," M. Garcia-Viloca, C. Alhambra, D. G. Truhlar, and J. Gao, *J. Chem. Phys.* **114**, 9953−9958 (2001).

614. "Comparison of Full Multiple Spawning, Trajectory Surface Hopping, and Converged Quantum Mechanics for Electronically Nonadiabatic Dynamics," M. D. Hack, A. M. Wensmann, D. G. Truhlar, M. Ben-Nun, and T. J. Martínez, *J. Chem. Phys.* **115**, 1172−1186 (2001).

615. "The Treatment of Classically Forbidden Electronic Transitions in Semiclassical Trajectory Surface Hopping Calculations," A W. Jasper, M. D. Hack, and D. G. Truhlar, *J. Chem. Phys.* **115**, 1804−1816 (2001).

616. "Solvent-Dependent Transition States for Decarboxylations," D. Sicinska, D. G. Truhlar, and P. Paneth, *J. Am. Chem. Soc.* **123**, 7683−7686 (2001).

618. "Variational Transition State Theory Evaluation of the Rate Constant for Proton Transfer in a Polar Solvent," R. P. McRae, G. K. Schenter, B. C. Garrett, Z. Svetlicic, and D. G. Truhlar, *J. Chem. Phys.* **115**, 8460−8480 (2001).

619. "The Role of Collective Solvent Coordinates and Nonequilibrium Solvation in Charge-Transfer Reactions," G. K. Schenter, B. C. Garrett, and D. G. Truhlar, *J. Phys. Chem. B* **105**, 9672−9685 (2001). (Feature Article.)

621. "Molecular Mechanics for Chemical Reactions. A Standard Strategy for Using Multi-Configuration Molecular Mechanics for Variational Transition State Theory with Optimized Multidimensional Tunneling," T. Albu, J. C. Corchado, and D. G. Truhlar, *J. Phys. Chem. A* **105**, 8465−8487 (2001).

622. "Test of Variational Transition State Theory with Multidimensional Tunneling Contributions Against an Accurate Full-dimensional Rate Constant Calculation for a Six-Atom System," J. Pu, J. C. Corchado, and D. G. Truhlar, *J. Chem. Phys.* **115**, 6266−6267 (2001).

623. "Canonical Variational Theory for Enzyme Kinetics with the Protein Mean Force and Multidimensional Quantum Mechanical Tunneling Dynamics. Theory and Application to Liver Alcohol Dehydrogenase," C. Alhambra, J. Corchado, M. L. Sánchez, M. Garcia-Viloca, J. Gao, and D. G. Truhlar, *J. Phys. Chem. B* **105,** 11326−11340 (2001).

624. "Quantum Mechanical Tunneling in Methylamine Dehydrogenase," C. Alhambra, M. L. Sánchez, J. C. Corchado, J. Gao, and D. G. Truhlar, *Chem. Phys. Lett.* **347**, 512−518 (2001); reprinted correctly: **355**, 388−394 (2002).

627. "Photodissociation of LiFH and NaFH van der Waals Complexes: A Semiclassical Trajectory Study," A W. Jasper, M. D. Hack, A. Chakraborty, D. G. Truhlar, and P. Piecuch, *J. Chem. Phys.* **115**, 7945−7952 (2001), **119**, 9321(E) (2003).

628. "The Incorporation of Quantum Effects in Enzyme Kinetics Modeling," D. G. Truhlar, J. Gao, C. Alhambra, M. Garcia-Viloca, J. Corchado, M. L. Sánchez, and J. Villà, *Acc. Chem. Res.* **35**, 341−349 (2002). (Special issue on Molecular Dynamics Simulations of Biomolecules.)

630. "Parameterized Direct Dynamics Study of Rate Constants of H with CH_4 from 250 to 2400 K," J. Pu and D. G. Truhlar, *J. Chem. Phys.* **116**, 1468−1478 (2002).

632. "What are the Best Affordable Multi-Coefficient Strategies for Calculating Transition State Geometries and Barrier Heights?" B. J. Lynch and D. G. Truhlar, *J. Phys. Chem. A* **106**, 842−846 (2002).

633. "How Well Does Microsolvation Represent Macrosolvation? A Test Case: Dynamics of Decarboxylation of 4-Pyridylacetic Acid Zwitterion" D. Sicinska, P. Paneth, and D. G. Truhlar, *J. Phys. Chem. B* **106**, 2708−2713 (2002).

634. "Interpolated Algorithms for Large-Curvature Tunneling Calculations," A. Fernandez-Ramos, D. G. Truhlar, J. C. Corchado, and J. Espinosa-Garcia, *J. Phys. Chem. A* **106**, 4957−4960 (2002).

635. "Coupled Quasidiabatic Potential Energy Surfaces for LiFH," A. W. Jasper, M. D. Hack, D. G. Truhlar, and P. Piecuch, *J. Chem. Phys.* **116**, 8353−8366 (2002).

636. "Fewest Switches with Time Uncertainty: A Modified Trajectory Surface Hopping Algorithm with Better Accuracy for Classically Forbidden Electronic Transitions," A. W. Jasper, S. N. Stechmann, and D. G. Truhlar, *J. Chem. Phys.* **116**, 5424−5431 (2002); erratum: **117**, 10247 (2002).

637. "Tests of Potential Energy Surfaces for $H + CH_4 \leftrightarrow CH_3 + H_2$: Deuterium and Muonium Kinetic Isotope Effects for the Forward and Reverse Reaction," J. Pu and D. G. Truhlar, *J. Chem. Phys.* **117**, 10675−10687 (2002).

639. "Dynamics of 1,2-Hydrogen Migration in Carbenes and Ring Expansion in Cyclopropylcarbenes," T. V. Albu, B. J. Lynch, D. G. Truhlar, A. C. Goren, D. A. Hrovat, W. T. Borden, and R. A. Moss, *J. Phys. Chem. A* **106**, 5323−5338 (2002).

640. "Validation of Variational Transition State Theory with Multidimensional Tunneling Contributions Against Accurate Quantum Mechanical Dynamics for $H + CH_4 \rightarrow H_2 + CH_3$ in an Extended Temperature Interval," J. Pu and D. G. Truhlar, *J. Chem. Phys.* **117**, 1479−1481 (2002).

641. "Reply to Comment on Molecular Mechanics for Chemical Reactions," D. G. Truhlar, *J. Phys. Chem. A* **106**, 5048−5051 (2002).

642. "Quantum Dynamics of Hydride Transfer Catalyzed by Bimetallic Electrophilic Catalysis: Synchronous Motion of Mg^{2+} and H^- in Xylose Isomerase," M. Garcia-Viloca, C. Alhambra, D. G. Truhlar, and J. Gao, *J. Am. Chem. Soc.* **124**, 7268−7269 (2002).

643. "Hydride Transfer Catalyzed by Xylose Isomerase: Mechanism and Quantum Effects," M. Garcia-Viloca, C. Alhambra, D. G. Truhlar, and J. Gao, J. *Comput. Chem.* **24**, 177−190 (2003). (Peter Kollman Memorial Issue.)

646. "Reduced Mass in the One-Dimensional Treatment of Tunneling," D. G. Truhlar and B. C. Garrett, *J. Phys. Chem. A* **107**, 4006−4007 (2003).

651. "Improved Treatment of Momentum at Classically Forbidden Electronic Transitions in Trajectory Surface Hopping Calculations," A. W. Jasper and D. G. Truhlar, *Chem. Phys. Lett.* **369**, 60−67 (2003).

654. "Generalized Transition State Theory in Terms of the Potential of Mean Force," G. K. Schenter, B. C. Garrett, and D. G. Truhlar, *J. Chem. Phys.* **119**, 5828−5833 (2003).

656. "Importance of Substrate and Cofactor Polarization in the Active Site of Dihydrofolate Reductase," M. Garcia-Viloca, D. G. Truhlar, and J. Gao, *J. Mol. Biol.* **327**, 549−560 (2003).

657. "Carbon Tunneling from a Single Quantum State," P. S. Zuev, R. S. Sheridan, T. V. Albu, D. G. Truhlar, D. A. Hrovat, W. T. Borden, *Science* **299**, 867−870 (2003).

660. "H + H_2 Thermal Reaction: A Convergence of Theory and Experiment," S. L. Mielke, K. A. Peterson, D. W. Schwenke, B. C. Garrett, D. G. Truhlar, J. V. Michael, M.-C. Su, and J. W. Sutherland, *Phys. Rev. Lett.* **91**, 63201/1−4 (2003).

661. "Free Energy Surface, Reaction Paths, and Kinetic Isotope Effect of Short-Chain Acyl-CoA Dehydrogenase," T. D. Poulsen, M. Garcia-Viloca, J. Gao, and D. G. Truhlar, *J. Phys. Chem. B* **107**, 9567−9578 (2003).

662. "Small Basis Sets for Calculations of Barrier Heights, Energies of Reaction, Electron Affinities, Geometries, and Dipole Moments," B. J. Lynch and D. G. Truhlar, *Theor. Chem. Acc.* **111**, 335−344 (2004). (Jacopo Tomasi Honorary Issue.)

664. "Narrow Subthreshold Quantum Mechanical Resonances in the Li + HF → H + LiF Reaction," L. Wei, A. W. Jasper, and D. G. Truhlar, *J. Phys. Chem. A* **107**, 7236−7247 (2003). (Donald J. Kouri Festschrift.)

667. "Sensitivity of Molecular Dynamics Simulations to the Choice of the X-ray Structure Used to Model an Enzymatic Reaction," M. Garcia-Viloca, T. D. Poulsen, D. G. Truhlar, and J. Gao, *Protein Sci.* **13**, 2341−2354 (2004).

669. "Reaction-Path Energetics and Kinetics of the Hydride Transfer Reaction Catalyzed by Dihydrofolate Reductase," M. Garcia-Viloca, D. G. Truhlar, and J. Gao, *Biochemistry* **42**, 13558−13575 (2003).

672. "Benchmark Results for Hydrogen Atom Transfer Between Carbon Centers and Validation of Electronic Structure Methods for Bond Energies and Barrier Heights," A. Dybala-Defratyka, P. Paneth, J. Pu, and D. G. Truhlar, *J. Phys. Chem. A* **108**, 2475−2486 (2004).

673. "How Enzymes Work: Analysis by Modern Rate Theory and Computer Simulations," M. Garcia-Viloca, J. Gao, M. Karplus, and D. G. Truhlar, *Science* **303**, 186−195 (2004).

675. "Army Ants Algorithm for Rare Event Sampling of Delocalized Nonadiabatic Transitions by Trajectory Surface Hopping and the Estimation of Sampling Errors by the Bootstrap Method," S. Nangia, A. W. Jasper, T. F. Miller III, and D. G. Truhlar, *J. Chem. Phys.* **120**, 3586−3597 (2004).

679. "Non-Born−Oppenheimer Trajectories with Self-Consistent Decay of Mixing," C. Zhu, A. W. Jasper, and D. G. Truhlar, *J. Chem. Phys.* **120**, 5543−5557 (2004).

680. "Tests of Second-Generation and Third-Generation Density Functionals for Thermochemical Kinetics," Y. Zhao, J. Pu, B. J. Lynch and D. G. Truhlar, *Phys. Chem. Chem. Phys.* **6**, 673−676 (2004).

681. "Development and Assessment of a New Hybrid Density Functional Method for Thermochemical Kinetics," Y. Zhao, B. J. Lynch and D. G. Truhlar, *J. Phys. Chem. A* **108**, 2715−2719 (2004).

682. "Efficient Molecular Mechanics for Chemical Reactions: Multiconfiguration Molecular Mechanics using Partial Electronic Structure Hessians," H. Lin, J. Pu, T. V. Albu, and D. G. Truhlar, *J. Phys. Chem. A* **108**, 4112−4124 (2004).

686. "Doubly Hybrid DFT: New Multi-Coefficient Correlation and Density Functional Methods for Thermochemistry and Thermochemical Kinetics," Y. Zhao, B. J. Lynch, and D. G. Truhlar, *J. Phys. Chem. A* **108**, 4786−4791 (2004).

687. "Coherent Switching with Decay of Mixing: An Improved Treatment of Electronic Coherence for Non-Born−Oppenheimer Trajectories," C. Zhu, S. Nangia, A. W. Jasper, and D. G. Truhlar, *J. Chem. Phys.* **121**, 7658−7670 (2004).

690. "Ensemble-Averaged Variational Transition State Theory with Optimized Multidimensional Tunneling for Enzyme Kinetics and Other Condensed-Phase Reactions," D. G. Truhlar, J. Gao, M. Garcia-Viloca, C. Alhambra, J. Corchado, M. L. Sanchez, and T. D. Poulsen, *Int. J. Quantum Chem.* **100**, 1136−1152 (2004). (*Proc. Sanibel Symp.*, 2004.)

691. "Introductory Lecture: Nonadiabatic Effects in Chemical Dynamics," A. W. Jasper, C. Zhu, S. Nangia, and D. G. Truhlar, *Faraday Discuss.* **127**, 1−22 (2004).

696. "Variational Transition State Theory," B. C. Garrett and D. G. Truhlar, *J. Mol. Struct.: THEOCHEM*, in press. (Special issue: Theory and Applications of Comp. Chem.: The First 40 Years.)

699. "Conical Intersections and Semiclassical Trajectories: Comparison to Accurate Quantum Dynamics and Analyses of the Trajectories," A. W. Jasper and D. G. Truhlar, *J. Chem. Phys.* **122**, 44101/1−16 (2005).

701. "Multi-Coefficient Extrapolated Density Functional Theory for Thermochemistry and Thermochemical Kinetics, " Y. Zhao, B. J. Lynch, and D. G. Truhlar, *Phys. Chem. Chem. Phys.* **7**, 43−52 (2005).

702. "Benchmark Calculations of Reaction Energies, Barrier Heights, and Transition State Geometries for Hydrogen Abstraction from Methanol by a Hydrogen Atom," J. Pu and D. G. Truhlar, *J. Phys. Chem. A* **109**, 773−778 (2005).

703. "Benchmark Database of Barrier Heights for Heavy Atom Transfer, Nucleophilic Substitution, Association, and Unimolecular Reactions and Its Use to Test Theoretical Methods," Y. Zhao, N. González-García, and D. G. Truhlar, *J. Phys. Chem. A* **109**, 2012−2018 (2005).

704. "Quantum Mechanical Reaction Rate Constants by Vibrational Configuration Interaction. Application to the OH + H_2 → H_2O + H Reaction as a Function of Temperature," A. Chakraborty and D. G. Truhlar, *Proc. Natl. Acad. Sci. U.S.A.*, **102**, 6744−6749 (2005). (Special Feature issue on Chem. Theory Comp.)

706. "Temperature Dependence of Carbon-13 Kinetic Isotope Effects of Importance to Global Climate Change," H. Lin, Y. Zhao, B. A. Ellingson, J. Pu, and D. G. Truhlar, *J. Am. Chem. Soc.* **127**, 2830−2831 (2005).

710. "Small Temperature Dependence of the Kinetic Isotope Effect for the Hydride Transfer Reaction Catalyzed by *Escherichia coli*, Dihydrofolate Reductase," J. Pu, S. Ma, J. Gao, and D. G. Truhlar, *J. Phys. Chem. B* **109**, 8551−8556 (2005).

711. "Dependence of Transition State Structure on Substrate: The Intrinsic C-13 Kinetic Isotope Effect is Different for Physiological and Slow Substrate of the Ornithine Decarboxylase Reaction Because of Different Hydrogen Bonding Structures," D. Sicinska, D. G. Truhlar, and P. Paneth, *J. Am. Chem. Soc.* **127**, 5414−5422 (2005).

714. "Non-Born−Oppenheimer Liouville−von Neumann Dynamics. Evolution of a Subsystem Controlled by Linear and Population-Driven Decay of Mixing with Decoherent and Coherent Switching," C. Zhu, A. W. Jasper, and D. G. Truhlar, *J. Chem. Theory Comp.* **1**, 527−540 (2005).

716. "Non-Born−Oppenheimer Molecular Dynamics," A. W. Jasper, S. Nangia, C. Zhu, and D. G. Truhlar, *Acc. Chem. Res.*, in press. (Special issue on Comp. Theor. Chem.)

723. "A New Algorithm for Efficient Direct Dynamics Calculations of Large-Curvature Tunneling and Its Application to Radical Reactions with 9−15 Atoms," A. Fernández-Ramos and D. G. Truhlar, *J. Chem. Theory Comput.* **1**, 1063−1078 (2005).

724. "Electronic Decoherence Time for Non-Born−Oppenheimer Trajectories," A. W. Jasper and D. G. Truhlar, *J. Chem. Phys.* **123**, 64103/1−4 (2005).

726. "Nonperfect Synchronization of Reaction Center Rehybridization in the Transition State of the Hydride Transfer Catalyzed by Dihydrofolate Reductase," J. Pu, S. Ma, M. Garcia-Viloca, J. Gao, and D. G. Truhlar, *J. Am. Chem. Soc.* **127**, 14879−14886 (2005).

728. "Potential of Mean Force Calculation for the Proton and Hydride Transfer Reactions Catalyzed by Medium Chain Acyl-Coa Dehydrogenase: The Effect of Mutations on Enzyme Catalysis," S. Bhattacharyya, S. Ma, M. T. Stankovich, D. G. Truhlar, and J. Gao, *Biochemistry*, in press.

730. "Combined Valence Bond-Molecular Mechanics Potential Energy Surface and Direct Dynamics Study of Rate Constants and Kinetic Isotope Effects for the H + C_2H_6 Reaction," A. Chakraborty, Y. Zhao, H. Lin, and D. G. Truhlar, *J. Chem. Phys.*, in press.

731. "Can a Single-Reference Approach Provide a Balanced Description of Ground and Excited States? A Comparison of the Completely Renormalized Equation-of-Motion Coupled-Cluster Method with Multireference Quasidegenerate Perturbation Theory near a Conical Intersection and along a Photodissociation Coordinate in Ammonia," S. Nangia, D. G. Truhlar, M. J. McGuire, and P. Piecuch, *J. Phys. Chem. A* **109**, 11647−11650 (2005).

Scattering and Energy Transfer

1. "Rearrangement Collisions: Effect of Core Terms, and Conservation of Particle Flux on Approximate Theories," D. G. Truhlar, D. C. Cartwright, and A. Kuppermann, *Phys. Rev.* **175**, 113−133 (1968).

4. "Differential and Integral Cross Sections for Excitation of the 2 ^{1}P State of Helium by Electron Impact," D. G. Truhlar, J. K. Rice, A. Kuppermann, S. Trajmar, and D. C. Cartwright, *Phys. Rev. A* **1**, 778−802 (1970).

6. "Electron Scattering by H_2 with and without Vibrational Excitation. I. Quantum Mechanical Theory," D. G. Truhlar and J. K. Rice, *J. Chem. Phys.* **52**, 4480−4501 (1970). Erratum: **55**, 2005 (1971).

7. "Electron Scattering by H_2 with and without Vibrational Excitation. II. Experimental and Theoretical Study of Elastic Scattering," S. Trajmar, D. G. Truhlar, and J. K. Rice, *J. Chem. Phys.* **52**, 4502−4515 (1970), **55**, 2004(E) (1971).

8. "Electron Scattering by H_2 with and without Vibrational Excitation. III. Experimental and Theoretical Study of Inelastic Scattering," S. Trajmar, D. G. Truhlar, J. K. Rice, and A. Kuppermann, *J. Chem. Phys.* **52**, 4516−4533 (1970).

14. "The Importance of Polarization for Electron Scattering in the Intermediate Energy Region," D. G. Truhlar, J. K. Rice, S. Trajmar, and D. C. Cartwright, *Chem. Phys. Lett.* **9**, 299−305 (1971).

16. "Forcing Conservation of Particle Flux in Perturbation Theory Calculations of Inelastic Scattering," D. G. Truhlar, *Phys. Rev. A* **4**, 1886−1891 (1971).

19. "Effect of Charge Polarization on Inelastic Scattering: Differential and Integral Cross Sections for Excitation of the 2 ^{1}S State of Helium by Electron Impact," J. K. Rice, D. G. Truhlar, D. C. Cartwright, and S. Trajmar, *Phys. Rev. A* **5**, 762−782 (1972).

24. "Applications of the Expansion Technique of Harris and Michels to Electron-Hydrogen Inelastic Scattering," R. L. Smith and D. G. Truhlar, *Phys. Lett. A* **39**, 35−37 (1972).

25. "Application of the Quasiminimum Principle to Calculations on Electron Scattering by Atomic Hydrogen," D. G. Truhlar and R. L. Smith, *Phys. Rev. A* **6**, 233−239 (1972).

26. "Convenient Determination of Resonance States in Atomic Collisions," D. G. Truhlar, *Chem. Phys. Lett.* **15**, 483−485 (1972).

27. "Electron Scattering by Molecules with and without Vibrational Excitation. IV. Elastic Scattering and Excitation of the First Vibrational Level of N_2 and CO at 20 eV," D. G. Truhlar, S. Trajmar, and W. Williams, *J. Chem. Phys.* **57**, 3250−3259 (1972).

28. "Electron Scattering by Molecules with and without Vibrational Excitation. V. Elastic Scattering and Nonresonant Vibrational Excitation of N_2 at 30−83 eV," D. G. Truhlar, *J. Chem. Phys.* **57**, 3260−3263 (1972).

29. "Ab Initio and Semiempirical Calculations of the Static Potential for Electron Scattering of the Nitrogen Molecule," D. G. Truhlar, F. A. Van-Catledge, and T. H. Dunning, *J. Chem. Phys.* **57**, 4788−4799 (1972), **69**, 2941(E) (1978).

30. "Test of Massey's Method for Calculating the Static Potential for Electron Scattering by N_2," D. G. Truhlar, *Chem. Phys. Lett.* **15**, 486−489 (1972).

34. "Electron Scattering by Molecules with and without Vibrational Excitation. VI. Elastic Scattering by CO at 6−80 eV," D. G. Truhlar, W. Williams, and S. Trajmar, *J. Chem. Phys.* **57**, 4307−4312 (1972).

35. "Program for Evaluation of Non-Exchange Type Integrals Required in Electron-Atom Scattering Theory Using Slater-Type Orbitals as Basis Functions," R. L. Smith and D. G. Truhlar, *Comput. Phys. Commun.* **5**, 80−87 (1973), **8**, 333−336(E) (1974).

38. "Vibrational Excitation in CO by Electron Impact in the Energy Range 10−90 eV," A. Chutjian, D. G. Truhlar, W. Williams, and S. Trajmar, *Phys. Rev. Lett.* **29**, 1580−1583 (1972), **33**, 1524(E) (1974).

39. "Program for Calculating Differential and Integral Cross Sections for Quantum Mechanical Scattering Problems from Reactance or Transition Matrices," M. A. Brandt, D. G. Truhlar, and R. L. Smith, *Comput. Phys. Commun.* **5**, 456−477 (1973). Erratum and addendum: **7**, 177 (1974).

40. "Semiclassical Treatment of Rainbow Maxima in Differential Cross Sections for Inelastic Scattering," D. G. Truhlar, *J. Chem. Phys.* **58**, 3109 (1973).

43. "Quantum Mechanical and Experimental Study of Elastic Scattering and Excitation of the 2^1P State of He by Electron Impact at 29−40 eV," D. G. Truhlar, S. Trajmar, W. Williams, S. Ormonde, and B. Torres, *Phys. Rev. A* **8**, 2475−2482 (1973).

44. "Electron Scattering With and Without Vibrational Excitation. VIII. Comment on a Theory of Small-Energy-Transfer Collisions Dominated by Long-Range Forces," D. G. Truhlar, *Phys. Rev. A* **7**, 2217−2219 (1973).

45. "Tests of Approximate Methods for the Calculation of the Static Potential for Electron Scattering by CO," D. G. Truhlar and F. A. Van-Catledge, *J. Chem. Phys.* **59**, 3207−3213 (1973), **69**, 2942(E) (1978).

47. "Importance of Long-Range Forces and Short-Range Forces in Electron Scattering: Elastic Scattering by N_2 at 10 and 30 eV," M. A. Brandt and D. G. Truhlar, *Chem. Phys. Lett.* **23**, 48−52 (1973).

49. "New Methods for Calculating Scattering Cross-Sections for Rearrangement Collisions," D. G. Truhlar and J. Abdallah, Jr., *Phys. Rev. A* **9**, 297−300 (1974).

50. "The Use of Consistent Phase Conventions in Calculating Angular Distributions of Scattering Cross Sections and Applications to Electron-Hydrogen Atom Scattering," M. A. Brandt and D. G. Truhlar, *Phys. Rev. A* **9**, 1188−1194 (1974).

52. "Program ACRL to Calculate Differential and Integral Cross Sections Adapted to Run on IBM Computers," M. A. Brandt, D. G. Truhlar, and R. L. Smith, *Comput. Phys. Commun.* **7**, 172−173 (1974).

53. "Applications of the Variational Least Squares Method to Inelastic Scattering," J. Abdallah, Jr. and D. G. Truhlar, *J. Chem. Phys.* **60**, 4670−4675 (1974).

54. "Finite Difference Boundary Value Method for Determination of Resonance Widths in Atomic Collisions," D. G. Truhlar, *Chem. Phys. Lett.* **26**, 377−380 (1974).

55. "Elastic Scattering of Electrons by Hydrogen Molecules at Intermediate Energies," D. G. Truhlar and J. K. Rice, *Phys. Lett. A* **47A**, 372−374 (1974).

56. "The Use of Contracted Basis Functions in Algebraic Variational Scattering Calculations," J. Abdallah, Jr. and D. G. Truhlar, *J. Chem. Phys.* **61**, 30−36 (1974).

58. "Hartree−Fock Generalized Oscillator Strengths for Electron Impact Excitation of the 2^1P State of Helium," D. G. Truhlar and D. C. Cartwright, *Phys. Rev. A* **10**, 1908−1910 (1974).

60. "Ab Initio Cross Sections for Excitation of the 2p state of Hydrogen by Electron Impact at Intermediate Energies," M. A. Brandt and D. G. Truhlar, *Phys. Rev. A* **11**, 1340−1346 (1975).

61. "Continuum Exchange Integrals for Algebraic Variational Calculations of Electron-Atom Scattering Using Slater-Type Orbitals as Basis Functions," J. Abdallah, Jr. and D. G. Truhlar, *Comput. Phys. Commun.* **9**, 327−336 (1975).

62. "Tests of Semiclassical Treatments of Vibrational−Translational Energy Transfer in Collinear Collisions of Helium with Hydrogen Molecules," J. W. Duff and D. G. Truhlar, *Chem. Phys.* **9**, 243−273 (1975).

64. "Approximations for the Exchange Potential in Electron Scattering," M. E. Riley and D. G. Truhlar, *J. Chem. Phys.* **63**, 2182−2191 (1975).

65. "Use of Semiclassical Collision Theory to Compare Analytic Fits to the Interaction Potential for Vibrational Excitation of H_2 by He," J. W. Duff and D. G. Truhlar, *J. Chem. Phys.* **63**, 4418−4429 (1975).

66. "Classical Probability Matrix: Prediction of Quantum-State Distributions by a Moment Analysis of Classical Trajectories," D. G. Truhlar and J. W. Duff, *Chem. Phys. Lett.* **36**, 551−554 (1975).

70. "Infinite-Order Sudden Approximation for Rotational Excitation of Hydrogen Molecules by Electrons in the Energy Range 10−40 eV," D. G. Truhlar, R. E. Poling, and M. A. Brandt, *J. Chem. Phys.* **64**, 826−829 (1976).

72. "Electron Scattering by Nitrogen Molecules in the Energy Range 30−75 eV: Theory and Application to Elastic Scattering," M. A. Brandt, D. G. Truhlar, and F. A. Van-Catledge, *J. Chem. Phys.* **64**, 4957−4967 (1976).

73. "Test of the Infinite-Order Sudden Approximation for Electron Scattering at Intermediate Energy," M. A. Brandt and D. G. Truhlar, *Chem. Phys.* **13**, 461−467 (1976).

76. "Effects of the Pauli Principle on Electron Scattering by Open-Shell Targets," M. E. Riley and D. G. Truhlar, *J. Chem. Phys.* **65**, 792−800 (1976).

79. "Classical S Matrix Theory: Application to Classically Forbidden Vibrational Excitation for He + HBr and H + Br_2," J. W. Duff and D. G. Truhlar, *Chem. Phys.* **17**, 249−254 (1976).

80. "Close-Coupling Calculations of Differential Cross Sections for Elastic Scattering and Rotational Excitation of Hydrogen Molecules by Electrons at 10 and 40 eV," D. G. Truhlar and M. A. Brandt, *J. Chem. Phys.* **65**, 3092−3101 (1976).

81. "Tests of INDO/1s and INDOXI/1s Methods for the Calculation of the Static Potential for Electron Scattering by CO," D. G. Truhlar and F. A. Van-Catledge, *J. Chem. Phys.* **65**, 5536−5538 (1976), **69**, 2942(E) (1978).

82. "Quantum Mechanical and Crossed-Beam Study of Vibrational Excitation of N_2 by Electron Impact at 30−75 eV," D. G. Truhlar, M. A. Brandt, S. K. Srivastava, S. Trajmar, and A. Chutjian, *J. Chem. Phys.* **66**, 655−663 (1977).

83. "Electron Scattering by N_2 at 5 and 10 eV: Rotational−Vibrational Close-Coupling Calculations and Crossed-Beam Studies of Vibrational Excitation," D. G. Truhlar, M. A. Brandt, A. Chutjian, S. K. Srivastava, and S. Trajmar, *J. Chem. Phys.* **65**, 2962−2969.

91. "Semiclassical Exchange Approximation for Inelastic Electron Scattering," D. G. Truhlar and N. A. Mullaney, *J. Chem. Phys.* **68**, 1574−1584 (1978).

97. "Ab Initio Calculation of the Vibrational Energy Transfer Rate of H_2 in Ar Using Monte Carlo Classical Trajectories and the Forced Quantum Oscillator Model," N. C. Blais and D. G. Truhlar, *J. Chem. Phys.* **69**, 846−854 (1978).

98. "Model Potentials for Electron Scattering: Converged Close Coupling Calculations for the Differential Cross Section for e^-N_2 at 30−50 eV," K. Onda and D. G. Truhlar, *J. Chem. Phys.* **69**, 1361−1373 (1978).

100. "Rotationally and Orbitally Adiabatic Basis Sets for Electron−Molecule Scattering," N. A. Mullaney and D. G. Truhlar, *Chem. Phys. Lett.* **58**, 512−517 (1978).

101. "Close Coupling Calculations with an INDOX/1s Static Potential, Semiclassical Exchange, and a Semiempirical Polarization Potential for Electron-CO_2 Elastic Scattering and Rotational Excitation," K. Onda and D. G. Truhlar, *J. Phys. B* **12**, 283−290 (1979).

102. "Adiabatic Polarization Potentials for Electron Scattering by N_2 and CO," D. G. Truhlar and F. A. Van-Catledge, *J. Chem. Phys.* **69**, 3575−3578 (1978).

108. "SCF Treatment of Charge Polarization Effects in Intermediate-Energy Electron Scattering Calculations with Applications to N_2," K. Onda and D. G. Truhlar, *J. Chem. Phys.* **70**, 1681−1689 (1979).

111. "The Use of Rotationally and Orbitally Adiabatic Basis Functions to Calculate Rotational Excitation Cross Sections for Atom-Molecule Collisions," N. A. Mullaney and D. G. Truhlar, *Chem. Phys.* **39**, 91−104 (1979).

116. "Low-Energy Electron−Molecule Scattering: Comparison of Coupled Channel Treatments of e^-N_2 Scattering at 13.6 eV Using Various Approximations to the Static and Exchange Potentials and an Approximate Polarization Potential," J. R. Rumble and D. G. Truhlar, *J. Chem. Phys.* **70**, 4101−4107 (1979), **72**, 3441(E) (1980).

119. "Rotational Excitation of Hydrogen Molecules in Collisions with Hydrogen Atoms," S. Green and D. G. Truhlar, *Ap. J.* **231**, L101−L013 (1979).

123. "Effective Potential Approach to Electron−Molecule Scattering Theory," D. G. Truhlar, K. Onda, R. A. Eades, and D. A. Dixon, *Int. J. Quantum Chem., Symp.* **13**, 601−632 (1979).

124. "Electron−Molecule Scattering at Intermediate Energy. Centrifugal Dominant Channel Decoupling and the INDOX Polarized SCF Model Applied to N_2 at 50 eV," K. Onda and D. G. Truhlar, *J. Chem. Phys.* **71**, 5097−5106 (1979).

125. "State-to-State Cross Sections for Electron Impact on N_2. Close Coupling and Polarized Born Calculations for Rotational and Vibrational Excitation and Pure Elastic Scattering at Nonresonant Energies," K. Onda and D. G. Truhlar, *J. Chem. Phys.* **71**, 5107−5123 (1979).

129. "Investigation of the Assumptions of the Multiple-Scattering Method for Electron−Molecule Scattering Cross Sections," J. R. Rumble and D. G. Truhlar, *J. Chem. Phys.* **72**, 3206−3210 (1980), **73**, 3022(E) (1980).

132. "Comparison of Local-Exchange Approximations for Intermediate-Energy Electron−Molecule Differential Cross Sections," K. Onda and D. G. Truhlar, *J. Chem. Phys.* **72**, 1415−1417 (1980).

134. "State-to-State Cross Sections for Elastic and Inelastic Electron Scattering by N_2 at 20−35 eV, Including Resonant Enhancement of Vibrational Excitation," K. Onda and D. G. Truhlar, *J. Chem. Phys.* **72**, 5249−5262 (1980).

136. "Matrix Effective Potential for Electronic Response in Electron Scattering with Application to He at 30−400 eV Impact Energy," D. G. Truhlar and K. Onda, *Phys. Lett.* **76A**, 119−120 (1980).

137. "Comparison of Local Exchange Potentials for Electron-N_2 Scattering," J. R. Rumble, Jr. and D. G. Truhlar, *J. Chem. Phys.* **72**, 5223−5227 (1980).

138. "New Approaches to the Quantum Mechanical Treatment of Charge Polarization in Intermediate-Energy Electron Scattering," K. Onda and D. G. Truhlar, *Phys. Rev. A* **22**, 86−100 (1980).

139. "Comparison of Convergence for the Schwinger, Optimized Anomaly-Free, and Optimized Minimum-Norm Variational Methods for Potential Scattering," D. Thirumalai and D. G. Truhlar, *Chem. Phys. Lett.* **70**, 330−335 (1980), **77**, 432(E) (1981).

143. "Quantum Mechanical Study of Elastic Scattering and Rotational Excitation of CO by Electrons," K. Onda and D. G. Truhlar, *J. Chem. Phys.* **73**, 2688−2695 (1980).

144. "New Version of Program for Calculating Differential and Integral Cross Sections for Quantum Mechanical Scattering Problems from Reactance and Transition Matrices," K. Onda, D. G. Truhlar, and M. A. Brandt, *Comput. Phys. Commun.* **21**, 97−108 (1980).

146. "Use of Vibrationally Adiabatic Basis Functions for Inelastic Atom-Molecule Scattering," N. M. Harvey and D. G. Truhlar, *Chem. Phys. Lett.* **74**, 252−256 (1980).

149. "Quasiclassical Trajectory Calculations and Quantal Wavepacket Calculations for Vibrational Energy Transfer at Energies above the Dissociation Threshold," J. C. Gray, G. A. Fraser, D. G. Truhlar, and K. C. Kulander, *J. Chem. Phys.* **73**, 5726−5733 (1980).

150. "Excitation of the Asymmetric Stretch Mode of CO_2 by Electron Impact," D. Thirumalai, K. Onda, and D. G. Truhlar, *J. Phys. B* **13**, L619−L622 (1980).

153. "Elastic Scattering and Rotational Excitation of a Polyatomic Molecule by Electron Impact: Acetylene," D. Thirumalai, K. Onda, and D. G. Truhlar, *J. Chem. Phys.* **74**, 526−534 (1981).

154. "Ab Initio Treatment of Electronically Inelastic K + H Collisions Using a Direct Integration Method for the Solution of the Coupled-Channel Scattering Equations in Electronically Adiabatic Representations," B. C. Garrett, M. J. Redmon, D. G. Truhlar, and C. F. Melius, *J. Chem. Phys.* **74**, 412−424 (1981).

155. "Vibrational Energy Transfer and an Improved Information-Theoretic Moment Method: Comparison of the Accuracy of Several Methods for Determining State-to-State Transition Probabilities from Quasiclassical Trajectories," D. G. Truhlar, B. P. Reid, D. E. Zurawski, and J. C. Gray, *J. Phys. Chem.* **85**, 786−791 (1981).

161. "Electron Scattering by CO_2: Elastic Scattering, Rotational Excitation, and Excitation of the Asymmetric Stretch at 10 eV Impact Energy," D. Thirumalai, K. Onda, and D. G. Truhlar, *J. Chem. Phys.* **74**, 6792−6805 (1981).

162. "Calculation of Vibrational Excitation of N_2 by Electron Impact at 5−50 eV using Extended-Basis-Set Hartree−Fock Wavefunctions," J. R. Rumble, Jr., D. G. Truhlar, and M. A. Morrison, *J. Phys. B* **14**, L301−L305 (1981).

163. "Dispersion-Equation Approach to Obtaining Complex Optical Potentials for Electron Scattering," S. M. Valone, D. Thirumalai, and D. G. Truhlar, *Int. J. Quantum Chem., Symp.* **15**, 341−353 (1981).

166. "Improved Calculation of the Cross Section for Excitation of the Asymmetric Stretch of CO_2 by Electron Impact," D. Thirumalai and D. G. Truhlar, *J. Chem. Phys.* **75**, 5207−5209 (1981).

171. "Quenching of the Resonance State of Potassium by Muonium," B. C. Garrett, D. G. Truhlar, and C. F. Melius, *Phys. Rev. A* **24**, 2853−2856 (1981).

172. "Monte Carlo Trajectory Calculation of State-to-State Cross Sections for Vibrational−Rotational-Translational Energy Transfer in Ar−H_2 Collisions," N. C. Blais and D. G. Truhlar, *J. Phys. Chem.* **86**, 638−647 (1982). (Simon H. Bauer Commemorative Issue.)

174. "Full-Response Pseudochannels: A New Method for Converging Coupled-Channels Scattering Calculations. Theory and Examples," D. Thirumalai and D. G. Truhlar, *J. Chem. Phys.* **76**, 385−389 (1982).

180. "The Quenching of Na (3^2P) by H_2: Interactions and Dynamics," D. G. Truhlar, J. W. Duff, N. C. Blais, J. C. Tully, and B. C. Garrett, *J. Chem. Phys.* **77**, 764−776 (1982).

181. "Localized Second-Order Optical Potential for Electron Scattering in Terms of Imaginary-Frequency Susceptibilities," S. M. Valone, D. G. Truhlar, and D. Thirumalai, *Phys. Rev. A* **25**, 3003−3014 (1982).

183. "Rapid Convergence of V−V Energy Transfer Calculated Using Adiabatic Basis Functions and an Accurate Two-State Model for Low-Energy Resonant V−V Energy Transfer," D. Thirumalai and D. G. Truhlar, *J. Chem. Phys.* **76**, 5287−5294 (1982).

184. "Application of the Matrix-Effective-Potential Formalism to Electron-Neon Scattering at 150−700 eV Impact Energy and Comparison to Optical Potential Calculations," D. Thirumalai and D. G. Truhlar, *Phys. Rev. A* **25**, 3058−3071 (1982).

185. "Energy-Dependent Polarization Potential, Dispersion-Relation Absorption Potential, and Matrix Effective Potential for Electron-Neon Scattering at 10−100 eV," D. Thirumalai and D. G. Truhlar, *Phys. Rev. A* 26, 793−807 (1982), **28**, 3140−3142(E) (1983).

186. "Polarization and Absorption Effects in Electron-Helium Scattering at 30−400 eV," D. Thirumalai, D. G. Truhlar, M. A. Brandt, R. A. Eades, and D. A. Dixon, *Phys. Rev. A* **25**, 2946−2958 (1982).

188. "Tests of the Semiclassical Polarization Approximation for Electron Scattering by Helium and Neon," D. Thirumalai and D. G. Truhlar, *Phys. Rev. A* **27**, 158−166 (1983).

194. "Electron Scattering by Methane. Elastic Scattering and Rotational Excitation Cross Sections Calculated with Ab Initio Interaction Potentials," N. Abusalbi, R. A. Eades, T. Nam, D.

Thirumalai, D. A. Dixon, D. G. Truhlar, and M. Dupuis, *J. Chem. Phys.* **78**, 1213−1227 (1983).

196. "Test of the Linear Sum Rule for Vibrational Energy Transfer by Trajectory Calculations," D. G. Truhlar and N. C. Blais, *J. Chem. Phys.* **77**, 2430−2431 (1982).

199. "Effective Exchange Potentials for Electronically Inelastic Scattering," D. W. Schwenke, G. Staszewska, and D. G. Truhlar, *J. Chem. Phys.* **78**, 275−279 (1983).

200. "Improved Parametrization of Diatomics-in-Molecules Potential Energy Surface for Na(3p ^{2}P) + H_2 → Na(3s ^{2}S) + H_2," N. C. Blais, D. G. Truhlar, and B. C. Garrett, *J. Chem. Phys.* **78**, 2956−2961 (1983).

203. "Rotational Energy Transfer in Collisions of Internally Excited Molecules. Effect of Initial Conditions and Potential Energy Surface," D. L. Thompson, N. C. Blais, and D. G. Truhlar, *J. Chem. Phys.* **78**, 1335−1338 (1983).

205. "Tests of the Quasiclassical Trajectory Cross-Correlation Moment Method Against Accurate Quantum Dynamics for V−V Energy Transfer in HF−HF Collisions," D. W. Schwenke, D. Thirumalai, D. G. Truhlar, and M. E. Coltrin, *J. Chem. Phys.* **78**, 3078−3083 (1983).

206. "Algorithm for Locating Narrow Resonances in Coupled Channel Quantal Scattering Calculations," D. G. Truhlar and D. W. Schwenke, *Chem. Phys. Lett.* **95**, 83−86 (1983).

211. "Nonempirical Model for the Imaginary Part of the Optical Potential for Electron Scattering," G. Staszewska, D. W. Schwenke, D. Thirumalai, and D. G. Truhlar, *J. Phys. B* **16**, L281−L287 (1983).

212. "Optical Model for Electron Scattering by Ar at 30−3000 eV: Test of the Adiabatic Model for Charge Polarization and a Quasi-Free Scattering Model for Inelastic Effects," G. Staszewska, D. W. Schwenke, and D. G. Truhlar, *Int. J. Quantum Chem., Symp.* **17**, 163−176 (1983).

213. "Recent Progress in Atomic and Molecular Collisions and the Interface with Electronic Structure Theory," D. G. Truhlar, *Int. J. Quantum Chem., Symp.* **17**, 77−87 (1983).

214. "Dispersion-Equation Approach to Obtaining Polarization Potentials for Quantum Mechanical Electron Scattering Calculations," G. Staszewska, D. W. Schwenke, and D. G. Truhlar, *Phys. Rev. A* **28**, 169−175 (1983).

215. "Quasifree-Scattering Model for the Imaginary Part of the Optical Potential for Electron Scattering," G. Staszewska, D. W. Schwenke, D. Thirumalai, and D. G. Truhlar, *Phys. Rev. A* **28**, 2740−2751 (1983).

216. "State-to-State Differential and Integral Cross Sections for Vibrational Rotational Excitation and Elastic Scattering of Electrons by N_2 at 5−50 eV: Calculations using Extended-Basis-Set Hartree−Fock Wavefunctions," J. R. Rumble, Jr., D. G. Truhlar, and M. A. Morrison, *J. Chem. Phys.* **79**, 1846−1858 (1983).

217. "Trajectory-Surface-Hopping Study of Na(3p ^{2}P) + H_2 → Na(3 ^{2}S) + $H_2(v', j', \theta)$," N. C. Blais and D. G. Truhlar, *J. Chem. Phys.* **79**, 1334−1342 (1983).

218. "An Approximate Potential Energy Surface for He−I_2 Collisions," D. W. Schwenke and D. G. Truhlar, *Chem. Phys. Lett.* **98**, 217−220 (1983).

223. "Accurate, Smooth, Local, Energy-Dependent Optical Potentials for Electron Scattering," D. W. Schwenke, D. Thirumalai, and D. G. Truhlar, *Phys. Rev. A* **28**, 3258−3267 (1983).

233. "Localized Gaussian Wavepacket Methods for Inelastic Collisions Involving Anharmonic Oscillators," R. T. Skodje and D. G. Truhlar, *J. Chem. Phys.* **80**, 3123−3136 (1984).

237. "Investigation of the Shape of the Imaginary Part of the Optical Model Potential for Electron Scattering by Rare Gases," G. Staszewska, D. W. Schwenke, and D. G. Truhlar, *Phys. Rev. A* **29**, 3078−3091 (1984).

238. "Complex Optical Potential Model for Electron-Molecule Scattering. Elastic Scattering and Rotational Excitation of H_2 at 10−100 eV," G. Staszewska, D. W. Schwenke, and D. G. Truhlar, *J. Chem. Phys.* **81**, 335−343 (1984).

239. "Effect of Electron Correlation in the Target Wavefunction on Electron−Molecule Scattering," J. R. Rumble, Jr., W. J. Stevens, and D. G. Truhlar, *J. Phys. B* **17**, 3151−3157 (1984).

241. "Single-Root, Real-Basis-Function Method with Correct Branch-Point Structure for Complex Resonance Energies," A. D. Isaacson and D. G. Truhlar, *Chem. Phys. Lett.* **110**, 130−134 (1984).

244. "Quantum Mechanical Differential and Integral Cross Sections for State-to-State Vibrational Excitation of I_2 by He," D. W. Schwenke and D. G. Truhlar, *J. Chem. Phys.* **81**, 5586−5595 (1984).

256. "The Collapsed Close Coupling Method: A Systematic Alternative to the Multichannel Optical Potential for Solutions of the Schroedinger Equation in a Truncated Subspace," G. Staszewska, D. W. Schwenke, and D. G. Truhlar, *Phys. Rev. A* **31**, 1348−1353 (1985). Erratum: **31**, 4036 (1985).

259. "An Ab Initio Potential Energy Surface and Dynamics Calculations for Vibrational Excitation of I_2 by He," F. B. Brown, D. W. Schwenke, and D. G. Truhlar, *Theor. Chim. Acta* **68**, 23−44 (1985).

267. "The Effect of Wigner Singularities on Low-Temperature Vibrational Relaxation Rates," D. W. Schwenke and D. G. Truhlar, *J. Chem. Phys.* **83**, 3454−3461 (1985).

269. "Eigenmode Analysis of Vibrational and Rotational Energy Relaxation in Nonlinear Systems," K. Haug and D. G. Truhlar, *J. Phys. Chem.* **89**, 3198−3201 (1985).

274. "Pseudochannel Approach to Scattering Problems: The Calculation of Coupling Elements from Ground-State Expectation Values," G. Staszewska, D. W. Schwenke, and D. G. Truhlar, *Phys. Rev. A* **33**, 1378−1381 (1986).

276. "On the Multidimensional Surface Intersection Problem and Classical Trajectory Surface Hopping," C. A. Mead and D. G. Truhlar, *J. Chem. Phys.* **84**, 1055−1056 (1986).

282. "Converged Close Coupling Calculations for V−V Energy Transfer: 2 HF($v = 1$) → HF($v = 2$) + HF($v = 0$)," D. W. Schwenke and D. G. Truhlar, *Theor. Chim. Acta* **69**, 175−178 (1986).

283. "Accuracy of the Energy-Corrected Sudden Scaling Procedure for Rotational Excitation of CO by Collisions with Ar," S. Green, D. L. Cochrane, and D. G. Truhlar, *J. Chem. Phys.* **84**, 3865−3869 (1986).

286. "Strategies and Performance Norms for Efficient Utilization of Vector Pipeline Computers as Illustrated by the Classical Mechanical Simulation of Rotationally Inelastic Collisions," D. L. Cochrane and D. G. Truhlar, *Parallel Comput.* **6**, 63−85 (1988).

296. "Converged Calculations of Rotational Energy Transfer in HF−HF Collisions," D. W. Schwenke and D. G. Truhlar, *J. Comput. Chem.* **8**, 282−290 (1987).

299. "Rapid Convergence of Discrete-Basis Representations of the Amplitude Density for Quantal Scattering Calculations," G. Staszewska and D. G. Truhlar, *Chem. Phys. Lett.* **130**, 341−345 (1986).

305. "Energy-Adapted Basis Sets for Quantal Scattering Calculations," G. Staszewska and D. G. Truhlar, *J. Chem. Phys.* **86**, 1646−1648 (1987).

308. "Convergence of L^2 Methods for Scattering Problems," G. Staszewska and D. G. Truhlar, *J. Chem. Phys.* **86**, 2793−2804 (1987).

309. "Fixed-Nuclei and Laboratory-Frame Formalisms for Electron Scattering by a Spherical Top, with Full Incorporation of Symmetry," N. Abusalbi, D. W. Schwenke, C. A. Mead, and D. G. Truhlar, *Theor. Chim. Acta* **71**, 333−358 (1987).

310. "Application of Fixed-Nuclei Scattering Theory to Electron-Methane Elastic and Inelastic Differential Cross Sections at 10 eV Impact Energy," N. Abusalbi, D. W. Schwenke, C. A. Mead, and D. G. Truhlar, *Theor. Chim. Acta* **71**, 359−374 (1987).

312. "Dispersion Relation Techniques for Approximating the Optical Model Potential for Electron Scattering," D. Thirumalai, G. Staszewska, and D. G. Truhlar, *Comments At. Mol. Phys.* **20**, 217−243 (1987).

313. "Comparison of Close Coupling and Quasiclassical Trajectory Calculations for Rotational Energy Transfer in the Collision of Two HF Molecules on a Realistic Potential Energy Surface," D. W. Schwenke, D. G. Truhlar, and M. E. Coltrin, *J. Chem. Phys.* **87**, 983−992 (1987).

315. "Completely L^2 Golden Rule Method for Resonance Energies and Widths," S. C. Tucker and D. G. Truhlar, *J. Chem. Phys.* **86**, 6251−6257 (1987).

316. "Converged Calculations of Vibrational Energy Transfer Probabilities for the Collision of two HF($v = 1$) Molecules," D. W. Schwenke and D. G. Truhlar, *Theor. Chim. Acta* **72**, 1−12 (1987).

320. "Storage Management Strategies in Large-Scale Quantum Dynamics Calculations," D. W. Schwenke, K. Haug, D. G. Truhlar, R. H. Schweitzer, J. Z. H. Zhang, Y. Sun, and D. J. Kouri, *Theor. Chim. Acta* **72**, 237−251 (1987).

329. "L^2 Golden Rule Method to Calculate Partial Widths for the Decay of Resonance States," S. C. Tucker and D. G. Truhlar, *J. Chem. Phys.* **88**, 3667−3677 (1988).

330. "A New Potential Energy Surface for Vibration-Vibration Coupling in HF−HF Quantal Scattering Calculations," D. W. Schwenke and D. G. Truhlar, *J. Chem. Phys.* **88**, 4800−4813 (1988).

336. "Supercomputer Chemistry at the University of Minnesota," J. Almlöf, D. G. Truhlar, H. T. Davis, K. F. Jensen, M. Tirrell, and T. Lybrand, *Int. J. Supercomput. Appl.* **2**, 5−15 (1988).

368. "Dynamical Basis Sets for Algebraic Variational Calculations in Quantum Mechanical Scattering Theory," Y. Sun, D. J. Kouri, D. G. Truhlar, and D. W. Schwenke, *Phys. Rev. A* **41**, 4857−4862 (1990).

376. "Do Classical Oscillators with Quantum Effective Potentials Simulate Quantal Oscillators in Energy Transfer Collisions?" D. L. Cochrane and D. G. Truhlar, *J. Chem. Phys.* **92**, 7716−7717 (1990).

382. "Time-Dependent Wavepacket Algorithm for Inelastic Molecule-Molecule Scattering," Y. Sun, D. J. Kouri, D. W. Schwenke, and D. G. Truhlar, *Comput. Phys. Commun.* **63**, 51−62 (1991).

385. "A Stationarity Principle for Quantum Mechanical Resonance States," D. G. Truhlar and C. A. Mead, *Phys. Rev. A* **42**, 2593−2602 (1990).

436. "Converged Quantum Mechanical Calculations of Electronic-to-Vibrational, Rotational Energy Transfer Probabilities in a System with a Conical Intersection," D. W. Schwenke, S. L. Mielke, G. J. Tawa, R. S. Friedman, P. Halvick, and D. G. Truhlar, *Chem. Phys. Lett.* **203**, 565−572 (1993).

440. "Energy Transfer through Exciplex Funnel States," S. L. Mielke, G. J. Tawa, D. G. Truhlar, and D. W. Schwenke, *J. Am. Chem. Soc.* **115**, 6436−6437 (1993).

441. "Partial Widths of Feshbach Funnel Resonances in the Na(3p)·H_2 Exciplex," S. L. Mielke, G. J. Tawa, D. G. Truhlar, and D. W. Schwenke, *Int. J. Quantum Chem., Symp.* **27**, 621−632 (1993).

455. "Algebraic Variational and Propagation Formalisms for Quantal Dynamics Calculations of Electronic-to-Vibrational, Rotational Energy Transfer and Application to the Quenching of the 3p State of Sodium by Hydrogen Molecules," G. J. Tawa, S. L. Mielke, D. G. Truhlar, and D. W. Schwenke, *J. Chem. Phys.* **100**, 5751−5777 (1994).

459. "A Converged Full-Dimensional Calculation of the Vibrational Energy Levels of $(HF)_2$," W. C. Necoechea and D. G. Truhlar, *Chem. Phys. Lett.* **224**, 297−304 (1994); erratum: **231**, 125−126 (1994).

503. "Validation of Trajectory Surface Hopping Methods Against Accurate Quantum Mechanical Dynamics and Semiclassical Analysis of Electronic-to-Vibrational Energy Transfer," M. S. Topaler, M. D. Hack, T. C. Allison, Y.-P. Liu, S. L. Mielke, D. W. Schwenke, and D. G. Truhlar, *J. Chem. Phys.* **106**, 8699−8709 (1997).

585. "Stabilization Methods for Quantum Mechanical Resonance States of Four-Body Systems," Y. L. Volobuev and D. G. Truhlar, *Comput. Phys. Commun.* **128**, 516−526 (2000). (Special issue on Parallel Computing in *Chem. Phys.*)

ICPEAC

I1. "Determination of Differential Elastic and Vibrational Excitation Cross Sections for e−H_2 Scattering," S. Trajmar, D. G. Truhlar, J. K. Rice, A. Kuppermann, and R. T. Brinkman, *Abstr. Pap. Int. Conf. Phys. Electron. At. Collisions*, sixth, 87−90 (1969).

I2. "Electron Scattering by $X^2\Sigma_g^+$ H_2 at 10 eV with Excitation of Nuclear Motion," D. G. Truhlar, J. K. Rice, S. Trajmar, and A. Kuppermann, *Abstr. Pap. Int. Conf. Phys. Electron. At. Collisions*, sixth, 148−152 (1969).

I3. "Cross Sections for Excitation of the 2 ^{2}S State of Hydrogen by Electron Impact," D. G. Truhlar and A. Kuppermann, *Abstr. Pap. Int. Conf. Phys. Electron. At. Collisions*, sixth, 247−250 (1969).

I4. "Vibrational Excitation of Diatomic Molecules by Electrons in the 10 to 100 eV Energy Range," S. Trajmar, W. Williams, D. G. Truhlar, and D. C. Cartwright, *Abstr. Pap. Int. Conf. Phys. Electron. At. Collisions*, seventh, 1069−1070 (1970).

I5. "Streamlines of Probability Current Density and Tunneling Fractions for the Collinear $H + H_2 \rightarrow H_2 + H$ Reaction," A. Kuppermann, J. T. Adams, and D. G. Truhlar, in *Abstr. Pap. Int. Conf. Phys. Electron. At. Collisions*, eighth, 149−150 (1973).

I6. "Coupling of Electronically Adiabatic States in Atomic and Molecular Collisions. Numerical Tests of the Origin Dependence of the Derivative Coupling Terms," B. C. Garrett, M. J. Redmon, D. G. Truhlar, and C. F. Melius, *Abstr. Pap. Int. Conf. Phys. Electron. At. Collisions*, 12th, 962−963 (1981).

I7. "Vibrational Excitation of N_2 by 5 to 50 eV Electrons," J. R. Rumble, Jr., D. G. Truhlar, and W. J. Stevens, *Abstr. Pap. Int. Conf. Phys. Electron. At. Collisions*, 12th, 316−317 (1981).

I8. "Vibrational−Rotational Excitation of N_2 by Electrons at 5−50 eV," J. Rumble, Jr. and D. G. Truhlar, *Abstr. Pap. Int. Conf. Phys. Electron. At. Collisions*, 13th, 223 (1983).

I9. "Electron Scattering by N_2: Calculations using MCSCF Target Wavefunction," J. Rumble, Jr., D. G. Truhlar, and W. J.

Stevens, *Abstr. Pap. Int. Conf. Phys. Electron. At. Collisions*, 13th, 224 (1983).

Diffusion

263. "Large Tunneling Effects in the Migration of Chemisorbed Hydrogen on a Metal," J. G. Lauderdale and D. G. Truhlar, *J. Am. Chem. Soc.* **107**, 4590−4591 (1985).

272. "Diffusion of Hydrogen, Deuterium, and Tritium on the (100) Plane of Copper: Reaction-Path Formulation, Variational Transition State Theory, and Tunneling Calculations," J. G. Lauderdale and D. G. Truhlar, *Surf. Sci.* **164**, 558−588 (1985).

279. "Embedded-Cluster Model for the Effect of Phonons on Hydrogen Surface Diffusion on Copper," J. G. Lauderdale and D. G. Truhlar, *J. Chem. Phys.* **84**, 1843−1849 (1986).

322. "Surface Diffusion of H on Copper: The Effect of Phonon-Adsorbate Coupling on the Diffusion Rate," T. N. Truong and D. G. Truhlar, *J. Phys. Chem.* **91**, 6229−6237 (1987).

333. "Surface Diffusion of H, D, and T on a Metal Surface: The Role of Metal Motions in the Kinetic Isotope Effects," T. N. Truong and D. G. Truhlar, *J. Chem. Phys.* **88**, 6611−6619 (1988).

364. "A New Ab Initio Potential Energy Surface for H on Ru(0001) and Its Use for Variational Transition State Theory and Semiclassical Tunneling Calculations of the Surface Diffusion of H and D," T. N. Truong, D. G. Truhlar, J. R. Chelikowsky, and M. Y. Chou, *J. Phys. Chem.* **94**, 1973−1981 (1990).

379. "The Effects of Steps, Coupling to Substrate Vibrations, and Surface Coverage on Surface Diffusion Rates and Kinetic Isotope Effects: Hydrogen Diffusion on Ni," T. N. Truong and D. G. Truhlar, *J. Chem. Phys.* **93**, 2125−2138 (1990).

449. "Effect of Phonon Coupling on Hydrogen Tunneling Rates at Gas−Surface Interfaces," S. E. Wonchoba and D. G. Truhlar, *J. Chem. Phys.* **99** 9637−9651 (1993).

473. "Surface Diffusion of H on Ni(100). Interpretation of the Transition Temperature," S. E. Wonchoba, W.-P. Hu, and D. G. Truhlar, *Phys. Rev. B* **51**, 9985−10002 (1995).

487. "General Potential-Energy Function for H/Ni and Dynamics Calculations of Surface Diffusion, Bulk Diffusion, Subsurface-to-Surface Transport, and Absorption," S. E. Wonchoba and D. G. Truhlar, *Phys. Rev. B* **53**, 11222−11241 (1996).

Geometric Phase

109. "On the Determination of Born−Oppenheimer Nuclear Motion Wavefunctions Including Complications Due to Conical Intersections and Identical Nuclei," C. A. Mead and D. G. Truhlar, *J. Chem. Phys.* **70**, 2284−2296 (1979). Erratum: **78**, 6344 (1983). This article is reprinted in *Geometric Phases in Physics*, edited by A. Shapere and F. Wilczek (World Scientific, Singapore, 1989), pp 90−103.

533. "Comment on 'On the Longuet-Higgins Phase and Its Relation to the Electronic Adiabatic-Diabatic Transformation Angle' [*J. Chem. Phys.* **107**, 2694 (1997)]," B. Kendrick, C. A. Mead, and D. G. Truhlar, *J. Chem. Phys.* **110**, 7594−7597 (1999).

Nanoparticles

674. "Validation of Theoretical Methods for the Structure and Energy of Aluminum Nanoparticles," N. E. Schultz, G. Staszewska, P. Staszewski, and D. G. Truhlar, *J. Phys. Chem. B* **108**, 4850−4861 (2004).

688. "Analytic Potential Energy Functions for Aluminum Clusters," A. W. Jasper, P. Staszewski, G. Staszewska, N. E. Schultz, and D. G. Truhlar, *J. Phys. Chem. B* **108**, 8996−9010 (2004).

693. "Many-Body Tight-Binding Model for Aluminum Nanoparticles," G. Staszewska, P. Staszewski, N. E. Schultz, and Donald G. Truhlar, *Phys. Rev. B* **71**, 045423/1−14 (2005).

705. "Analytic Potential Energy Functions for Simulating Aluminum Nanoparticles," A. W. Jasper, N. E. Schultz, and D. G. Truhlar, *J. Phys. Chem. B* **109**, 3915−3920 (2005).

Electronic and Molecular Structure and Spectroscopy

12. "Oscillators with Quartic Anharmonicity: Approximate Energy Levels," D. G. Truhlar, *J. Mol. Spectrosc.* **38**, 415−421 (1971).

17. "Finite Difference Boundary Value Method for Solving One-Dimensional Eigenvalue Equations," D. G. Truhlar, *J. Comput. Phys.* **10**, 123−132 (1972).

23. "Vibrational Matrix Elements of the Quadrupole Moment Functions of H_2, N_2, and CO," D. G. Truhlar, *Int. J. Quantum Chem.* **6**, 975−988 (1972).

33. "Computed Bond Energies and Vibrational Frequencies for ClHCl, BrHBr, and IHI, Including Isotope Effects and Anharmonicity," D. G. Truhlar, P. C. Olson, and C. A. Parr, *J. Chem. Phys.* **57**, 4479−4483 (1972).

37. "Application of the Configuration-Interaction Method and the Random Phase Approximation to the Ab Initio Calculation of Electronic Excitation Energies of H_2O," D. G. Truhlar, *Int. J. Quantum Chem.* **7**, 807−817 (1973).

46. "Ab Initio Hartree−Fock Calculations of Electronic Wave Functions for the c $^3\Pi_u$ State of H_2," D. G. Truhlar, *Int. J. Quantum Chem.* **7**, 1175−1182 (1973).

67. "Mixing of Ionic and Covalent Configurations for NaH, KH, and MgH^+," R. W. Numrich and D. G. Truhlar, *J. Phys. Chem.* **79**, 2745−2766 (1975).

68. "Anharmonic Force Constants of Polyatomic Molecules: Test of the Procedure for Deducing a Force Field from the Vibration−Rotation Spectrum," D. G. Truhlar, R. W. Olson, A. C. Jeannotte II, and J. Overend, *J. Am. Chem. Soc.* **98**, 2373−2379 (1976).

69. "Application of the Finite-Difference Boundary Value Method to the Calculation of Born−Oppenheimer Vibrational Eigenenergies for the Double-Minimum E, F $^1\Sigma_g^+$ State of the Hydrogen Molecule," D. G. Truhlar and W. D. Tarara, *J. Chem. Phys.* **64**, 237−241 (1976).

77. "Ab initio Effective Core Potentials: Reduction of All-Electron Molecular Structure Calculations to Calculations Involving Only Valence Electrons," L. R. Kahn, P. Baybutt, and D. G. Truhlar, J. *Chem. Phys.* **65**, 3826−3853 (1976).

92. "Detailed Study of the Interaction of Covalent and Ionic States in Collisions of Na and K with H," R. W. Numrich and D. G. Truhlar, *J. Phys. Chem.* **82**, 168−176 (1978).

113. "Ab Initio SCF Polarizabilities and Electron−Molecule Adiabatic Polarization Potentials. I. H_2," D. G. Truhlar, D. A. Dixon, and R. A. Eades, *J. Phys. B* **12**, 1913−1925 (1979).

114. "Ab Initio SCF Polarizabilities and Electron−Molecule Adiabatic Polarization Potentials. II. Li_2," D. A. Dixon, R. A. Eades, and D. G. Truhlar, *J. Phys. B* **12**, 2741−2753 (1979).

115. "Ab Initio SCF Polarizabilities and Electron−Molecule Adiabatic Polarization Potentials. III. N_2," R. A. Eades, D. G. Truhlar, and D. A. Dixon, *Phys. Rev. A* **20**, 867−878 (1979).

117. "Calculations of Potential Energy Curves for the Ground States of NaH^+ and KH^+ and Π States of NaH and KH," C. F. Melius, R. W. Numrich, and D. G. Truhlar, *J. Phys. Chem.* **83**, 1221−1227 (1979).

147. "SCF−CI Calculations for Vibrational Eigenvalues and Wavefunctions of Systems Exhibiting Fermi Resonance," T. C. Thompson and D. G. Truhlar, *Chem. Phys. Lett.* **75**, 87−90 (1980).

151. "Numerical Evaluation of Matrix Elements over Eigenfunctions of One-Dimensional Vibrational Problems," D. G. Truhlar and K. Onda, *Phys. Rev. A* **23**, 973−974 (1981).

187. "Ab Initio Adiabatic Polarization Potentials for Be and Mg," R. A. Eades, D. A. Dixon, and D. G. Truhlar, *J. Phys. B* **15**, 3365−3375 (1982).

190. "Conditions for the Definition of a Strictly Diabatic Electronic Basis for Molecular Systems," C. A. Mead and D. G. Truhlar, *J. Chem. Phys.* **77**, 6090−6098 (1982).

191. "Optimization of Vibrational Coordinates, with an Application to the Water Molecule," T. C. Thompson and D. G. Truhlar, *J. Chem. Phys.* **77**, 3031−3035 (1982).

243. "An Optimized Quadrature Scheme for Matrix Elements over the Eigenfunctions of General Anharmonic Potentials," D. W. Schwenke and D. G. Truhlar, *Comput. Phys. Commun.* **34**, 57−66 (1984).

246. "On the Form of the Adiabatic and Diabatic Representations and the Validity of the Adiabatic Approximation for X_3 Jahn−Teller Systems," T. C. Thompson, D. G. Truhlar, and C. A. Mead, *J. Chem. Phys.* **82**, 2392−2407 (1985).

252. "Systematic Study of Basis Set Superposition Errors in the Calculated Interaction Energy of Two HF Molecules," D. W. Schwenke and D. G. Truhlar, *J. Chem. Phys.* **82**, 2418−2426 (1985), **84**, 4113(E) (1986), **86**, 3760(E) (1987).

261. "Consistent Analytic Representation of the Two Lowest Potential Energy Surfaces for Li_3, Na_3, and K_3," T. C. Thompson, G. Izmirlian, Jr., S. J. Lemon, D. G. Truhlar, and C. A. Mead, *J. Chem. Phys.* **82**, 5597−5603 (1985).

264. "A New Semiempirical Method of Correcting Large-Scale Configuration Interaction Calculations for Incomplete Dynamic Correlation of Electrons," F. B. Brown and D. G. Truhlar, *Chem. Phys. Lett.* **117**, 307−313 (1985).

270. "Semiclassical Reaction-Path Methods Applied to Calculate the Tunneling Splitting in NH_3," F. B. Brown, S. C. Tucker, and D. G. Truhlar, *J. Chem. Phys.* **83**, 4451−4455 (1985).

291. "The Potential Energy Surface of the Jahn−Teller-Distorted $^2E'$ Ground State of Copper Trimer," D. G. Truhlar, T. C. Thompson, and C. A. Mead, *Chem. Phys. Lett.* **127**, 287−291 (1986).

295. "Correlation Balance in Basis Sets for Electronic Structure Calculations," M. S. Gordon and D. G. Truhlar, *Int. J. Quantum Chem.* **31**, 81−90 (1987).

298. "Reaction-Path Analysis of the Tunneling Splitting in Fluxional Molecules: Application to the Degenerate Rearrangement of Hydrogen Fluoride Dimer," G. C. Hancock, P. Rejto, R. Steckler, F. B. Brown, D. W. Schwenke, and D. G. Truhlar, *J. Chem. Phys.* **85**, 4997−5003 (1986).

302. "The Hartree−Fock Dissociation of F_2," M. S. Gordon and D. G. Truhlar, *Theor. Chim. Acta* **71**, 1−5 (1987).

328. "An Analytic Representation of the Six-Dimensional Potential Energy Surface of Hydrogen Fluoride Dimer," G. C. Hancock, D. G. Truhlar, and C. E. Dykstra, *J. Chem. Phys.* **88**, 1786−1796 (1988).

334. "A Vibrational Configuration Interaction Program for Energies and Resonance Widths," S. C. Tucker, T. C. Thompson, J. G. Lauderdale, and D. G. Truhlar, *Comput. Phys. Commun.* **51**, 233−256 (1988).

345. "Reaction-Path Analysis of the Effect of Monomer Excitation on the Tunneling Splitting of Hydrogen Fluoride Dimer," G. C. Hancock and D. G. Truhlar, *J. Chem. Phys.* **90**, 3498−3505 (1989).

386. "Reaction Path Power Series Analysis of NH_3 Inversion," R. Steckler and D. G. Truhlar, *J. Chem. Phys.* **93**, 6570−6577 (1990).

388. "Projection Operator Method for Geometry Optimization with Constraints," D.-h. Lu, M. Zhao, and D. G. Truhlar, *J. Comput. Chem.* **12**, 376−384 (1991).

397. "Molecular Modeling of Solvation. $Cl^-(D_2O)$," X. G. Zhao, A. Gonzàlez-Lafont, D. G. Truhlar, and R. Steckler, *J. Chem. Phys.* **94**, 5544−5558 (1991).

408. "The Calculation of Highly Excited Bound-State Energy Levels for a Triatomic Molecule by Using Three-Arrangement Basis Sets and Contracted Basis Functions," P. N. Day and D. G. Truhlar, *J. Chem. Phys.* **95**, 6615−6621 (1991).

432. "Comment on: van der Waals Functional Forms for Molecular Simulations," D. G. Truhlar, *J. Chem. Phys.* **98**, 2491 (1993).

438. "Quantum Chemical Conformational Analysis of Glucose in Aqueous Solution," C. J. Cramer and D. G. Truhlar, *J. Am. Chem. Soc.* **115**, 5745−5753 (1993).

454. "Structural Distortion of CH_3I in an Ion−Dipole Precursor Complex," W.-P. Hu and D. G. Truhlar, *J. Phys. Chem.* **98**, 1049−1052 (1994).

457. "Quantum Chemical Conformational Analysis of 1,2-Ethanediol: Correlation and Solvation Effects on the Tendency to Form Internal Hydrogen Bonds in the Gas Phase and Aqueous Solution," C. J. Cramer and D. G. Truhlar, *J. Am. Chem. Soc.* **116**, 3892−3900 (1994).

465. "Class IV Charge Models: A New Semiempirical Approach in Quantum Chemistry," J. W. Storer, D. J. Giesen, C. J. Cramer, and D. G. Truhlar, *J. Comput.-Aided Mol. Des.* **9**, 87−110 (1995).

471. "Improved General Scaling Factors and Systematic Tests of the SAC Method for Estimating Correlation Energies of Molecules," I. Rossi and D. G. Truhlar, *Chem. Phys. Lett.* **234**, 64−70 (1995).

474. "General Method for Removing Resonance Singularities in Quantum Mechanical Perturbation Theory," K. M. Kuhler, D. G. Truhlar, and A. D. Isaacson, *J. Chem. Phys.* **104**, 4664−4671 (1996).

476. "Relative Stability of Alternative Chair Forms and Hydroxymethyl Conformations of β-D-glucopyranose," S. E. Barrows, F. J. Dulles, C. J. Cramer, A. D. French, and D. G. Truhlar, *Carbohydr. Res.* **276**, 219−251 (1995).

477. "Degeneracy-Corrected Perturbation Theory for Electronic Structure Calculations," X. Assfeld, J. E. Almlöf, and D. G. Truhlar, *Chem. Phys. Lett.* **241**, 438−444 (1995).

482. "An Improved Potential Energy Surface for the Degenerate Rearrangement of $(HF)_2$," W. C. Necoechea and D. G. Truhlar, *Chem. Phys. Lett.* **248**, 182−188 (1996).

485. "The MIDI! Basis Set for Quantum Mechanical Calculations of Molecular Geometries and Partial Charges," R. E. Easton, D. J. Giesen, A. Welch, C. J. Cramer, and D. G. Truhlar, *Theor. Chim. Acta* **93**, 281−301 (1996).

488. "Quantum Chemical Conformational Analysis and X-Ray Structure of 4-Methyl-3-Thiosemicarbazide," C. C. Chambers, E. Archibong, S. M. Mazhari, A. Jabalameli, J. D. Zubkowski, R. H. Sullivan, E. J. Valente, C. J. Cramer, and D. G. Truhlar, *J. Mol. Struct.: THEOCHEM* **388**, 161−167 (1996).

493. "Correlated Capped Subsystem Calculations as a Way to Include Electron Correlation Locally: A Test for Substituent Effects on Bond Energies," E. L. Coitiño, D. G. Truhlar, and K. Morokuma, *Chem. Phys. Lett.* **259**, 159−164 (1996).

495. "Exo-anomeric Effects on Energies and Geometries of Different Conformations of Glucose and Related Systems in

the Gas Phase and Aqueous Solution," C. J. Cramer, D. G. Truhlar, and A. D. French, *Carbohydr. Res.* **298**, 1−14 (1997).

499. "Correlated Capped Subsystem Method for the Calculation of Substituent Effects on Bond Energies," M. Noland, E. L. Coitiño, and D. G. Truhlar, *J. Phys. Chem. A* **101**, 1193−1197 (1997).

501. "New Methods for Potential Functions for Simulating Biological Molecules," G. D. Hawkins, C. J. Cramer, and D. G. Truhlar, *J. Chim. Phys.* **94**, 1448−1481(1997). (CECAM Workshop: Potential Functions for Simulation of Biomolecular Systems.)

502. "Tunneling Splittings in Predissociated HF Dimer," Y. Volobuev, W. C. Nechoechea, and D. G. Truhlar, *J. Phys. Chem. A* **101**, 3045−3048 (1997).

504. "Quantum Mechanical and ^{13}C Dynamic NMR Study of 1,3-Dimethylthiourea Conformational Isomerizations," C. C. Chambers, E. F. Archibong, A. Jabalameli, R. H. Sullivan, D. J. Giesen, C. J. Cramer, and D. G. Truhlar, *J. Mol. Struct.: THEOCHEM* **425**, 61−68 (1998). (Special issue: Current Trends in Computational Chemistry.)

512. "Systematic Analysis of Bond Energies Calculated by the Integrated Molecular Orbital-Molecular Orbital Method," E. L. Coitiño and D. G. Truhlar, *J. Phys. Chem. A* **101**, 4641−4645 (1997).

518. "New Class IV Charge Model for Extracting Accurate Partial Charges from Wave Functions," J. Li, T. Zhu, C. J. Cramer, and D. G. Truhlar, *J. Phys. Chem. A* **102**, 1820−1831 (1998).

523. "Integrated Molecular Orbital Method with Harmonic Cap for Molecular Forces and its Application to Geometry Optimization and the Calculation of Vibrational Frequencies," J. C. Corchado and D. G. Truhlar, *J. Phys. Chem. A* **102**, 1895−1898 (1998).

525. "MIDI! Basis Set for Silicon, Bromine, and Iodine," J. Li, C. J. Cramer, and D. G. Truhlar, *Theor. Chem. Acc.* **99**, 192−196 (1998).

527. "Density Functional Solvation Model Based on CM2 Atomic Charges," T. Zhu, J. Li, G. D. Hawkins, C. J. Cramer, and D. G. Truhlar, *J. Chem. Phys.* **109**, 9117−9133 (1998); errata: **111**, 5624 (1999) and **113**, 3930 (2000).

535. "Factors Controlling the Relative Stability of Anomers and Hydroxymethyl Conformers of Glucopyranose," S. E. Barrows, J. W. Storer, C. J. Cramer, A. D. French, and D. G. Truhlar, *J. Comput. Chem.* **19**, 1111−1129 (1998). (Special issue in honor of N. L. Allinger.)

541. "Basis Set Extrapolation," D. G. Truhlar, *Chem. Phys. Lett.* **294**, 45−48 (1998).

542. "A Class IV Charge Model for Molecular Excited States," J. Li, B. Williams, C. J. Cramer, and D. G. Truhlar, *J. Chem. Phys.* **110**, 724−733 (1999), 111, 5624(E) (1999).

545. "Quantum Chemical Analysis of Para-Substitution Effects on the Electronic Structure of Phenylnitrenium Ions in the Gas Phase and Aqueous Solution," M. B. Sullivan, K. Brown, C. J. Cramer, and D. G. Truhlar, *J. Am. Chem. Soc.* **120**, 11778−11783 (1998), **121**, 11026(E) (1999).

548. "Infrared Absorption Line Strengths of the Na···FH van der Waals Molecule," M. S. Topaler, P. Piecuch, and D. G. Truhlar, *J. Chem. Phys.* **110**, 5634−5638 (1999).

550. "Geometry Optimization with an Infinite Basis Set," Y.-Y. Chuang and D. G. Truhlar, *J. Phys. Chem. A* **103**, 651−652 (1999).

558. "Optimized Parameters for Scaling Correlation Energy," P. L. Fast, J. Corchado, M. L. Sanchez, and D. G. Truhlar, *J. Phys. Chem. A* **103**, 3139−3143 (1999).

559. "Simple Approximation of Core-Correlation Effects on Binding Energies," P. L. Fast and D. G. Truhlar, *J. Phys. Chem. A* **103**, 3802−3803 (1999).

560. "Accurate Dipole Moments from Hartree−Fock Calculations by Means of Class IV Charges," J. Li, J. Xing, C. J. Cramer, and D. G. Truhlar, *J. Chem. Phys.* **111**, 885−892 (1999).

561. "Multi-Coefficient Correlation Method for Quantum Chemistry," P. L. Fast, J. C. Corchado, M. L. Sánchez, and D. G. Truhlar, *J. Phys. Chem. A* **103**, 5129−5136 (1999).

563. "The Gaussian-2 Method with Proper Dissociation, Improved Accuracy, and Less Cost," P. L. Fast, M. L. Sánchez, J. C. Corchado, and D. G. Truhlar, *J. Chem. Phys.* **110**, 11679−11681 (1999).

564. "Multi-Coefficient Gaussian-3 Method for Calculating Potential Energy Surfaces," P. L. Fast, M. L. Sánchez, and D. G. Truhlar, *Chem. Phys. Lett.* **306**, 407−410 (1999).

567. "Perspective on 'Principles for a Direct SCF Approach to LCAO-MO Ab Initio Calculations,' by J. Almlöf, K. Faegri, Jr., and K. Korsell [*J. Comput. Chem.* 1982, 3:385−399]," *Theor. Chem. Acc.* **103**, 349−352 (2000). [New Century issue.]

568. "Infinite Basis Limits in Electronic Structure Theory," P. L. Fast, M. L. Sánchez, and D. G. Truhlar, *J. Chem. Phys.* **111**, 2921−2926 (1999), **113**, 3931(E) (2000).

571. "Two-Response-Time Model Based on CM2/INDO/S2 Electrostatic Potentials for the Dielectric Polarization Component of Solvatochromic Shifts on Vertical Excitation Energies," J. Li, C. J. Cramer, and D. G. Truhlar, *Int. J. Quantum Chem.* **77**, 264−280 (2000). (Festschrift in Honor of Michael C. Zerner's 60th Birthday.)

580. "Multilevel Geometry Optimization," J. M. Rodgers, P. L. Fast, and D. G. Truhlar, *J. Chem. Phys.* **112**, 3141−3147 (2000).

586. "Improved Coefficients for the Scaling All Correlation and Multi-Coefficient Correlation Methods," C. M. Tratz, P. L. Fast, and D. G. Truhlar, *PhysChemComm.* **2**(14), 70−79 (1999).

594. "Thermochemical Analysis of Core Correlation and Scalar Relativistic Effects on Molecular Atomization Energies," J. M. L. Martin, A. Sundermann, P. L. Fast, and D. G. Truhlar, *J. Chem. Phys.* **113**, 1348−1358 (2000).

595. "MC-QCISD: Multi-Coefficient Correlation Method Based on Quadratic Configuration Interaction with Single and Double Excitations," P. L. Fast and D. G. Truhlar, *J. Phys. Chem. A* **104**, 6111−6116 (2000).

600. "Convergence of Variational Calculations of the Ground-State Energy of HF Dimer," Y. Volobuev, W. C. Necoechea, and D. G. Truhlar, *Chem. Phys. Lett.* **330**, 471−474 (2000).

601. "On the Nonexistence of Strictly Diabatic Molecular Electronic Bases," B. K. Kendrick, C. A. Mead, and D. G. Truhlar, *Chem. Phys. Lett.* **330**, 629−632 (2000).

610. "Multi-Coefficient Correlation Method: Comparison of Specific-Range Reaction Parameters to General Reaction Parameters for CnHxOy Compounds," P. L. Fast, N. Schultz, and D. G. Truhlar, *J. Phys. Chem. A* **105**, 4143−4149 (2001).

617. "The Direct Calculation of Diabatic States Based on Configurational Uniformity," H. Nakamura and D. G. Truhlar, *J. Chem. Phys.* **115**, 10353−10372 (2001).

620. "POTLIB 2001: A Potential Energy Surface Library for Chemical Systems," R. J. Duchovic, Y. L. Volobuev, G. C. Lynch, T. C. Allison, J. C. Corchado, D. G. Truhlar, A. F. Wagner, and B. C. Garrett, *Comput. Phys. Commun.* **144**, 169−187 (2002), **156**, 319−322(E) (2004).

625. "MIDIX Basis Set for Lithium Atom: Accurate Geometries and Atomic Partial Charges for Lithium Compounds with Minimal Computational Cost," J. D. Thompson, P. Winget, and D. G. Truhlar, *PhysChemComm.* **4**(16), 72−77 (2001).

626. "Properties of Nonadiabatic Couplings and the Generalized Born−Oppenheimer Approximation," B. K. Kendrick, C. A. Mead, and D. G. Truhlar, *Chem. Phys.* **277**, 31−41 (2002).

631. "Charge Model 3: A Class IV Charge Model Based on Hybrid Density Functional Theory with Variable Exchange," P. Winget, J. D. Thompson, J. D. Xidos, C. J. Cramer, and D. G. Truhlar, *J. Phys. Chem. A* **106**, 10707−10717 (2002).

638. "Obtaining the Right Orbitals is the Key to Calculating Accurate Binding Energies for Cu^+ Ion," B. J. Lynch and D. G. Truhlar, *Chem. Phys. Lett.* **361**, 251−258 (2002).

644. "Direct Diabatization of Electronic States by the Fourfold Way. II. Dynamical Correlation and Rearrangement Processes," H. Nakamura and D. G. Truhlar, *J. Chem. Phys.* **117**, 5576−5593 (2002).

647. "Structures and Aggregation States of Fluoromethyllithium and Chloromethyllithium Carbenoids in the Gas Phase and in Ethereal Solvent," L. M. Pratt, B. Ramachandran, J. D. Xidos, C. J. Cramer, and D. G. Truhlar, *J. Org. Chem.* **67**, 7607−7612 (2002).

648. "More Reliable Partial Atomic Charges When Using Diffuse Basis Functions," J. D. Thompson, J. D. Xidos, T. M. Sonbuchner, C. J. Cramer, and D. G. Truhlar, *PhysChemComm.* **5**(18), 117−134 (2002).

649. "The Effectiveness of Diffuse Basis Functions for Calculating Relative Energies by Density Functional Theory," B. J. Lynch, Y. Zhao, and D. G. Truhlar, *J. Phys. Chem. A* **107**, 1384−1388 (2003).

650. "Lateral Confinement of an Interfacial Electron Wavefunction by a Surface Dipole Lattice," G. Dutton, J. Pu, D. G. Truhlar, and X.-Y. Zhu, *J. Chem. Phys.* **118**, 4337−4340 (2003).

652. "Parameterization of Charge Model 3 for AM1, PM3, BLYP, and B3LYP," J. D. Thompson, C. J. Cramer, and D. G. Truhlar, *J. Comput. Chem.* **24**, 1291−1304 (2003).

653. "Robust and Affordable Multi-Coefficient Methods for Thermochemistry and Thermochemical Kinetics: The MCCM/3 Suite and SAC/3," B. J. Lynch and D. G. Truhlar, *J. Phys. Chem. A* **107**, 3898−3906 (2003).

655. "Force Field Variations along the Torsional Coordinates of CH_3OH and CH_3CHO," T. V. Albu and D. G. Truhlar, *J. Mol. Sprectrosc.* **219**, 129−131 (2003).

658. "Extension of the Fourfold Way For Calculation Of Global Diabatic Potential Energy Surfaces of Complex, Multi-Arrangement, Non-Born−Oppenheimer Systems: Application to HNCO (S_0, S_1)," H. Nakamura and D. G. Truhlar, *J. Chem. Phys.* **118**, 6816−6829 (2003).

663. "A Class IV Charge Model for Boron Based on Hybrid Density Functional Theory," J. M. Brom, B. J. Schmitz, J. D. Thompson, C. J. Cramer, and D. G. Truhlar, *J. Phys. Chem. A* **107**, 6483−6488 (2003).

666. "Small Representative Benchmarks for Thermochemical Calculations," B. J. Lynch and D. G. Truhlar, *J. Phys. Chem. A* **107**, 8996−8999 (2003), **108**, 1460(E) (2003).

668. "The Relative Likelihood of Encountering Conical Intersections and Avoided Intersections on the Potential Energy Surfaces of Polyatomic Molecules," D. G. Truhlar and C. A. Mead, *Phys. Rev. A* **68**, 32501/1−2 (2003).

671. "Generalized Hybrid Orbital (GHO) Method for Combining Ab Initio Hartree−Fock Wave Functions with Molecular Mechanics," J. Pu, J. Gao, and D. G. Truhlar, *J. Phys. Chem. A* **108**, 632−650 (2004).

678. "Class IV Charge Model for the Self-Consistent Charge Density-Functional Tight-Binding Model," J. A. Kalinowski, B. Lesyng, J. D. Thompson, C. J. Cramer, and D. G. Truhlar, *J. Phys. Chem. A* **108**, 2545−2549 (2004).

684. "Combining Self-Consistent-Charge Density-Functional Tight-Binding (SCC-DFTB) with Molecular Mechanics by the Generalized Hybrid Orbital (GHO) Method," J. Pu, J. Gao, and D. G. Truhlar, *J. Phys. Chem. A* **108**, 5454−5463 (2004).

689. "New Effective Core Method (Effective Core Potential and Valence Basis Set) for Aluminum Clusters and Nanoparticles and Al Molecules Containing C, H, and O," N. E. Schultz and D. G. Truhlar, *J. Chem. Theory Comput.* **1**, 41−53 (2005).

692. "Hybrid Meta Density Functional Theory Methods for Thermochemistry, Thermochemical Kinetics, and Noncovalent Interactions: The MPW1B95 and MPWB1K Models and Comparative Assessments for Hydrogen Bonding and van der Waals Interactions," Y. Zhao and D. G. Truhlar, *J. Phys. Chem. A* **108**, 6908−6918 (2004).

695. "Use of Block Hessians for the Optimization of Molecular Geometries," *J. Chem. Theory Comput.* **1**, 54−60 (2005).

697. "Accurate Partial Atomic Charges for High-Energy Molecules Using Class IV Charge Models with the MIDI! Basis Set," C. P. Kelly, C. J. Cramer, and D. G. Truhlar, *Theor. Chem. Acc.* **113**, 133−151 (2005).

700. "The 6−31B(d) Basis Set and the BMC-QCISD and BMC−CCSD Multi-Coefficient Correlation Methods," B. J. Lynch, Y. Zhao, and D. G. Truhlar, *J. Phys. Chem. A* **109**, 1643−1649 (2005).

707. "Redistributed Charge and Dipole Schemes for Combined Quantum Mechanical and Molecular Mechanical Calculations," H. Lin and D. G. Truhlar, *J. Phys. Chem. A* **109**, 3991−4004 (2005).

708. "Generalized Hybrid Orbital Method for Combined Quantum Mechanical and Molecular Mechanical Calculations Based on Density Functional Theory and Hybrid Density Functional Theory," J. Pu, J. Gao, and D. G. Truhlar, *ChemPhysChem.* **6**, 1853−1865 (2005). (Michele Parrinello Festschrift.)

709. "Benchmark Databases for Nonbonded Interactions and Their Use to Test Density Functional Theory," Y. Zhao and D. G. Truhlar, *J. Chem. Theory Comput.* **1**, 415−432 (2005).

712. "Databases for Transition Element Bonding: Metal−Metal Bond Energies and Bond Lengths and Their Use to Test Hybrid, Hybrid Meta, and Meta Density Functionals and Generalized Gradient Approximations," N. E. Schultz, Y. Zhao, and D. G. Truhlar, *J. Phys. Chem. A* **109**, 4388−4403 (2005).

713. "Design of Density Functionals that are Broadly Accurate for Thermochemistry, Thermochemical Kinetics, and Nonbonded Interactions," Y. Zhao and D. G. Truhlar, *J. Phys. Chem. A* **109**, 5656−5667 (2005).

715. "Multi-Coefficient Extrapolated DFT Studies of $\pi\cdots\pi$ Interactions: The Benzene Dimer," Y. Zhao and D. G. Truhlar, *J. Phys. Chem. A* **109**, 4209−4212 (2005).

718. "How Well Can New-Generation Density Functional Methods Describe Stacking Interactions in Biological Systems?" Y. Zhao and D. G. Truhlar, *Phys. Chem. Chem. Phys.* **7**, 2701−2705 (2005).

719. "Infinite-Basis Calculations of Binding Energies for the Hydrogen Bonded and Stacked Tetramers of Formic Acid and Formamide and Their Use for Validation of Hybrid DFT and Ab Initio Methods," Y. Zhao and D. G. Truhlar, *J. Phys. Chem. A* **109**, 6624−6627 (2005).

720. "How Well Can Density Functional Methods Describe Hydrogen Bonds to π Acceptors?" Y. Zhao, O. Tishchenko, and D. G. Truhlar, *J. Phys. Chem. B* **109**, 19046−19051 (2005).

721. "Improved Density Functionals for Water," E. E. Dahlke and D. G. Truhlar, *J. Phys. Chem. A* **109**, 15677−15683 (2005).

722. "QM/MM: What Have We Learned, Where are We, and Where Do We Go from Here?" H. Lin and D. G. Truhlar, *Theor. Chem. Acc.*, in press. (*Proc. Electron. Comp. Chem. Conf.*, 10th, keynote paper.)

727. "Density Functionals for Inorganometallic and Organometallic Chemistry," N. E. Schultz, Y. Zhao, and D. G. Truhlar, *J. Phys. Chem. A*, **109**, 11127−11143 (2005).

729. "Exchange Correlation Functional with Broad Accuracy for Metallic and Nonmetallic Compounds, Kinetics, and Noncovalent Interactions," Y. Zhao, N. E. Schultz, and D. G. Truhlar, *J. Chem. Phys.*, **123**, 161103/1−4 (2005).

Computational Thermochemistry, Solvation

118. "Importance of Quartic Anharmonicity for Bending Partition Functions in Transition-State Theory," B. C. Garrett and D. G. Truhlar, *J. Phys. Chem.* **83**, 1915−1924 (1979).

164. "Tests of Approximation Schemes for Vibrational Energy Levels and Partition Functions for Triatomics: H_2O and SO_2," A. D. Isaacson, D. G. Truhlar, K. Scanlon, and J. Overend, *J. Chem. Phys.* **75**, 3017−3024 (1981).

167. "The Accuracy of the Pitzer-Gwinn Method for Partition Functions of Anharmonic Vibrational Modes," A. D. Isaacson and D. G. Truhlar, *J. Chem. Phys.* **75**, 4090−4094 (1981).

231. "Vibrational Partition Functions Calculated from Limited Information," A. D. Isaacson and D. G. Truhlar, *J. Chem. Phys.* **80**, 2888−2896 (1984).

390. "A Simple Approximation for the Vibrational Partition Function of a Hindered Internal Rotation," D. G. Truhlar, *J. Comput. Chem.* **12**, 266−270 (1991).

391. "Simple Perturbation Theory Estimates of Equilibrium Constants from Force Fields," D. G. Truhlar and A. D. Isaacson, *J. Chem. Phys.* **94**, 357−359 (1991).

409. "Molecular Orbital Theory Calculations of Aqueous Solvation Effects on Chemical Equilibria," C. J. Cramer and D. G. Truhlar, *J. Am. Chem. Soc.* **113**, 8552−8554, 9901(E) (1991).

418. "An SCF Solvation Model for the Hydrophobic Effect and Absolute Free Energies of Aqueous Solvation," C. J. Cramer and D. G. Truhlar, *Science* **256**, 213−217 (1992).

420. "PM3-SM3: A General Parameterization for Including Aqueous Solvation Effects in the PM3 Molecular Orbital Model," C. J. Cramer and D. G. Truhlar, *J. Comput. Chem.* **13**, 1089−1097 (1992).

423. "AM1-SM2 and PM3-SM3 Parameterized SCF Solvation Models for Free Energies in Aqueous Solution," C. J. Cramer and D. G. Truhlar, *J. Comput.-Aided Mol. Des.* **6**, 629−666 (1992).

424. "Quantum Free Energy Calculations: Optimized Fourier Path Integral Monte Carlo Computation of Coupled Vibrational Partition Functions," R. Q. Topper and D. G. Truhlar, *J. Chem. Phys.* **97**, 3647−3667 (1992).

425. "Quantum Free Energy Calculations: A Three-Dimensional Test Case," R. Q. Topper, G. J. Tawa, and D. G. Truhlar, *J. Chem. Phys.* **97**, 3668−3673 (1992), **113**, 3930(E) (2000).

428. "Polarization of the Nucleic Acid Bases in Aqueous Solution," C. J. Cramer and D. G. Truhlar, *Chem. Phys. Lett.* **198**, 74−80 (1992), **202**, 567(E) (1993).

433. "Quantum Steam Tables. Free Energy Calculations for H_2O, D_2O, H_2S, and H_2Se by Adaptively Optimized Monte Carlo Fourier Path Integrals," R. Q. Topper, Q. Zhang, Y.-P. Liu, and D. G. Truhlar, *J. Chem. Phys.* **98**, 4991−5005 (1993).

434. "The Accuracy of Second Order Perturbation Theory for Multiply Excited Vibrational Energy Levels and Partition Functions for a Symmetric Top Molecular Ion," Q. Zhang, P. N. Day, and D. G. Truhlar, *J. Chem. Phys.* **98**, 4948−4958 (1993).

447. "Correlation and Solvation Effects on Heterocyclic Equilibria in Aqueous Solution," C. J. Cramer and D. G. Truhlar, *J. Am. Chem. Soc.* **115**, 8810−8817 (1993).

456. "Entropic Contributions to Free Energies of Solvation," D. J. Giesen, C. J. Cramer, and D. G. Truhlar, *J. Phys. Chem.* **98**, 4141−4147 (1994).

463. "Improved Methods for Semiempirical Solvation Models," D. A. Liotard, G. D. Hawkins, G. C. Lynch, C. J. Cramer, and D. G. Truhlar, *J. Comput. Chem.* **16**, 422−440 (1995).

467. "General Semiempirical Quantum Mechanical Solvation Model for Nonpolar Solvation Energies. *n*-Hexadecane," D. J. Giesen, J. W. Storer, C. J. Cramer, and D. G. Truhlar, *J. Am. Chem. Soc.* **117**, 1057−1068 (1995).

475. "A Semiempirical Quantum Mechanical Solvation Model for Solvation Free Energies in All Alkane Solvents," D. J. Giesen, C. J. Cramer, and D. G. Truhlar, *J. Phys. Chem.* **99**, 7137−7146 (1995).

481. "Pairwise Solute Descreening of Solute Charges from a Dielectric Medium," G. D. Hawkins, C. J. Cramer, and D. G. Truhlar, *Chem. Phys. Lett.* **246**, 122−129 (1995).

492. "Model for Aqueous Solvation Based on Class IV Atomic Charges and First-Solvation Shell Effects," C. C. Chambers, G. D. Hawkins, C. J. Cramer, and D. G. Truhlar, *J. Phys. Chem.* **100**, 16385−16398 (1996).

496. "Parameterized Models of Aqueous Free Energies of Solvation Based on Pairwise Descreening of Solute Atomic Charges from a Dielectric Medium," G. D. Hawkins, C. J. Cramer, and D. G. Truhlar, *J. Phys. Chem.* **100**, 19824−19839 (1996).

497. "A Universal Organic Solvation Model," D. J. Giesen, M. Z. Gu, C. J. Cramer, and D. G. Truhlar, *J. Org. Chem.* **61**, 8720−8721 (1996); erratum: **65**, 5886 (2000).

500. "A Solvation Model for Chloroform Based on Class IV Atomic Charges," D. J. Giesen, C. C. Chambers, C. J. Cramer, and D. G. Truhlar, *J. Phys. Chem. B* **101**, 2061−2069 (1997).

508. "What Controls the Partitioning of Nucleic Acid Bases Between Chloroform and Water?," D. J. Giesen, C. C. Chambers, C. J. Cramer, and D. G. Truhlar, *J. Phys. Chem. B* **101**, 5084−5088 (1997).

509. "Parameterized Model for Aqueous Free Energies of Solvation Using Geometry-Dependent Atomic Surface Tensions with Implicit Electrostatics," G. D. Hawkins, C. J. Cramer, and D. G. Truhlar, *J. Phys. Chem. B* **101**, 7147−7157 (1997).

513. "A Universal Solvation Model for the Quantum Mechanical Calculation of Free Energies of Solvation in Non-Aqueous Solvents," D. J. Giesen, G. D. Hawkins, D. A. Liotard, C. J. Cramer, and D. G. Truhlar, *Theor. Chem. Acc.* **98**, 85−109 (1997); erratum: **101**, 309 (1999).

517. "Universal Quantum Mechanical Model for Solvation Free Energies Based on Gas-Phase Geometries," G. D. Hawkins, C. J. Cramer, and D. G. Truhlar, *J. Phys. Chem. B* **102**, 3257−3271 (1998).

526. "OMNISOL: Fast Prediction of Free Energies of Solvation and Partition Coefficients," G. D. Hawkins, D. A. Liotard, C. J. Cramer, and D. G. Truhlar, *J. Org. Chem.* **63**, 4305−4313 (1998).

528. "Universal Reaction Field Model Based on Ab Initio Hartree−Fock Theory," J. Li, G. D. Hawkins, C. J. Cramer, and D. G. Truhlar, *Chem. Phys. Lett.* **288**, 293−298 (1998).

549. "Application of a Universal Solvation Model to Nucleic Acid Bases. Comparison of Semiempirical Molecular Orbital Theory, Ab Initio Hartree−Fock Theory, and Density Functional Theory," J. Li, C. J. Cramer, and D. G. Truhlar, *Biophys. Chem.* **78**, 147−155 (1999). (Special issue on Implicit Solvent Representation in Biomolecular Chemistry.)

553. "Extension of the Platform of Applicability of the SM5.42R Universal Solvation Model," J. Li, T. Zhu, G. D. Hawkins, P. Winget, D. A. Liotard, C. J. Cramer, and D. G. Truhlar, *Theor. Chem. Acc.* **103**, 9−63 (1999).

554. "Analytical Energy Gradients of a Self-Consistent Reaction-Field Solvation Model Based on CM2 Charges," T. Zhu, J. Li, D. A. Liotard, C. J. Cramer, and D. G. Truhlar, *J. Chem. Phys.* **110**, 5503−5513 (1999).

570. "A Universal Solvation Model Based on Class IV Charges and the Intermediate Neglect of Differential Overlap for Spectroscopy Molecular Orbital Method," J. Li, T. Zhu, C. J. Cramer, and D. G. Truhlar, *J. Phys. Chem. A* **104**, 2178−2182 (2000). (W. A. Goddard III Birthday Issue.)

572. "A Universal Solvation Model Based on the Conductor-like Screening Model," D. M. Dolney, G. D. Hawkins, P. Winget, D. A. Liotard, C. J. Cramer, and D. G. Truhlar, *J. Comput. Chem.* **21**, 340−366 (2000).

573. "Prediction of Vapor Pressures from Self-Solvation Free Energies Calculated by the SM5 Series of Universal Solvation Models," P. Winget, G. D. Hawkins, C. J. Cramer, and D. G. Truhlar, *J. Phys. Chem. B* **104**, 4726−4734 (2000).

576. "Statistical Thermodynamics of Bond Torsion Modes," Y.-Y. Chuang and D. G. Truhlar, *J. Chem. Phys.* **112**, 1221−1228 (2000), **121**, 7036(E) (2004).

578. "Computational Electrochemistry: Aqueous One-Electron Oxidation Potentials for Substituted Anilines," P. Winget, E. J. Weber, C. J. Cramer, and D. G. Truhlar, *Phys. Chem. Chem. Phys.* **2**, 1231−1239, 1871(E) (2000).

584. "Parallel Fourier-Path-Integral Monte Carlo Calculations of Absolute Free Energies and Chemical Equilibria," J. Srinivasan, Y. L. Volobuev, S. L. Mielke, and D. G. Truhlar, *Comput. Phys. Commun.* **128**, 446−464 (2000). (Special issue on Parallel Computing in Chem. Phys.)

592. "Extrapolation and Perturbation Schemes for Accelerating the Convergence of Quantum Mechanical Free Energy Calculations via the Fourier Path-Integral Monte Carlo Method," S. L. Mielke, J. Srinivasan, and D. G. Truhlar, *J. Chem. Phys.* **112**, 8758−8764 (2000).

593. "Prediction of Soil Sorption Coefficients Using a Universal Solvation Model," P. Winget, C. J. Cramer, and D. G. Truhlar, *Environ. Sci. Technol.* **34**, 4733−4740 (2000).

602. "A New Fourier Path Integral Method, A More General Scheme for Extrapolation, and Comparison of Eight Path Integral Methods for the Quantum Mechanical Calculation of Free Energies," S. L. Mielke and D. G. Truhlar, *J. Chem. Phys.* **114**, 621−630 (2001).

613. "Displaced-Points Path Integral Methods for Including Quantum Effects in the Monte Carlo Evaluation of Free Energies," S. L. Mielke and D. G. Truhlar, *J. Chem. Phys.* **115**, 652−682 (2001).

629. "Parameterization of a Universal Solvation Model for Molecules Containing Silicon," P. Winget, C. J. Cramer, and D. G. Truhlar, *J. Phys. Chem. B* **106**, 5160−5168 (2002).

645. "Electrostatic Component of Solvation: Comparison of SCRF Models," C. Curutchet, C. J. Cramer, D. G. Truhlar, M. F. Ruiz-Lopez, M. Orozco, and F. J. Luque, *J. Comput. Chem.* **24**, 284−297 (2003).

659. "Molecular Modeling of Environmentally Important Processes: Reduction Potentials" by A. Lewis, J. A. Bumpus, D. G. Truhlar, and C. J. Cramer, *J. Chem. Educ.* **81**, 596−604 (2004); erratum: in press.

665. "Predicting Aqueous Solubilities from Aqueous Free Energies of Solvation and Experimental or Calculated Vapor Pressures of Pure Substances," J. D. Thompson, C. J. Cramer, and D. G. Truhlar, *J. Chem. Phys.* **119**, 1661−1670 (2003).

670. "A 'Path-by-Path' Monotone Extrapolation Sequence for Feynman Path Integral Calculations of Quantum Mechanical Free Energies" S. L. Mielke and D. G. Truhlar, *Chem. Phys. Lett.* **378**, 317−322 (2003).

676. "Calculation of Converged Rovibrational Energies and Partition Function for Methane using Vibrational−Rotational Configuration Interaction," A. Chakraborty, D. G. Truhlar, J. M. Bowman, and S. Carter, *J. Chem. Phys.* **121**, 2071−2084 (2004).

677. "Predicting Air−Water Adsorption Coefficients Using a Universal Solvation Model and Surface Area Methods," C. P. Kelly, C. J. Cramer, and D. G. Truhlar, *J. Phys. Chem. B* **108**, 12882−12897 (2004).

683. "New Universal Solvation Model and Comparison of the Accuracy of the SM5.42R, SM5.43R, C−PCM, D-PCM, and IEF−PCM Continuum Solvation Models for Aqueous and Organic Solvation Free Energies and for Vapor Pressures," J. D. Thompson, C. J. Cramer, and D. G. Truhlar, *J. Phys. Chem. A* **108**, 6532−6542 (2004).

685. "Computation of Equilibrium Oxidation and Reduction Potentials for Reversible and Dissociative Electron-Transfer Reactions in Solution," P. Winget, C. J. Cramer, D. G. Truhlar, *Theor. Chem. Acc.* **112**, 217−227 (2004). (Jean-Louis Rivail Honorary Issue.)

694. "Accurate Vibrational−Rotational Partition Functions and Standard-State Free Energy Values for H_2O_2 from Monte Carlo Path-Integral Calculations," V. A. Lynch, S. L. Mielke, and D. G. Truhlar, *J. Chem. Phys.* **121**, 5148−5162 (2004).

698. "Density-Functional and Hybrid-DFT SM5.43R Continuum Solvation Models for Aqueous and Organic Solvents," J. D. Thompson, C. J. Cramer, and D. G. Truhlar, *Theor. Chem. Acc.* **113**, 107−131 (2005).

717. "High-Precision Quantum Thermochemistry on Non-Quasiharmonic Potentials: Converged Path Integral Free Energies and a Systematically Convergent Family of Generalized Pitzer-Gwinn Approximations," V. A. Lynch, S. L. Mielke, and D. G. Truhlar, *J. Phys. Chem. A* **109**, 10092−10099 (2005).

725. "SM6: A Density Functional Theory Continuum Solvation Model for Calculating Aqueous Solvation Free Energies of Neutrals, Ions, and Solute-Water Clusters," C. P. Kelly, C. J. Cramer, and D. G. Truhlar, *J. Chem. Theory Comput.* **1**, 1133−1152 (2005).

732. "Adding Explicit Solvent Molecules to Continuum Solvent Calculations for the Calculation of Aqueous Acid Dissociation Constants," C. P. Kelly, C. J. Cramer, and D. G. Truhlar, *J. Phys. Chem. A*, in press.

Books Edited

B1. *Chemical Applications of Atomic and Molecular Electrostatic Potentials*, edited by P. Politzer and D. G. Truhlar (Plenum Press, New York, 1981). ix + 472 pages.

B2. *Potential Energy Surfaces and Dynamics Calculations*, edited by D. G. Truhlar (Plenum Press, New York, 1981). xiii + 866 pages.

B3. *Resonances in Electron−Molecule Scattering, van der Waals Complexes, and Reactive Chemical Dynamics*, edited by D. G. Truhlar (*ACS Symp. Ser.* Volume 263, Washington, D.C., 1984). xi + 522 pages.

B4. *Supercomputer Research in Chemistry and Chemical Engineering*, edited by K. F. Jensen and D. G. Truhlar (*ACS Symp. Ser.* Volume 353, Washington, D.C., 1987). vii + 436 pages.

B5. *Mathematical Frontiers in Computational Chemical Physics*, edited by D. G. Truhlar (Springer-Verlag, New York, 1988). xi + 349 pages. [IMA Vol. Math. Its Appl. 15 (1988).]

B6. *Practical Iterative Methods for Large Scale Computations*, edited by D. L. Boley, D. G. Truhlar, Y. Saad, R. E. Wyatt, and L. A. Collins (North-Holland, Amsterdam, 1989). x + 481 pages.

B7. *Structure and Reactivity in Aqueous Solution: Characterization of Chemical and Biological Systems*, edited by C. J. Cramer and D. G. Truhlar (*ACS Symp. Ser.* Volume 568, Washington, D.C., 1994). x + 438 pages.

B8. *Domain-Based Parallelism and Problem Decomposition Methods in Computational Science and Engineering*, edited by D. E. Keyes, Y. Saad, and D. G. Truhlar (Society for Industrial and Applied Mathematics, Philadelphia, PA, 1995). xvi + 323 pages.

B9. *Multiparticle Quantum Scattering with Applications to Nuclear, Atomic, and Molecular Physics*, edited by D. G. Truhlar and B. Simon (Springer, New York, 1997). x + 401 pages. [IMA Vol. Math. Its Appl. 89 (1997).]

B10. *Rational Drug Design*, edited by D. G. Truhlar, W. J. Howe, A. J. Hopfinger, J. Blaney, and R. A. Dammkoehler (Springer, New York, 1999). xii + 206 pages. [IMA Vol. Math. Its Appl. 108 (1999).]

B11. *Monte Carlo Methods in Chemical Physics*, edited by D. M. Ferguson, J. I. Siepmann, and D. G. Truhlar (John Wiley & Sons, New York, 1999). xii + 555 pages. [Advances in Chemical Physics series, volume 105.]

B12. *Transition State Modeling for Catalysis*, edited by D. G. Truhlar and K. Morokuma (*ACS Symp. Ser.* Volume 721, Washington, D.C., 1999). xv + 521 pages.

B13. *Parallel Computing in Chemical Physics*, edited by F. Hossfeld, R. Ahlrichs, P. Taylor, and D. G. Truhlar (Elsevier, Amsterdam, 2000). 530 pages.

Theses

1. "The Spectra and Products of the Chemiluminescent Vapor Phase Reaction of Sodium with Methylene Chloride," D. G. Truhlar, B. A. Thesis, St. Mary's College, Winona, MN, 1965, unpublished.

2. "Quantum Mechanical Calculations for Rearrangement Collisions of Electrons, Atoms, and Molecules," D. G. Truhlar, Ph.D. Thesis, California Institute of Technology, Pasadena, CA, Dec. 1, 1969, unpublished. [*Diss. Abstr. Int., B* **31**, 1217 (1970).]

Other Reports

R1. "Computational Chemistry: Many Roads to Travel," D. G. Truhlar, *IEEE Comp. Sci. Eng.* **1**(3), 80 (1994).

R2. "Watching the Molecules Move: International Symposium on Computational Molecular Dynamics," D. G. Truhlar, *Comp. Sci. Eng.* **1**(4), 76−78 (1994).

R3. "POLYRATE 6.5: A New Version of Computer Program for the Calculation of Chemical Reaction Rates for Polyatomics," R. Steckler, W.-P. Hu, Y.-P. Liu, G. C. Lynch, B. C. Garrett, A. D. Isaacson, V. S. Melissas, D.-h. Lu, T. N. Truong, S. N. Rai, G. C. Hancock, J. G. Lauderdale, T. Joseph, and D. G. Truhlar, *Comput. Phys. Commun.* **88**, 341−343 (1995).

R4. "MORATE 6.5: A New Version of Computer Program for Direct Dynamics Calculations of Chemical Reaction Rate Constants," W.-P. Hu, G. C. Lynch, Y.-P. Liu, I. Rossi, J. J. P. Stewart, R. Steckler, B. C. Garrett, A. D. Isaacson, D.-h. Lu, V. S. Melissas, and D. G. Truhlar, *Comput. Phys. Commun.* **88**, 344−346 (1995).

R5. "Scientific Computation: An Interdisciplinary Approach at Minnesota," D. G. Truhlar, *Behavior Research Methods, Instruments & Computers* **29**, 3−5 (1997).

R6. "International Conference on Parallel Computing," D. G. Truhlar, *IEEE Comp. Sci. Eng.* **4**(1), 98−100 (1997).

R7. "The Role of Electrostatics in Chemistry," C. J. Cramer and D. G. Truhlar, *Theor. Chem. Acc.* **98**, 206−211 (1997).

R8. "Computational Drug-Design Workshop," D. G. Truhlar, *IEEE Comp. Sci. Eng.* **4**(4), 84−87 (1997).

R9. "Quantum Catalysis," D. G. Truhlar, *IEEE Comp. Sci. Eng.* **5**(2), 98−100 (1998).

R10. "Electronically Nonadiabatic Dynamics and Resonance Lifetimes," D. G. Truhlar, in *Molecular Quantum States at Dissociation*, edited by R. Prosmiti, J. Tennyson, and D. C. Clary (CCP6, Daresbury, 1998), pp 59−62.

R11. "Present-Day View of Transition State Theory," in *Physical Chemistry*, 2nd ed., R. S. Berry, S. A. Rice, and J. Ross (Oxford University Press, New York, 2000), pp 913−915.

R12. "Computational Chemistry," D. G. Truhlar and V. McKoy, *Comp. Sci. Eng.* **2**(6), 19−21 (2000).