

List of Publications of George C. Schatz

Books

1. *Quantum Mechanics in Chemistry*, G. C. Schatz and M. A. Ratner, Prentice Hall, Englewood Cliffs, NJ, 1993, xix + 325 pages; republished by Dover, 2002 with additions and corrections. ISBN 0-486-42003-5.

2. *Highly Excited Molecules: Relaxation, Reaction and Structure*, A. S. Mullin and G. C. Schatz, ACS Symposium Series 678, American Chemical Society, Washington, DC, 1997, xii + 330 pages.

3. *Introduction to Quantum Mechanics in Chemistry*, M. A. Ratner and G. C. Schatz, Prentice Hall, Upper Saddle River, NJ, 2001, x + 296 pages.

Papers in Journals

1. Electron Paramagnetic Resonance of Magnetically Dilute Cupric ($3d^9$, 2D) Ion in Single Crystals of Zinc 3-Pyridine Sulfonate, G. C. Schatz and J. A. McMillan, *J. Chem. Phys.*, **55**, 2343–6 (1971).

2. Chemiluminescence Excited by Atomic Fluorine, G. C. Schatz and M. Kaufman, *J. Phys. Chem.*, **76**, 3586–90 (1972).

3. Quantum Initial Conditions in Quasi-Classical Trajectory Calculations, J. M. Bowman, Aron Kuppermann, and G. C. Schatz, *Chem. Phys. Lett.*, **19**, 20–25 (1973).

4. Large Quantum Effects in the Collinear $F + H_2 \rightarrow FH + H$ Reaction, G. C. Schatz, J. M. Bowman and Aron Kuppermann, *J. Chem. Phys.*, **58**, 4023–5 (1973).

5. Role of Direct and Resonant (Compound State) Processes and of Their Interferences in the Quantum Dynamics of the collinear $H + H_2$ Exchange Reaction, G. C. Schatz and A. Kuppermann, *J. Chem. Phys.*, **59**, 964–5 (1973).

6. Violation of Microscopic Reversibility and the Use of Reverse Quasi-Classical Trajectories for Calculating Reaction Cross Sections, J. M. Bowman, G. C. Schatz and A. Kuppermann, *Chem. Phys. Lett.*, **24**, 378–80 (1974).

7. Coplanar and Collinear Quantum Mechanical Reactive Scattering: The Importance of Virtual Vibrational Channels in the $H + H_2$ Exchange Reaction, Aron Kupperman, G. C. Schatz and M. Baer, *J. Chem. Phys.*, **61**, 4362–3 (1974).

8. Quantum Mechanical Reactive Scattering: An Accurate Three-Dimensional Calculation, Aron Kuppermann and G. C. Schatz, *J. Chem. Phys.*, **62**, 2502–4 (1975).

9. Exact Quantum, Quasi-Classical and Semi-Classical Reaction Probabilities for the Collinear $F + H_2 \rightarrow FH + H$ Reaction, G. C. Schatz, J. M. Bowman and Aron Kuppermann, *J. Chem. Phys.*, **63**, 674–84 (1975).

10. Exact Quantum, Quasi-Classical and Semi-Classical Reaction Probabilities for the Collinear $F + D_2 \rightarrow FD + D$ Reaction, G. C. Schatz, J. M. Bowman and Aron Kuppermann, *J. Chem. Phys.*, **63**, 685–96 (1975).

11. Dynamical Resonances in Collinear, Coplanar and Three Dimensional Quantum Mechanical Reactive Scattering, G. C. Schatz and Aron Kupperman, *Phys. Rev. Lett.*, **35**, 1266–9 (1975).

12. The Quantum Dynamics of Atom Plus Diatom Chemical Reactions, G. C. Schatz, Ph.D. Thesis, California Institute of Technology, 1975.

13. Quantum Mechanical Reactive Scattering for Planar Atom plus Diatom Systems: I. Theory, Aron Kuppermann, G. C. Schatz and M. Baer, *J. Chem. Phys.*, **65**, 4596–4623 (1976).

14. Quantum Mechanical Reactive Scattering for Planar Atom plus Diatom Systems: II. Accurate Cross Sections for $H + H_2$, G. C. Schatz and A. Kuppermann, *J. Chem. Phys.*, **65**, 4624–4641 (1976).

15. Quantum Mechanical Reactive Scattering for Three-Dimensional Atom plus Diatom Systems, I. Theory, G. C. Schatz and Aron Kuppermann, *J. Chem. Phys.*, **65**, 4642–4667 (1976).

16. Quantum Mechanical Reactive Scattering for Three-Dimensional Atom plus Diatom Systems: II. Accurate Cross Sections for $H + H_2$, G. C. Schatz and Aron Kuppermann, *J. Chem. Phys.*, **65**, 4668–4692 (1976).

17. Franck–Condon Factors in Studies of Dynamics of Chemical Reactions I. General Theory, Application to Collinear Atom–Diatom Reactions, G. C. Schatz and J. Ross, *J. Chem. Phys.*, **66**, 1021–1036 (1977).

18. Franck–Condon Factors in Studies of Dynamics of Chemical Reaction II. Vibration–Rotation Distributions in Atom–Diatom Reactions, G. C. Schatz and J. Ross, *J. Chem. Phys.*, **66**, 1037–1053 (1977).

19. Angular Momentum Decoupling Approximations in the Quantum Dynamics of Reactive Systems, A. Kuppermann, G. C. Schatz and J.P. Dwyer, *Chem. Phys. Lett.*, **45**, 71–73 (1977).

20. Franck–Condon Factors in Studies of Dynamics of Chemical Reactions III. Analysis of Information Theory for Vibration–Rotation Distributions and Isotopic Branching Ratios, G. C. Schatz and J. Ross, *J. Chem. Phys.*, **66**, 2943–2958 (1977).

21. On Stochastic Reductions in Molecular Collision Theory: Projection Operator Formalism: Application to Classical and Quantum Forced Oscillator Model, G. C. Schatz, F. J. McLafferty and J. Ross, *J. Chem. Phys.* **66**, 3609–3623 (1977).

22. The Generalized Cumulant Expansion Approach to Stochastic Reductions in Molecular Collision Dynamics: Applications to Collisional Energy Transfer, G. C. Schatz, *J. Chem. Phys.*, **66**, 5220–5225 (1977).

23. On Self-Consistent and Stochastic Treatments of V-T Energy Transfer in Collinear Atom–Diatom Collisions, G. C. Schatz, *Chem. Phys.*, **24**, 263 (1977).

24. The Direct Histogram Method for Quasiclassical Collision Dynamics: Application to Collinear Atom–Diatom Scattering, G. C. Schatz and C. Vaughn, *Chem. Phys. Lett.*, **54**, 327–331 (1978).

25. A Direct Method for Determining Moments of Final State Distributions in Molecular Collisions, G. C. Schatz, *Mol. Phys.*, **35**, 477–500 (1978).

26. The Importance of Anharmonicity on the Rates of Energy Transfer in Rare Gas/ CO_2 Systems, G. C. Schatz and M. D. Moser, *J. Chem. Phys.*, **68**, 1992–1993 (1978).

27. A Generalized Langevin Equation Approach to Molecular Collision Dynamics, G. C. Schatz, *Chem. Phys.*, **31**, 295–307 (1978).

28. Stochastic Theory of Collisional Energy Transfer: Nature of Convergence of Master Equation Transition Probabilities and Moments as a Function of Cumulant Expansion Order, G. C. Schatz, *Chem. Phys. Lett.*, **58**, 368–374 (1978).

29. Theory of Raman Scattering by Molecules Adsorbed on Electrode Surfaces, F. W. King, R. P. Van Duyne and G. C. Schatz, *J. Chem. Phys.*, **69**, 4472–4481 (1978).
30. A Method for Determining “Good” Action-Angle Variables and Semiclassical Eigenvalues in Nonseparable Systems, G. C. Schatz and M. D. Moser, *Chem. Phys.*, **35**, 239–251 (1978).
31. Theory of Raman Scattering by Molecules Adsorbed at Electrode Surfaces. Model Calculations for Resonance Raman Scattering by an Adsorbed Diatomic, F. W. King and G. C. Schatz, *Chem. Phys.*, **38**, 245–256 (1979).
32. Franck–Condon Factors in Studies of Dynamics of Chemical Reactions. V. Simple Construction of Quasiadiabatic Potential Energy Surfaces and Numerical Evaluation of Franck–Condon Integrals, C. L. Vila, J. L. Kinsey, J. Ross and G. C. Schatz, *J. Chem. Phys.*, **70**, 2414–2424 (1979).
33. Comment on “Theory of Collisions Between an Atom and a Diatomic Molecule in the Body-Fixed Coordinate System,” G. C. Schatz and A. Kuppermann, *J. Chem. Phys.*, **70** 3151–3152 (1979).
34. Stochastic Theory of Vibrational Energy Transfer in Collinear Atom–Diatom Collisions: The Role of Non-Markovian Effects, F. W. King and G. C. Schatz, *Mol. Phys.*, **38**, 257–272 (1979).
35. Classical Perturbation Theory of Good Action-Angle Variables: Applications to Semiclassical Eigenvalues and to Collisional Energy Transfer in Polyatomic Molecules, G. C. Schatz and T. Mulloney, *J. Phys. Chem.*, **83**, 989–999 (1979).
36. Collisional Energy Transfer in Polyatomic Molecules: A Study of Anharmonicity Effects in Kr + CO₂, G. C. Schatz and T. Mulloney, *J. Chem. Phys.*, **71**, 5257–5267 (1979).
37. A Method for Determining Semiclassical Tunnelling Probabilities in Atom–Diatom Reactions, R. I. Altkorn and G. C. Schatz, *J. Chem. Phys.*, **72**, 3337–3347 (1980).
38. How Symmetric Stretch Excitation in a Triatomic Molecule Can be More Efficient Than Asymmetric Stretch Excitation in Enhancing Reaction Rates in Atom Plus Triatom Reactions, G. C. Schatz, *J. Chem. Phys.*, **71**, 542–543 (1979).
39. Theoretical Studies of the O + H₂ Reaction, S. P. Walch, A. F. Wagner, T. H. Dunning and G. C. Schatz, *J. Chem. Phys.*, **72**, 2894–2896 (1980).
40. Vibrational Deactivation on Chemically Reactive Potential Surfaces: An Exact Quantum Study of a Low Barrier Collinear Model of H + FH, D + FD, H + FD, and D + FH, G. C. Schatz and A. Kuppermann, *J. Chem. Phys.*, **72**, 2737–2743 (1980).
41. Classical Rotational and Centrifugal Sudden Approximations for Atom-Molecule Collisional Energy Transfer, T. Mulloney and G. C. Schatz, *Chem. Phys.*, **45**, 213–223 (1980).
42. Collisional Energy Transfer as a Probe of Ergodicity in Molecular Vibrational Motions, G. C. Schatz, *Chem. Phys. Lett.* **67**, 248–251 (1979).
43. An *ab initio* Calculation of the Rate Constant for the OH + H₂ → H₂O + H Reaction, G. C. Schatz and S. P. Walch, *J. Chem. Phys.*, **72**, 776–777 (1980).
44. A Reference Trajectory Approach to Langevin Equations in Gas phase Collision Dynamics, G. C. Schatz and M. D. Moser, *J. Chem. Phys.*, **73**, 2792–2801 (1980).
45. A Quasiclassical Trajectory Study of Collisional Excitation in Li⁺ + CO₂, G. C. Schatz, *J. Chem. Phys.*, **72**, 3929–3938 (1980).
46. Image Field Theory of Enhanced Raman Scattering by Molecules Adsorbed on Metal Surfaces: Detailed Comparison with Experimental Results, G. C. Schatz and R. P. Van Duyne, *Surf. Sci.*, **101**, 425–438 (1980).
47. A Quasi-Classical Trajectory Study of Product Vibrational Distributions in the OH + H₂ → H₂O + H Reaction, G. C. Schatz and H. Elgersma, *Chem. Phys. Phys. Lett.*, **73**, 21–24 (1980).
48. On the Mode Specificity of Reaction Rate Enhancements, G. C. Schatz, *J. Chem. Soc., Faraday Discuss.*, **67**, 140–141 (1979).
49. On the Use of Mass Scaled Cluster Coordinates to Describe Polyatomic Molecule Reaction Dynamics: Application to O + CS₂ → SO + CS, Henry Elgersma and George C. Schatz, *Chem. Phys.*, **54**, 201–216 (1981).
50. *Ab initio* Calculation of Transition State Normal Mode Properties and Rate Constants for the H(T) + CH₄(CD₄) Abstraction and Exchange Reactions, George C. Schatz, Stephen P. Walch and Albert F. Wagner, *J. Chem. Phys.*, **73**, 4536–4547 (1980).
51. A Quasiclassical Trajectory Study of Reagent Vibrational Excitation Effects in the OH + H₂ → H₂O + H Reaction, George C. Schatz, *J. Chem. Phys.*, **74**, 1133–1139 (1981).
52. Tunable Laser Excitation Profile of Surface Enhanced Raman Scattering from Pyridine Adsorbed on a Copper Electrode, Craig S. Allen, George C. Schatz and Richard P. Van Duyne, *Chem. Phys. Lett.*, **75**, 201–205 (1980).
53. An Analytical Fit to an Accurate *ab initio* (¹A₁) Potential Surface of H₂O. Michael J. Redmon and George C. Schatz, *Chem. Phys.*, **54**, 365–374 (1981).
54. A Quasiclassical Trajectory Study of Product Rotational, Angular and Projection Distributions in the OH + H₂ → H₂O + H Reaction, G. C. Schatz and H. Elgersma, In *Potential Energy Surfaces and Dynamics Calculations*, D. G. Truhlar, Ed., Plenum, New York, 1981, pp 311–374.
55. Overview of Reactive Scattering, G. C. Schatz, In *Potential Energy Surfaces and Dynamics Calculations*, D. G. Truhlar, Ed., Plenum, New York, 1981, pp 287–310.
56. The Evaluation of Fitting Functions for the Representation of an O + H₂ Potential Energy Surface, A. F. Wagner, G. C. Schatz and J. M. Bowman, *J. Chem. Phys.*, **74**, 4960–4983 (1981).
57. A Comparative Study of the Reaction Dynamics of Several Potential Energy Surfaces of O (³P) + H₂ → OH + H. I, G. C. Schatz, A.F. Wagner, S. P. Walch and J. M. Bowman, *J. Chem. Phys.*, **74**, 4984–4996 (1981).
58. Collisional Excitation of H₂O by O-Atom Impact: Classical Dynamics on an Accurate *Ab-Initio* Potential Energy Surface, M. J. Redmon, R. J. Bartlett, B. C. Garrett, G. D. Purvis, P. M. Saatzter, G. C. Schatz, and I. Shavitt, In *Potential Energy Surfaces and Dynamics Calculations*, D. G. Truhlar, Ed., Plenum, New York, 1981, pp 771–804.
59. Quasiclassical Trajectory Studies of State to State Collisional Energy Transfer in Polyatomic Molecules, G. C. Schatz, In *Molecular Collision Dynamics*, Topics in Current Physics, Vol. 33, J. M. Bowman, Ed., Springer, Heidelberg, 1983, pp 25–60.
60. Quasiclassical Trajectory Study of Collisional Excitation in O(³P) + CO₂, G. C. Schatz and M. J. Redmon, *Chem. Phys.*, **58**, 195–202 (1981).
61. Tests of Collinear Quasiclassical Trajectory Transmission Coefficient Correction to Transition State Theory, J. M. Bowman, Guan-Zhi Ju, Ki Tung Lee, A. F. Wagner and G. C. Schatz, *J. Chem. Phys.*, **75**, 141–147 (1981).
62. 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).

63. A Quasiclassical Trajectory Study of Mode Specific Reaction Rate Enhancements in $\text{H} + \text{H}_2\text{O} (\nu_1, \nu_2, \nu_3) \rightarrow \text{OH} + \text{H}_2$, H. Elgersma and G. C. Schatz, *Int. J. Quantum Chem. Symp.*, **15**, 611–619 (1981).

64. A Comparative Study of the Reaction Dynamics of the $\text{O}(\text{}^3\text{P}) + \text{H}_2 \rightarrow \text{OH} + \text{H}$ Reaction on Several Potential Energy Surfaces. II. Exact Quantum and Quasiclassical Collinear Reaction Probabilities, K. T. Lee, J. M. Bowman, A. F. Wagner and G. C. Schatz, *J. Chem. Phys.*, **76**, 3563–3582 (1982).

65. A Comparative Study of the Reaction Dynamics of the $\text{O}(\text{}^3\text{P}) + \text{H}_2 \rightarrow \text{OH} + \text{H}$ Reaction on Several Potential Energy Surfaces. III. Collinear Exact Quantum Transmission Coefficient Correction to Transition State Theory, K.T. Lee, J. M. Bowman, A. F. Wagner, and G. C. Schatz, *J. Chem. Phys.*, **76**, 3583–3596 (1982).

66. The Role of Surface Roughness in Surface Enhanced Raman Spectroscopy (SERS): The Importance of Multiple Plasmon Resonances, U. Laor and G. C. Schatz, *Chem. Phys. Lett.*, **82**, 566–570 (1981).

67. The Image Field Effect: How Important Is It? G. C. Schatz, In *Surface Enhanced Raman Scattering*, R. K. Chang and T. E. Furtak, Eds., Plenum, New York, 1982, pp 35–50.

68. The Effect of Randomly Distributed Surface Bumps on Local Field Enhancements in Surface Enhanced Raman Spectroscopy, U. Laor and G. C. Schatz, *J. Chem. Phys.*, **76**, 2888–2899 (1982).

69. Energy Transfer, Stabilization and Dissociation in Collisions of He with Highly Excited HO_2 , C. R. Gallucci and G. C. Schatz, *J. Phys. Chem.*, **86**, 2352–2358 (1982).

70. An ab initio Determination of the Rate Constant for $\text{H}_2 + \text{C}_2\text{H} \rightarrow \text{H} + \text{C}_2\text{H}_2$, L. B. Harding, G. C. Schatz and R. A. Chiles, *J. Chem. Phys.*, **76**, 5172–5173 (1982).

71. An ab initio Determination of the Rate Constant for $\text{H} + \text{H}_2\text{CO} \rightarrow \text{H}_2 + \text{HCO}$, L. B. Harding and G. C. Schatz, *J. Chem. Phys.*, **76**, 4296–4297 (1982).

72. Time Dependent Hartree–Fock Calculations of Surface Enhanced Raman Intensities: I. H_2 Adsorbed on a Model Li Cluster, P. K. K. Pandey and G. C. Schatz, *Chem. Phys. Lett.*, **88**, 193–197 (1982).

73. Ab initio Calculation of the Transition State Properties and Addition Rate Constants for $\text{H} + \text{C}_2\text{H}_2$ and Selected Isotopic Analogs, L. B. Harding, A. F. Wagner, J. M. Bowman and G. C. Schatz and K. Christoffel, *J. Phys. Chem.*, **86** 4312–4327 (1982).

74. A Study of the Dynamics of UV Laser Photolysis of NOCl and NOBr , M. D. Moser, E. Weitz and G. C. Schatz, *J. Chem. Phys.*, **78**, 757–766 (1983).

75. An Effective Molecular Orbital Basis Selection Scheme to Calculate Resonant Frequency Dependent Polarizabilities and Polarizability Derivatives by Time Dependent Hartree–Fock Theory, P. K. K. Pandey and G. C. Schatz, *Chem. Phys. Lett.*, **91**, 286–290 (1982).

76. Orientation Dependence of Surface Enhanced Raman Intensities: Results from *Ab Initio* Calculations, P. K. K. Pandey and G. C. Schatz, *J. Electron Spectrosc. Relat. Phenom.*, **29**, 351–355 (1983).

77. The Quantum Dynamics of $\text{H} + \text{H}_2 (\nu = 1)$: A Coupled States Study of Cross Sections and Rate Constants, G. C. Schatz, *Chem. Phys. Lett.*, **94**, 183–187 (1983).

78. A Theoretical Study of Deuterium Isotope Effects in the Reactions $\text{H}_2 + \text{CH}_3$ and $\text{H} + \text{CH}_4$, G. C. Schatz, A. F. Wagner and T. H. Dunning, *J. Phys. Chem.*, **88**, 221–232 (1984).

79. Analytical Potential Energy Surfaces for Ethynyl (C_2H), Acetylene (C_2H_2) and Vinyl (C_2H_3), K. A. White and G. C. Schatz, *J. Phys. Chem.*, **88**, 2049–2057 (1984).

80. Dynamical Instabilities and Structural Changes in Molecules, B. Barbooy, G. C. Schatz, M. A. Ratner and R. B. Gerber, *Mol. Phys.*, **50**, 353 (1983).

81. Dissociation Dynamics of Vibrationally Excited Van der Waals Clusters: $\text{I}_2\text{XY} \rightarrow \text{X} + \text{Y}$ ($\text{X}, \text{Y} = \text{He}, \text{Ne}$); G. C. Schatz, V. Buch, M. A. Ratner and R. B. Gerber, *J. Chem. Phys.*, **79**, 1808–1822 (1983).

82. The Origin of Cross Section Threshold in $\text{H} + \text{H}_2$: Why Quantum Dynamics Appears to be More Vibrationally Adiabatic than Classical Dynamics, G. C. Schatz, *J. Chem. Phys.*, **79**, 5386–5391 (1983).

83. Comments on Two Treatments of Symmetry Rules in Chemical Reactions, H. I. Metiu, G. C. Schatz and J. Ross, *J. Chem. Phys.*, **79**, 2854–2856 (1983).

84. A New Approach to the Determination of Good Action - Angle Variables for Coupled Oscillator Systems, L. C. Geiger and G. C. Schatz, *Chem. Phys.*, **79**, 431–448 (1983).

85. Plasmon Resonance Broadening in Spheroidal Metal Particles, W. A. Kraus and G. C. Schatz, *Chem. Phys. Lett.*, **99**, 353–357 (1983).

86. Plasmon Resonance Broadening in Small Metal Particles, W. A. Kraus and G. C. Schatz, *J. Chem. Phys.*, **79**, 6130–6139 (1983).

87. A Detailed Analysis of the Raman Enhancement Mechanisms Associated with the Interaction of a Raman Scatterer with a Resonant Metal Cluster: Results for $\text{Li}_n\text{-H}_2$. P. K. K. Pandey and G. C. Schatz, *J. Chem. Phys.*, **80**, 2959–2972 (1984).

88. A Quasiclassical Trajectory Study of Collisional Excitation in $\text{H} + \text{CO}$, L. C. Geiger and G. C. Schatz, *J. Phys. Chem.*, **88**, 214–221 (1984).

89. A Quasiclassical Trajectory Study of the State to State Dynamics of $\text{H} + \text{H}_2\text{O} \rightarrow \text{OH} + \text{H}_2$, G. C. Schatz, M. C. Colton and J. L. Grant, *J. Phys. Chem.*, **88**, 2971–2977 (1984).

90. Coupled Channel Distorted Wave Calculations for the Three Dimensional $\text{H} + \text{H}_2$ Reaction, G. C. Schatz, L. M. Hubbard, P. S. Dardi and W. H. Miller, *J. Chem. Phys.*, **81**, 231–240 (1984).

91. Theoretical Studies of Surface Enhanced Raman Scattering, G. C. Schatz, *Acc. Chem. Res.*, **17**, 370–376 (1984).

92. Semiclassical Vibrational Eigenvalues of Triatomic Molecules: Application of the FFT Method to SO_2 , H_2O , H_3^+ and CO_2 , C. W. Eaker and G. C. Schatz, *J. Chem. Phys.*, **81**, 2394–2399 (1984).

93. A Coupled States Quantum Reactive Scattering Study of $\text{H} + \text{D}_2 \rightarrow \text{HD} + \text{D}$ at $E_{\text{rel}} (\nu = j = 0) = 0.55 \text{ eV}$, G. C. Schatz, *Chem. Phys. Lett.*, **108**, 532–534 (1984).

94. Resonances in the Collisional Excitation of CO by Fast H Atoms, L. C. Geiger, G. C. Schatz and B. C. Garrett, In *Resonances in Electron-Molecule Scattering, Van der Waals Complexes, and Reactive Chemical Dynamics*, ACS Symposium Series 263, D. G. Truhlar, Ed., American Chemical Society, Washington, DC, 1984, pp 421–440.

95. Electromagnetic Theory Calculations for Spheroids: An Accurate Study of Particle Size Dependence of SERS and Hyper-Raman Enhancements, E. J. Zeman and G. C. Schatz, In *Dynamics on Surfaces*, Proceedings of the 17th Jerusalem

Symposium on Quantum Chemistry and Biochemistry, B. Pullman, Ed., Reidel, Dordrecht, Holland, 1984, pp 413–424.

96. Fourier Transform Methods for Calculating Action Variables and Semiclassical Eigenvalues for Coupled Oscillator Systems, C. W. Eaker, G. C. Schatz, N. DeLeon and E. J. Heller, *J. Chem. Phys.*, **81**, 5913–5919 (1984).

97. Theories of Time Dependent Chemical Phenomena, G. C. Schatz, *The Register of Phi Lambda Upsilon*, Vol. 69, 1984, pp 13–16.

98. A Quasiclassical Trajectory Study of the $H_2^+ + H_2 \rightarrow H_3^+ + H$ Reaction, C. W. Eaker and G. C. Schatz, *J. Phys. Chem.*, **89**, 2612–2620 (1985).

99. A Quasiclassical Trajectory Study of Collisions of Fast H Atoms with CO Using an Accurate *Ab Initio* Potential Energy Surface, L. C. Geiger, G. C. Schatz and L. B. Harding, *Chem. Phys. Lett.*, **114**, 520–525 (1985).

100. Theoretical Studies of Fast H Atom Collisions with NO, M. C. Colton and G. C. Schatz, *J. Chem. Phys.*, **83**, 3413–3425 (1985).

101. A Quantum Reactive Scattering Study of $Mu + H_2 \rightarrow MuH + H$, G. C. Schatz, *J. Chem. Phys.*, **83**, 3441–3448 (1985).

102. A Quasiclassical Trajectory Study of Vibrational Predissociation and Collisional Relaxation in Ar-OCS, L. L. Gibson and G. C. Schatz, *J. Chem. Phys.*, **83**, 3433–3440 (1985).

103. Recent Quantum Scattering Calculations on the H + H_2 Reaction and Its Isotopic Counterparts, G. C. Schatz, In *Theory of Chemical Reaction Dynamics*, Proceedings of NATO Workshop, Orsay, France, 1986, D. C. Clary, Ed., D. Reidel, Dordrecht, The Netherlands, 1986, pp 1–26.

104. A Coupled States Distorted Wave Study of the $O(^3P) + H_2$ (D_2 , HD, DH) Reaction, G. C. Schatz, *J. Chem. Phys.*, **83**, 5677–5686 (1985).

105. The FFT Method for Determining Semiclassical Eigenvalues: Application to Asymmetric Top Rigid Rotors, R. J. Duchovic and G. C. Schatz, *J. Chem. Phys.*, **84**, 2239–2246 (1986).

106. Test of Variational Transition State Theory and Multi-dimensional Semiclassical Transmission Coefficients 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 Isotope Effects, B. C. Garrett, D. G. Truhlar and G. C. Schatz, *J. Am. Chem. Soc.*, **108**, 2876–2881 (1986).

107. Future Directions for Supercomputer Use in Chemistry, G. C. Schatz, *Proceedings of Workshop on Supercomputers in Chemistry*, Evanston, IL, 1984, National Science Foundation, Washington, DC, 1985.

108. Simulation in Materials Science, George C. Schatz, *Information and Communications*, The National Academies Press, Washington, DC, 2003, pp 146–151.

109. Theoretical Studies of Vibrational Excitation in Collisions of $O(^3P)$ with $H_2O(^1A_1)$, M. J. Redmon, B. C. Garrett and G. C. Schatz, *J. Chem. Phys.*, **84**, 764–773 (1986).

110. A Coupled States Reactive Scattering Study of Bending Excited Resonances in Three Dimensional H + H_2 , M. C. Colton and G. C. Schatz, *Chem. Phys. Lett.*, **124**, 256–9 (1986).

111. A Coupled States Calculation of Accurate Quantum Rate Constants for H + H_2 , M. C. Colton and G. C. Schatz, *Int. J. Chem. Kinet.*, **18**, 961–975 (1986).

112. A Theoretical Study of Complex Formation, Isotope Effects and Energy Partitioning in the $O(^1D) + H_2(D_2, HD)$ Reaction, M. S. Fitzcharles and G. C. Schatz, *J. Phys. Chem.*, **90**, 3634–3644 (1986).

113. Tunnelling in Bimolecular Collisions, G. C. Schatz, *Chem. Rev.*, **87**, 81–89 (1987).

114. Quantum Reactive Scattering for A + BCD \rightarrow AB + CD Reactions: Coupled Channel Distorted Wave Theory, G. A. Natanson and G. C. Schatz, *J. Chem. Phys.*, **85**, 2038–2053 (1986).

115. The Formation of Highly Excited H_3^+ in the Reaction $H_2^+(v) + H_2 \rightarrow H_3^+ + H$, G. C. Schatz, J. K. Badenhoop and C. W. Eaker, *Int. J. Quantum Chem. Symp.*, **31**, 57–63 (1987).

116. A Surface Hopping Quasiclassical Trajectory Study of the $H_2^+ + H_2$ and $(H_2 + D_2)^+$ Systems, C. W. Eaker and G. C. Schatz, *Chem. Phys. Lett.*, **127**, 343–346 (1986).

117. The Rate Constants for the H + H_2 Reaction and Its Isotopic Analogs at Low Temperatures: Wigner Threshold Low Behavior, T. Takayanagi, N. Masaki, K. Nakamura, M. Okamoto, S. Sato and G. C. Schatz, *J. Chem. Phys.*, **86**, 6133–9 (1987).

118. Superminicomputer Accelerates Combustion Research, G. C. Schatz, *Res. Dev. Mag.*, **28**, 8, 68–70 (1986).

119. An Accurate Electromagnetic Theory Study of Surface Enhancement Factors for Ag, Au, Cu, Li, Na, Al, Ga, In, Zn and Cd, E. J. Zeman and G. C. Schatz, *J. Phys. Chem.*, **91**, 634–642 (1987).

120. A Centrifugal Sudden Distorted Wave Study of the Reaction $Cl + HCl \rightarrow ClH + Cl$: Product Rotational Distributions, G. C. Schatz, B. Amaee and J. N. L. Connor, *Chem. Phys. Lett.*, **132**, 1–5 (1986).

121. Phase Space Bottlenecks: A Comparison of Quantum and Classical Intramolecular Dynamics for Collinear OCS, L. L. Gibson, G. C. Schatz, M. A. Ratner and M. J. Davis, *J. Chem. Phys.*, **86**, 3263–3272 (1987).

122. A Quasiclassical Trajectory Study of Final State Distributions in Collisions of Fast H(D) Atoms with HF(DF), G. C. Schatz, *J. Chem. Phys.*, **86**, 6738–6744 (1987).

123. The Centrifugal Sudden Distorted Wave Method for Calculating Cross Sections for Chemical Reactions: Angular Distributions for $Cl + HCl \rightarrow ClH + Cl$, G. C. Schatz, B. Amaee and J. N. L. Connor, *Comput. Phys. Commun.*, **47**, 45–53 (1987).

124. A Surface Enhanced Resonance Raman Study of Cobalt Phthalocyanine on Rough Ag Films. Theory and Experiment, E. J. Zeman, K. T. Carron, G. C. Schatz and R. P. Van Duyne, *J. Chem. Phys.*, **87**, 4189–4200 (1987).

125. Metastable H_3^+ Formation and Decay in the Reaction of Highly Excited H_2^+ with H_2 , J. K. Badenhoop, G. C. Schatz, and C. W. Eaker, *J. Chem. Phys.*, **87**, 5317–5324 (1987).

126. State to State Chemistry with Fast Hydrogen Atoms: Reaction and Collisional Excitation in H + CO_2 , G. C. Schatz, M. S. Fitzcharles, and L. B. Harding, *Faraday Discuss. Chem. Soc.*, **84**, 359–369 (1987).

127. Dynamics of Heavy + Light-Heavy Atom Transfer Reactions: The Reaction $Cl + HCl \rightarrow ClH + Cl$, B. Amaee, J. N. L. Connor, J. C. Whitehead, W. Jakubetz and G. C. Schatz, *Faraday Discuss. Chem. Soc.*, **84**, 387–403 (1987).

128. A Centrifugal Sudden Distorted Wave Study of the $Cl + HCl$ Reaction: Results for a Scaled and Fitted *Ab Initio* Potential Surface Having a Non-Collinear Reaction Path, G. C. Schatz, B. Amaee and J. N. L. Connor, *J. Phys. Chem.*, **92**, 3190–3195 (1988).

129. Spatially Resolved Surface Enhanced Second Harmonic Generation: Theoretical and Experimental Evidence for Electrodynamic Enhancement in the Near Infrared on a Laser Microfabricated Pt Surface, K. L. Haller, L. A. Bumm, R. I.

Altkorn, E. J. Zeman, G. C. Schatz, and R. P. Van Duyne, *J. Chem. Phys.*, **90**, 1237–1252 (1989).

130. A Surface Enhanced Hyper-Raman Scattering Study of Pyridine Adsorbed on Silver: Experiment and Theory, J. T. Golab, J. R. Sprague, K. T. Carron, G. C. Schatz and R. P. Van Duyne, *J. Chem. Phys.*, **88**, 7942–51 (1988).

131. A Theoretical Study of the Oriented Reaction $\text{HBr} + \text{CO}_2 + h\nu \rightarrow \text{OH} + \text{CO} + \text{Br}$, G. C. Schatz and M. S. Fitzcharles, In *Selectivity in Chemical Reactions*, NATO ASI C245, J. C. Whitehead, Ed., Kluwer, Dordrecht, The Netherlands, 1988, pp 353–364.

132. Energies and Lifetimes of Predissociative States of van der Waals Molecules: Self-Consistent Field Calculations for $\text{I}_2(\text{v})\text{He}$, $\text{I}_2(\text{v})\text{Ne}$, G. C. Schatz, R. B. Gerber and M. A. Ratner, *J. Chem. Phys.*, **88**, 3709–3714 (1988).

133. State-Selective Studies of $\text{T} \rightarrow \text{R, V}$ Energy Transfer: The $\text{H} + \text{CO}$ System, G. K. Chawla, G. C. McBane, P. L. Houston and G. C. Schatz, *J. Chem. Phys.*, **88**, 5481–5488 (1988).

134. A Program for Determining Primitive Semiclassical Eigenvalues for Vibrating/Rotating Nonlinear Triatomic Molecules, G. C. Schatz, *Comput. Phys. Commun.*, **51**, 135–147 (1988).

135. Quantum Effects in Gas phase Bimolecular Chemical Reactions, G. C. Schatz, *Annu. Rev. Phys. Chem.*, **39**, 317–340 (1988).

136. Theoretical Studies of the Dynamics of Chemical Reactions, T. H. Dunning, Jr., L. B. Harding, A. F. Wagner, G. C. Schatz, and J. M. Bowman, *Science*, **240**, 453–459 (1988).

137. Theoretical Studies of Collisional Energy Transfer in Highly Excited Molecules: The Importance of Intramolecular Vibrational Redistribution in Successive Collision Modeling of $\text{He} + \text{CS}_2$, M. Bruehl and G. C. Schatz, *J. Chem. Phys.*, **89**, 770–779 (1988).

138. Quantum Reactive Scattering Using Hyperspherical Coordinates: Results for $\text{H} + \text{H}_2$ and $\text{Cl} + \text{HCl}$, G. C. Schatz, *Chem. Phys. Lett.*, **150**, 92–98 (1988).

139. Oscillating Reactivity and Resonances in the Three Dimensional $\text{Cl} + \text{HCl}$ Reaction, G. C. Schatz, *Chem. Phys. Lett.*, **151**, 409–14 (1988).

140. Theoretical Studies of Collisional Energy Transfer in Highly Excited Molecules: Temperature and Potential Surface Dependence of Relaxation in He , Ne , $\text{Ar} + \text{CS}_2$, M. Bruehl and G. C. Schatz, *J. Phys. Chem.*, **92**, 3190–95 (1988).

141. Collision Induced Dissociation of H_2^+ and D_2^+ with H_2 using a Surface Hopping Trajectory Method, C. W. Eaker and G. C. Schatz, *J. Chem. Phys.*, **89**, 6713–6718 (1988).

142. The Analytic Representation of Potential Energy Surfaces for Chemical Reactions, G. C. Schatz, In *Advances in Molecular Electronic Structure Theory (Vol. 1): Calculation and Characterization of Potential Energy Surfaces*, T. H. Dunning, Jr., Ed., JAI Press, Greenwich, CT, 1990, pp 85–127.

143. The Analytical Representation of Electronic Potential Energy Surfaces, G. C. Schatz, *Rev. Mod. Phys.*, **61**, 669–688 (1989).

144. A Three Dimensional Reactive Scattering Study of the Photodetachment Spectrum of ClHCl^- , G. C. Schatz, *J. Chem. Phys.*, **90**, 3582–9 (1989).

145. Spectroscopy of High Vibrational Levels of the N-N Stretching Mode of N-N- ^{16}O and N-N- ^{18}O , N. L. S. Yamasaki, C. Manzanares, L. C. Baylor, G. C. Schatz, and E. Weitz, *J. Phys. Chem.*, **93**, 2204–9 (1989).

146. A Three Dimensional Quantum Reactive Scattering Study of the $\text{I} + \text{HI}$ Reaction and of the IHI^- Photodetachment Spectrum, G. C. Schatz, *J. Chem. Phys.*, **90**, 4847–4854 (1989).

147. A Reduced Dimensionality Quantum Reactive Scattering Study of the Insertion Reaction $\text{O}(^1\text{D}) + \text{H}_2 \rightarrow \text{OH} + \text{H}$, J. K. Badenhoop, H. Koizumi and G. C. Schatz, *J. Chem. Phys.*, **91**, 142–9 (1989).

148. Rotational Distributions in the Photodetachment of IHI^- and in the $\text{I} + \text{HI}$ Reaction: The influence of IHI Transition State Resonances, G. C. Schatz, *Isr. J. Chem.*, **29**, 361–7 (1989).

149. A Coupled Channel Quantum Scattering Study of Alignment Effects in $\text{Na}(^2\text{P}_{3/2}) + \text{He} \rightarrow \text{Na}(^2\text{P}_{1/2}) + \text{He}$ Collisions, G. C. Schatz, L. J. Kovalenko and S. R. Leone, *J. Chem. Phys.*, **91**, 6961–72 (1989).

150. Transition State Resonances in Collinear $\text{O}(^2\text{P}) + \text{HCl} \rightarrow \text{OH} + \text{Cl}$, H. Koizumi and G. C. Schatz, *Int. J. Quantum Chem.*, **23**, 137–45 (1989).

151. Nonadiabatic Effects in Photodissociation Dynamics: A Quantum Mechanical Study of ICN Photodissociation in the A Continuum, H. Guo and G. C. Schatz, *J. Chem. Phys.*, **92**, 1634–42 (1990).

152. A Centrifugal Sudden Distorted Wave Study of the $\text{Cl} + \text{HCl} \rightarrow \text{ClH} + \text{Cl}$ Reaction Using a “Tight-Bend” Potential Energy Surface, G. C. Schatz, B. Amaee, and J. N. L. Connor, *J. Chem. Phys.*, **92**, 4893–8 (1990).

153. Reduced-Dimensionality Quantum Calculations of the Thermal Rate Coefficient for the $\text{Cl} + \text{HCl} \rightarrow \text{ClH} + \text{Cl}$ Reaction: Comparison with Centrifugal-Sudden Distorted-Wave, Coupled Channel Hyperspherical, and Experimental Results, Q. Sun, J. M. Bowman, G. C. Schatz, J. R. Sharp and J. N. L. Connor, *J. Chem. Phys.*, **92**, 1677–86 (1990).

154. A Three-Dimensional Quantum Reactive Scattering Study of the $\text{I} + \text{DI}$ Reaction and of the IDI^- Photodetachment Spectrum, G. C. Schatz, *J. Chem. Soc., Faraday Trans.*, **86**, 1729–35 (1990).

155. Three Dimensional Quantum Scattering Studies of Transition State Resonances: Results for $\text{O} + \text{HCl} \rightarrow \text{OH} + \text{Cl}$, H. Koizumi and G. C. Schatz, In *Molecular Vibrations (Vol. IA)*, J. M. Bowman and M. A. Ratner, Eds., JAI Press, Greenwich, CT, 1990, pp 139–164.

156. The Evolution of Vibrational phase Space During the Collisional Relaxation of Highly Excited CS_2 , M. Bruehl and G. C. Schatz, *J. Chem. Phys.*, **92**, 6561–6573 (1990).

157. Quantum Theory of Photodetachment Spectra of Transition States, G. C. Schatz, *J. Phys. Chem.*, **94**, 6157–6164 (1990).

158. Time-dependent Dynamics of Methyl Iodide Photodissociation in the First Continuum, H. Guo and G. C. Schatz, *J. Chem. Phys.*, **93**, 393–402 (1990).

159. A Centrifugal Sudden Distorted Wave Study of Isotope Effects for the Reactions $\text{Cl} + \text{HCl} \rightarrow \text{ClH} + \text{Cl}$ and $\text{Cl} + \text{DCI} \rightarrow \text{CID} + \text{Cl}$, G. C. Schatz, B. Amaee and J. N. L. Connor, *J. Chem. Phys.*, **93**, 5544 (1990).

160. A Reduced Dimension Quantum Wavepacket Study of Photodissociation Dynamics of Diatomic Molecules on Surfaces, H. Guo and G. C. Schatz, *J. Chem. Phys.*, **94**, 379–387 (1991).

161. Observation of Highly Energetic Collisions in Classical Trajectory Studies of Collisional Energy Transfer, G. Lendvay and G. C. Schatz, *J. Phys. Chem.*, **94**, 8864–66 (1990).

162. Polarized Resonance Raman Spectrum as a Probe of Nonadiabatic Transitions in Photodissociation: A Theoretical Treatment, H. Guo and G. C. Schatz, *J. Phys. Chem.*, **95**, 3091–96 (1991).

163. Collisional Excitation of CO by 2.3 eV H Atoms, G. C. McBane, S. H. Kable, P. L. Houston and G. C. Schatz, *J. Chem. Phys.*, **94**, 1141–1149 (1991).
164. Influence of Transition State Resonances on Integral Cross Sections and Product Rovibrational Distributions for the $\text{Cl} + \text{HCl} \rightarrow \text{ClH} + \text{Cl}$ Reaction, G. C. Schatz, D. Sokolovski, and J. N. L. Connor, *J. Chem. Phys.*, **94**, 4311–19 (1991).
165. Resonances in Heavy + Light-Heavy Atom Reactions: Influence on Differential and Integral Cross Sections and on Transition State Photodetachment Spectra, G. C. Schatz, D. Sokolovski, and J. N. L. Connor, *Faraday Discuss. Chem. Soc.*, **91**, 17–30 (1991).
166. A Quasiclassical Trajectory Study of $\text{H} + \text{CO}_2 \rightarrow \text{OH} + \text{CO}$: Bulk Reaction Dynamics and the Effect of Van der Waals Precursor Formation, K. Kudla and G. C. Schatz, *J. Phys. Chem.*, **95**, 8267–73 (1991).
167. Quantum Nonadiabatic Effects in the Photodissociation of Vibrationally Excited CH_3I , H. Guo, K. Q. Lao, G. C. Schatz and A. D. Hammerich, *J. Chem. Phys.*, **94**, 6562–8 (1991).
168. A Quasiclassical Trajectory Study of the $\text{OH} + \text{CO}$ Reaction, K. Kudla, G. C. Schatz, and A. F. Wagner, *J. Chem. Phys.*, **95**, 1635–47 (1991).
169. A Coupled Channel Study of HN_2 Unimolecular Decay Based on a Global *Ab Initio* Potential Surface, H. Koizumi, G. C. Schatz, and S. P. Walch, *J. Chem. Phys.*, **95**, 4130–35 (1991).
170. A Mechanism for the Quenching of I^* in Photodissociation of Methyl Iodide on an MgO Surface, H. Guo and G. C. Schatz, *Chem. Phys. Lett.*, **184**, 245–250 (1991).
171. HN_2 and DN_2 Resonance Spectra: Scattering and Stabilization Calculations, H. Koizumi, G. C. Schatz, and J. M. Bowman, In *Isotope Effects in Gas-Phase Chemistry*, J. A. Kaye, Ed., ACS Symposium Series, No. 502, American Chemical Society, Washington, DC, 1992, pp 37–47.
172. Energy Dependence of Energy Transfer in Collisional Relaxation of Vibrationally Highly Excited CS_2 , G. Lendvay and G. C. Schatz, *J. Phys. Chem.* **95**, 8748–53 (1991).
173. An Analytical Representation of the Lowest Potential Energy Surface for the Reaction $\text{O}(^3\text{P}) + \text{HCl}(X1\Sigma) \rightarrow \text{OH}(X2\Pi) + \text{Cl}(^2\text{P})$, H. Koizumi, G. C. Schatz, and M. S. Gordon, *J. Chem. Phys.* **95**, 6421–28 (1991).
174. A Reduced Dimension Quantum Reactive Scattering Study of $\text{OH} + \text{CO} \rightarrow \text{H} + \text{CO}_2$, G. C. Schatz and J. Dyck, *Chem. Phys. Lett.*, **188**, 11–15 (1992).
175. Trajectory Studies of Collisional Relaxation of Highly Excited CS_2 by H_2 , CO , HCl , CS_2 and CH_4 , G. Lendvay and G. C. Schatz, *J. Chem. Phys.*, **96**, 4356–65 (1992).
176. A Quasiclassical Trajectory Study of OH Rotational Excitation in $\text{OH} + \text{CO}$ Collisions Using *Ab Initio* Potential Surfaces, K. Kudla, A. G. Koures, L. B. Harding and G. C. Schatz, *J. Chem. Phys.*, **96**, 7465–73 (1992).
177. A Quantum Scattering Study of the $\text{Cl} + \text{HCl} \rightarrow \text{ClH} + \text{H}$ Reaction: Centrifugal Sudden Hyperspherical Differential and Integral Cross Sections, Product Distributions and Rate Coefficients, G. C. Schatz, D. Sokolovski and J. N. L. Connor, In *Advances in Molecular Vibrations and Collision Dynamics: Quantum Reactive Scattering, Vol. IIB*, J. M. Bowman, Ed., JAI Press, Greenwich, CT, 1994, pp 1–26.
178. Comparison of Quasiclassical and Quantum Dynamics for Resonance Scattering in the $\text{Cl} + \text{HCl} \rightarrow \text{ClH} + \text{Cl}$ Reaction, W. Jakubetz, D. Sokolovski, J. N. L. Connor and G. C. Schatz, *J. Chem. Phys.*, **97**, 6451–9 (1992).
179. Choice of Gas Kinetic Rate Coefficients in the Vibrational Relaxation of Highly Excited Polyatomic Molecules, G. Lendvay and G. C. Schatz, *J. Phys. Chem.*, **96**, 3752–6 (1992).
180. A Quasiclassical Trajectory Study of Bond Specific Chemistry in the Reaction $\text{H} + \text{HOD} \rightarrow \text{H}_2 + \text{OD}$, $\text{HD} + \text{OH}$, K. Kudla and G. C. Schatz, *Chem. Phys. Lett.*, **193**, 507–11 (1992).
181. Critical Comparison of Approximate and Accurate Quantum Mechanical Calculations of Reaction Rates for a Model Activated Reaction in Solution, R. P. McRae, G. K. Schenter, B. C. Garrett, G. R. Haynes, G. A. Voth and G. C. Schatz, *J. Chem. Phys.*, **97**, 7392–7404 (1992).
182. *Ab Initio* and Semiempirical Molecular Orbital Studies of Surface Enhanced and Bulk HyperRaman Scattering from Pyridine, W.-H. Yang and G. C. Schatz, *J. Chem. Phys.*, **97**, 3831–45 (1992).
183. Comment on: Time-dependent Hartree Approximation Applied to the Photodissociation of ICN, H. Guo and G. C. Schatz, *J. Chem. Phys.*, **97**, 7853–4 (1992).
184. Time Dependent Methods for Calculating Thermal Rate Coefficients using Flux Correlation Functions, M. Thachuk and G. C. Schatz, *J. Chem. Phys.*, **97**, 7297–7313 (1992).
185. Electromagnetic mechanism of surface enhanced spectroscopy, G. C. Schatz and R. P. Van Duyne, In *Handbook of Vibrational Spectroscopy*, J. M. Chalmers and P. R. Griffiths, Eds., John Wiley & Sons, Ltd., New York, 2002, Vol. 1, pp 759–774.
186. *Ab Initio* Electronic Structure Calculations of Stationary Points and Barrier Heights for the ClHCl and HCl_2 Systems, M. A. Vincent, J. N. L. Connor, M. S. Gordon and G. C. Schatz, *Chem. Phys. Lett.*, **203**, 415–22 (1993).
187. *Ab Initio* Potential Energy Surface for IHI^- : Simulation of IHI^- Photodetachment Spectra, G. C. Schatz, S. Florance, T. J. Lee and C. W. Bauschlicher, Jr., *Chem. Phys. Lett.*, **202**, 495–500 (1993).
188. Collisional Energy Transfer from Highly Excited SF_6 , G. Lendvay and G. C. Schatz, *J. Chem. Phys.*, **98**, 1034–41 (1993).
189. Theoretical Studies of Energy Transfer and Reaction in $\text{H} + \text{H}_2\text{O}$ and $\text{H} + \text{D}_2\text{O}$ Collisions, K. Kudla and G. C. Schatz, *J. Chem. Phys.*, **98**, 4644–51 (1993).
190. Theoretical Studies of the Reactions $\text{H} + \text{CH} \rightarrow \text{C} + \text{H}_2$ and $\text{C} + \text{H}_2 \rightarrow \text{CH}_2$ Using an *Ab Initio* Global Ground State Potential Surface for CH_2 , L. B. Harding, R. Guadagnini and G. C. Schatz, *J. Phys. Chem.*, **97**, 5472–81 (1993).
191. Nearside-farside Analysis of Angular Scattering in Elastic, Inelastic and Reactive Molecular Collisions, J. N. L. Connor, P. McCabe, D. Sokolovski and G. C. Schatz, *Chem. Phys. Lett.*, **206**, 119–122 (1993).
192. A Quasiclassical Trajectory Study of Mode Specific Reaction Dynamics in the $\text{Cl} + \text{HOD}$ and $\text{H} + \text{HOD}$ Reactions, K. Kudla and G. C. Schatz, *Chem. Phys.*, **175**, 71–82 (1993).
193. Quantum and Quasiclassical Calculations on the $\text{OH} + \text{CO} \rightarrow \text{CO}_2 + \text{H}$ Reaction, D. C. Clary and G. C. Schatz, *J. Chem. Phys.*, **99**, 4578–89 (1993).
194. Evaluation of Thermal Rates for Reactions with Intermediate Wells: Removal of Bound State Contributions to Quantum Flux Correlation Functions, M. Thachuk, H. R. Mayne and G. C. Schatz, *J. Chem. Phys.*, **99**, 3516–25 (1993).
195. A Coupled Channel Hyperspherical Scattering Study of the $\text{Cl} + \text{HCl} \rightarrow \text{ClH} + \text{Cl}$ Reaction: Cumulative and State-Selected Probabilities, Integral Cross Sections and Product Rotational Distributions, G. C. Schatz, D. Sokolovski and J. N. L. Connor, *Can. J. Chem.*, **72**, 903–8 (1994).
196. Classical Trajectory Methods for Studying Energy Transfer from Highly Vibrationally Excited Molecules, G. Lendvay and G. C. Schatz, In *Vibrational Energy Transfer*

Involving Large and Small Molecules, Advances in Chemical Kinetics and Dynamics, Vol. 2B, J. A. Barker, Ed., JAI Press, Greenwich, CT, 1995, pp 481–513.

197. Product State Distributions in Chemical Reactions: The Reaction $\text{OH} + \text{CO} \rightarrow \text{H} + \text{CO}_2$, K. Kudla and G. C. Schatz, In *The Chemical Dynamics and Kinetics of Small Radicals*, K. Liu and A. F. Wagner, Eds., World Scientific, Singapore, 1995, pp 438–465.

198. Surface-Enhanced Second-Harmonic Diffraction: Selective Enhancement by Spatial Harmonics, A. C. R. Pipino and G. C. Schatz, *Phys. Rev. B*, **49**, 8320–8330 (1994).

199. Transition States of Chemical Reactions, G. C. Schatz, *Science*, **262**, 1828–9 (1993).

200. A Quasiclassical Trajectory Study of Product Energy and Angular Distributions in $\text{OH} + \text{H}_2(\text{D}_2)$, K. S. Bradley and G. C. Schatz, *J. Phys. Chem.*, **98**, 3788–95 (1994).

201. Differential Cross Sections for Fine Structure Transitions in $\text{O}(^3\text{P}_2) + \text{Ar}$ Collisions, Z. Ma, K. Liu, L. B. Harding, M. Komotos, and G. C. Schatz, *J. Chem. Phys.*, **100**, 8026–39 (1994).

202. Surface Profile Dependence of Photon/Plasmon-Polariton Coupling at a Corrugated Silver Surface, A. R. C. Pipino and G. C. Schatz, *J. Opt. Soc. Am. B*, **11**, 2036–45 (1994).

203. Comparison of Master Equation and Trajectory Simulation of the Relaxation of an Ensemble of Highly Vibrationally Excited Molecules, G. Lendvay and G. C. Schatz, *J. Phys. Chem.*, **98**, 6530–6 (1994).

204. Experimental and Theoretical Study of the $\text{O} + \text{HCl}$ Transition State Region by Photodetachment of OHCl^- , M. J. Davis, H. Koizumi, G. C. Schatz, S. E. Bradforth and D. M. Neumark, *J. Chem. Phys.*, **101**, 4708–21 (1994).

205. Evaluation of Resonance Contributions to Thermal Reaction Rates Using Quantum Flux Correlation Functions, M. Thachuk and G. C. Schatz, *J. Chem. Phys.*, **101**, 6577–85 (1994).

206. Global Potential Energy Surfaces for the Lowest $^1\text{A}'$, $^3\text{A}''$ and $^2\text{A}''$ States of HNO , R. Guadagnini, G. C. Schatz and S. P. Walch, *J. Chem. Phys.*, **102**, 774–83 (1995).

207. Quasiclassical Trajectory Studies of $\text{N} + \text{OH}$, $\text{O} + \text{NH}$ and $\text{H} + \text{NO}$ Collisions using Global *Ab Initio* Potential Energy Surfaces, R. Guadagnini, G. C. Schatz, and S. P. Walch, *J. Chem. Phys.*, **102**, 784–91 (1995).

208. Quasiclassical Trajectory Studies of State Resolved Bimolecular Reactions: Vibrational Distributions in Triatomic Products, G. C. Schatz, *J. Phys. Chem.*, **99**, 516–24 (1995).

209. The Influence of Atomic Fine-Structure on Bimolecular Rate Constants: The $\text{Cl}(^2\text{P}) + \text{HCl}$ Reaction, G. C. Schatz, *J. Phys. Chem.*, **99**, 7522–29, 1995.

210. Quantum Dynamics of a Planar Model for the Complex Forming $\text{OH} + \text{CO} \rightarrow \text{H} + \text{CO}_2$ Reaction, E.M. Goldfield, S. K. Gray and G. C. Schatz, *J. Chem. Phys.*, **102**, 8807–17 (1995).

211. New Uniform Semiclassical Theory of Resonance Angular Scattering for Reactive Molecular Collisions, D. Sokolovski, J. N. L. Connor and G. C. Schatz, *Chem. Phys. Lett.*, **238**, 127–131 (1995).

212. A Theoretical Study of the $\text{NH} + \text{NO}$ Reaction, K. S. Bradley, P. McCabe, G. C. Schatz, and S. P. Walch, *J. Chem. Phys.*, **102**, 6696–705 (1995).

213. Theoretical Studies of Polyatomic Bimolecular Reaction Dynamics, J. M. Bowman and G. C. Schatz, *Annu. Rev. Phys. Chem.* **46**, 169–95 (1995).

214. A Rigorous Electrodynamical Model for Periodic Structure Formation During UV-laser-induced Metal Atom Deposition,

A. C. R. Pipino, G. C. Schatz and R. P. Van Duyne, *Chem. Phys. Lett.* **237**, 137–44, 1995.

215. Complex Angular Momentum Analysis of Resonance Scattering in the $\text{Cl} + \text{HCl} \rightarrow \text{ClH} + \text{Cl}$ Reaction, D. Sokolovski, J. N. L. Connor and G. C. Schatz, *J. Chem. Phys.*, **103**, 5979–98 (1995).

216. Discrete Dipole Approximation for Calculating Absorption and Raman Intensities for Small Particles with Arbitrary Shapes, W.-H. Yang, G. C. Schatz and R. P. Van Duyne, *J. Chem. Phys.*, **103**, 869–75 (1995).

217. RRKM Studies of Product Branching in the $\text{NH} + \text{NO}$ Reaction, M. Simonson, K. S. Bradley and G. C. Schatz, *Chem. Phys. Lett.* **244**, 19–26 (1995).

218. Scattering Theory and Dynamics: Time-Dependent and Time-Independent Methods, G. C. Schatz, *J. Phys. Chem.*, **100**, 12839–47 (1996).

219. Surface-enhanced Second Harmonic Diffraction: Experimental Investigation of Selective Enhancement, A. C. R. Pipino, R. P. Van Duyne and G. C. Schatz, *Phys. Rev. B*, **53**, 4162–9 (1996).

220. Potential Energy Surface and Quasiclassical Trajectory Studies of the $\text{H}_2 + \text{CN}$ Reaction, M. ter Horst, G. C. Schatz, and L. B. Harding, *J. Chem. Phys.*, **105**, 558–71 (1996).

221. Mode-Specific Chemistry in the $\text{H} + \text{HCN}$ and $\text{H} + \text{N}_2\text{O}$ Reactions, M. ter Horst, K. S. Bradley and G. C. Schatz, in *Gas phase Chemical Reaction Systems*, Springer Series in Chemical Physics 61, J. Wolfrum, H.-R. Volpp, R. Rannacher, and J. Warnatz, Eds., Springer, Berlin, 1996, pp 144–154.

222. Optimized Surfaces for Second Harmonic Generation from Surface-Plasmon Polaritons: Theory and Experiment, A. C. R. Pipino, R. P. Van Duyne and G. C. Schatz, *Proc. SPIE*, **2622**, 254–61 (1995).

223. A Surface-Enhanced Hyper-Raman and Surface-Enhanced Raman Scattering Study of trans-1,2-bis(4 pyridyl) ethylene adsorbed onto Silver Film over Nanosphere Electrodes: Vibrational Assignments - Experiment and Theory, W-H Yang, J. Hulteen, G. C. Schatz and R. P. Van Duyne, *J. Chem. Phys.* **104**, 4313–23 (1996).

224. Centrifugal-sudden hyperspherical study of $\text{Cl} + \text{HCl} \rightarrow \text{ClH} + \text{Cl}$ reaction dynamics on “tight-bend” and “loose-bend” potential energy surfaces, D. Sokolovski, J. N. L. Connor and G. C. Schatz, *Chem. Phys.*, **207**, 461–76 (1996).

225. Approximate Quantum Scattering Studies of the $\text{CN} + \text{H}_2$ Reaction, T. Takayanagi, M. Ter Horst and G. C. Schatz, *J. Chem. Phys.*, **105**, 2309–16 (1996).

226. The Product Vibrational, Rotational and Translational Energy Distribution for the Reaction $\text{O}(^3\text{P}_j) + \text{O}_3 \rightarrow 2\text{O}_2$: Evidence for an O_4 Complex, J. A. Mack, Y. Huang, A. Wodtke, and G. C. Schatz, *J. Chem. Phys.*, **105**, 7495–7503 (1996).

227. A Quasiclassical Trajectory Study of $\text{H} + \text{N}_2\text{O}(v_1, v_2, v_3)$, K. S. Bradley and G. C. Schatz, *J. Phys. Chem.*, **100**, 12154–61 (1996).

228. Unusual Insertion Mechanism in the Reaction $\text{C}(^3\text{P}) + \text{H}_2 \rightarrow \text{CH} + \text{H}$, R. Guadagnini and G. C. Schatz, *J. Phys. Chem.*, **100**, 18944–49 (1996).

229. Theoretical Studies of Collisional Relaxation of Highly Excited SO_2 in an Ar Bath, G. Lendvay, G. C. Schatz and L. B. Harding, *Faraday Discuss. Chem. Soc.*, **102**, 389–403 (1995) (published in 1997).

230. Structural Information from Ion Mobility Measurements: Effects of the Long-Range Potential, M. F. Mesleh, J. M. Hunter, A. A. Shvartsburg, G. C. Schatz and M. F. Jarrold, *J. Phys. Chem.*, **100**, 16082–86 (1996).

231. A Global H₂O Potential Energy Surface for the Reaction O(¹D) + H₂ → OH + H, T.-S. Ho, T. Hollebeek, H. Rabitz, L. B. Harding and G. C. Schatz, *J. Chem. Phys.*, **105**, 10472–86 (1996).
232. Formulation of the Double Differential and other Cross Sections for the ClHCl[−] Photodetachment Process, G. G. Balint-Kurti and G. C. Schatz, *J. Chem. Soc., Faraday Trans.*, **93**, 755–64 (1997).
233. Coupled Potential Energy Surfaces and Quantum Reactive Scattering for the Cl(²P) + HCl → ClH + Cl(²P) Reaction, C. S. Maierle, G. C. Schatz, M. S. Gordon, P. M. McCabe, and J. N. L. Connor, *J. Chem. Soc., Faraday Trans.*, **97**, 709–20 (1997).
234. Quantum Scattering Studies of Collisional Energy Transfer from Highly Excited Polyatomic Molecules: Classical/Quantum Comparisons for Collinear He + CS₂, G. C. Schatz and G. Lendvay, *J. Chem. Phys.*, **106**, 3548–57 (1997).
235. Quantum reactive scattering studies of the CN + H₂ → HCN + H reaction: the role of the nonreactive CN bond, T. Takayanagi and G. C. Schatz, *Chem. Phys. Lett.*, **265**, 410–417 (1997).
236. Reaction Dynamics Calculations for the Reaction CN + H₂ → HCN + H: Applications of the Rotating-Bond Approximation, T. Takayanagi and G. C. Schatz, *J. Chem. Phys.*, **106**, 3227–36 (1997).
237. A Quasiclassical Trajectory Study of Product State Distributions from the CN + H₂ → HCN + H Reaction, G. A. Bethardy, A. F. Wagner, G. C. Schatz and M. A. ter Horst, *J. Chem. Phys.*, **106**, 6001–15 (1997).
238. Quantum Scattering Studies of Collisional Energy Transfer from Highly Excited Polyatomic Molecules: A Bend–Stretch Model of He + CS₂, G. Lendvay and G. C. Schatz, *Ber. Bunsen-Ges. Phys. Chem.*, **101**, 587–94 (1997).
239. Quasiclassical Trajectory Studies of H(D) + HF(DF) Collisions at 2 eV, G. C. Schatz, *J. Chem. Phys.* **106**, 2277 (1997).
240. A Quasiclassical Trajectory Study of H + CO₂: Angular and Translational Distributions, and OH angular momentum alignment, K. S. Bradley and G. C. Schatz, *J. Chem. Phys.*, **106**, 8464–72 (1997).
241. Mobilities of Carbon Cluster Ions: Critical Importance of the Molecular Attractive Potential, A. A. Shvartsburg, G. C. Schatz, M. F. Jarrold, *J. Chem. Phys.*, **108**, 2416–23 (1998).
242. Dynamics of Highly Excited States in Chemistry: An Overview, A. S. Mullin and G. C. Schatz, In *Highly Excited Molecules: Relaxation, Reaction and Structure*, ACS Symposium Series No. 678, A. S. Mullin and G. C. Schatz, Eds., American Chemical Society, Washington, DC, 1997, pp 1–24.
243. Quantum Scattering Studies of Collisional Energy Transfer from Highly Excited Polyatomic Molecules: Collinear He + CS₂ at Energies up to 92 kcal/mol, G. Lendvay, G. C. Schatz and T. Takayanagi, In *Highly Excited Molecules: Relaxation, Reaction and Structure*, ACS Symposium Series No. 678, A. S. Mullin and G. C. Schatz, Eds., American Chemical Society, Washington, DC, 1997, pp 202–219.
244. Experimental and Theoretical Angular and Translational Distributions for the Reaction CN + D₂ → DCN + D, Jeng-Han Wang, Kopin Liu, G. C. Schatz and M. Ter Horst, *J. Chem. Phys.*, **107**, 7869 (1997).
245. Photoinitiated Reaction Dynamics Between Aligned Adsorbates on Solid Surfaces: A Theoretical Exploration of the H + CO₂ System on LiF(001), Josie V. Setzler, Hua Guo, and G. C. Schatz, *J. Phys. Chem. B*, **101**, 5352–61 (1997).
246. A global A-state potential surface for H₂O: Influence of excited states on the O(¹D) + H₂ reaction, G. C. Schatz, A. Papaioannou, L. A. Pederson, L. B. Harding, T. Hollebeek, T.-S. Ho, and H. Rabitz, *J. Chem. Phys.*, **107**, 2340–50 (1997).
247. Computational Methods for Polyatomic Bimolecular Reactions, G. C. Schatz, M. ter Horst and T. Takayanagi, In *Modern Methods for Multidimensional Dynamics Computations in Chemistry*, D. L. Thompson, Ed., World Scientific, Singapore, 1998, pp 1–33.
248. Automatic Potential Energy Surface Generation Directly from ab initio Calculations Using Shepard Interpolation: A Test Calculation for the H₂ + H System, T. Ishida and G. C. Schatz, *J. Chem. Phys.*, **107**, 3558–68 (1997).
249. Quantum Effects in Gas phase Bimolecular Collision Processes: From State-to-State Properties to Microcanonical Averages, G. C. Schatz, In *Comparisons of Classical and Quantum Dynamics*, Advances in Classical Trajectory Methods, Vol. III, W. L. Hase, Ed., JAI Press, Greenwich CT, 1998, pp 205–229.
250. Adiabatic and Nonadiabatic Dynamics Studies of O(¹D) + H₂ → OH + H, G. C. Schatz, L. A. Pederson and P. J. Kuntz, *Faraday Discuss. Chem. Soc.*, **108**, 357–74 (1997).
251. A further theoretical exploration of the surface-aligned photoinitiated H + CO₂ reaction: Surface motion and temperature dependence, J. V. Setzler, J. Bechtel, H. Guo and G. C. Schatz, *J. Chem. Phys.* **107**, 9176–84 (1997).
252. Structures of the Clusters Produced by Laser Desorption of Fullerenes: [2 + 2] Cycloadducts of Pre-Shrunk Cages, A. A. Shvartsburg, L. A. Pederson, R. R. Hudgins, G. C. Schatz, and M. F. Jarrold, *J. Phys. Chem.*, **102**, 7919–23 (1998).
253. Quantum Scattering Studies of Spin–Orbit Effects in the Cl(²P) + HCl → ClH + Cl(²P) Reaction, G. C. Schatz, P. McCabe and J. N. L. Connor, *Faraday Discuss. Chem. Soc.*, **110**, 139–157 (1998).
254. Vibrational Predissociation Rates and Final State Distributions for He-ICl and He-I₂ Using a Computationally Simple Method, Jeonghee Seong, Hosung Sun, Mark A. Ratner, George C. Schatz, and R. B. Gerber, *J. Phys. Chem.*, **102**, 9345–52 (1998).
255. Ab initio and RRKM Studies of the reactions of C, CH and ¹CH₂ with acetylene, R. Guadagnini, G. C. Schatz, and S. P. Walch, *J. Phys. Chem.*, **A102**, 5857–66 (1998).
256. A Quasiclassical Trajectory Study of H + H₂O → OH + H₂: Angular Distributions and OH Angular Momentum Alignment, Kimberly S. Bradley and George C. Schatz, *J. Chem. Phys.*, **108**, 7994–8003 (1998).
257. A Combined Experimental and Theoretical Study of the Simplest Nitrogen Atom Reaction, M. Alagia, N. Balucani, L. Cartechini, P. Casavecchia, G. G. Volpi, L. A. Pederson, G. C. Schatz, G. Lendvay, L. B. Harding, T. Hollebeek, T.-S. Ho, H. Rabitz, *J. Chem. Phys.*, **110**, 8857–60 (1999).
258. Calculating Dipole and Quadrupole Polarizabilities Relevant to Surface Enhanced Raman Spectroscopy, Gary S. Kedziora and George C. Schatz, *Spectrochim. Acta*, **A55**, 625–638 (1999).
259. Monte Carlo sampling methods for determining potential energy surfaces using Shepard interpolation. The O(¹D) + H₂ system. T. Ishida and G. C. Schatz, *Chem. Phys. Lett.*, **298**, 285–92 (1998).
260. Coupled *ab initio* potential energy surfaces for the reaction Cl(²P) + HCl → ClH + Cl(²P) A. J. Dobbyn, J. N. L. Connor, N. A. Besley, P. J. Knowles and G. C. Schatz, *Phys. Chem. Chem. Phys.*, **1**, 957–966 (1999).

261. Nanosphere lithography: Surface plasmon resonance spectrum of a periodic array of silver nanoparticles by UV-vis extinction spectroscopy and electrodynamic modeling, T. R. Jensen, G. C. Schatz and R. P. Van Duyne, *J. Phys. Chem.*, **B103**, 2394–2401 (1999).
262. Reactive and inelastic collisions of H atoms with vibrationally excited water molecules, G. Lendvay, K. S. Bradley and G. C. Schatz, *J. Chem. Phys.*, **110**, 2963–70 (1999).
263. Helicity decoupled quantum dynamics and capture model cross sections and rate constants for $O(^1D)+H_2 \rightarrow OH + H$, S. K. Gray, E. M. Goldfield, G. C. Schatz and G. G. Balint-Kurti, *Phys. Chem. Chem. Phys.*, **1**, 1141–1148 (1999).
264. Nanosphere lithography: effect of the external dielectric medium on the surface plasmon resonance spectrum of a periodic array of silver nanoparticles, T. R. Jensen, M. L. Duval, K. L. Kelly, A. Lazarides, G. C. Schatz and R. P. Van Duyne, *J. Phys. Chem.*, **103**, 9846–53 (1999).
265. Perspective on “Exchange Reactions with Activation Energy. I. Simple Barrier Potential for (H, H₂)” M. Karplus, R. N. Porter and R. D. Sharma, *J. Chem. Phys.* **43**, 3259–87 (1965); George C. Schatz, *Theor. Chem. Acc.*, **103**, 270–272 (2000).
266. Wavepacket Methods for the Direct Calculation of Energy Transfer Moments in Molecular Collisions. Kimberly S. Bradley, George C. Schatz, and Gabriel G. Balint-Kurti, *J. Phys. Chem.*, **103**, 947–952 (1999).
267. Potential energy surface and quasiclassical trajectory studies of the $N(^2D) + H_2$ Reaction, L. A. Pederson, G. C. Schatz, T-S Ho, T. Hollebeek, H. Rabitz, L. B. Harding and G. Lendvay, *J. Chem. Phys.*, **110**, 9091–100 (1999).
268. Reaction of H with Highly Vibrationally Excited Water: Activated or Not?, G. C. Schatz, G. Wu, G. Lendvay, De-Cai Fang and L. B. Harding, *Faraday Discuss. Chem. Soc.*, **113**, 151–66 (1999).
269. Quantum Scattering Study of Electronic Coriolis and Nonadiabatic Coupling Effects in $O(^1D) + H_2 \rightarrow OH + H$, K. Drukker and G. C. Schatz, *J. Chem. Phys.*, **111**, 2451–63 (1999).
270. Electrostatics of Noble Metal Nanoparticles and Nanoparticle Clusters, T. Jensen, L. Kelly, A. Lazarides and G. C. Schatz, *J. Cluster Sci.*, **10**, 295–317 (1999).
271. Reaction Dynamics of $O(^1D) + HD$. I. the Insertion Pathway, Yen-Tsung Hsu, Kopin Liu, Lisa A. Pederson, George C. Schatz, *J. Chem. Phys.*, **111**, 7921–30 (1999).
272. Reaction Dynamics of $O(^1D) + HD$. II. Effects of Excited Surfaces, Yen-Tsung Hsu, Kopin Liu, Lisa A. Pederson, George C. Schatz, *J. Chem. Phys.*, **111**, 7930–44 (1999).
273. Potential energy surface of the A state of NH₂, and the role of excited states in the $N(^2D) + H_2$ Reaction, L. A. Pederson, G. C. Schatz, T. Hollebeek, T.-S. Ho, H. Rabitz, and L. B. Harding, *J. Phys. Chem.*, **112**, 2301–7 (2000).
274. A local interpolation scheme using no derivatives in quantum chemical calculations, T. Ishida and G. C. Schatz, *Chem. Phys. Lett.* **314**, 369–375 (1999).
275. Quantum Wave Packet Study of Nonadiabatic Effects in $O(^1D) + H_2 \rightarrow OH + H$, S. K. Gray, C. Petrongolo, K. Drukker and G. C. Schatz, *J. Phys. Chem.*, **103**, 9448–9459 (1999).
276. Fitting potential energy surfaces, G. C. Schatz, In *Reaction and Molecular Dynamics*, Lecture Notes in Chemistry, Vol. 14, A. Lagana and A. Riganelli, Eds., Springer, Berlin, 2000, pp 15–32.
277. Quantum Mechanics of Interacting Systems: Scattering Theory, G. C. Schatz, In *Encyclopedia of Chemical Physics and Physical Chemistry, Vol. I: Fundamentals*, J. H. Moore and N. D. Spencer, Eds., Institute of Physics Publishing, Bristol, PA, 2001, pp 827–864.
278. DNA-linked metal nanosphere materials: structural basis for the optical properties, A. A. Lazarides and G. C. Schatz, *J. Phys. Chem.*, **104**, 460–7 (2000).
279. DNA-linked metal nanosphere materials: FFT solution for the optical response, A. A. Lazarides and G. C. Schatz, *J. Chem. Phys.* **112**, 2987–2993 (2000).
280. Quantum scattering on coupled ab initio potential energy surfaces for the $Cl(^2P) + HCl \rightarrow ClH + Cl(^2P)$ reaction, T. W. J. Whiteley, A. J. Dobbyn, J. N. L. Connor and G. C. Schatz, *Phys. Chem. Chem. Phys.*, **2**, 549–556 (2000).
281. Modeling Nanoparticle Optical Properties, K. Lance Kelly, Traci R. Jensen, Anne A. Lazarides and George C. Schatz, In *Metal Nanoparticles: Synthesis, Characterization and Applications*, D. Feldheim and C. Foss, Eds., Marcel-Dekker, New York, 2002, pp 89–118.
282. What controls the optical properties of DNA-linked gold nanoparticle assemblies? J. J. Storhoff, A. A. Lazarides, R. C. Mucic, C. A. Mirkin, R. L. Letsinger, and G. C. Schatz, *J. Am. Chem. Soc.*, **122**, 4640–50 (2000).
283. Optical Properties of Metal Nanoparticles and Nanoparticle Aggregates Important in Biosensors, Anne A. Lazarides, K. Lance Kelly, Traci R. Jensen and George C. Schatz, *THEOCHEM*, **529**, 59–63 (2000).
284. Quantum scattering study of collisional energy transfer in $He + NO_2$: The importance of the vibronic mixing, C. Petrongolo and G. C. Schatz, *J. Chem. Phys.* **112**, 5672–8 (2000).
285. Detecting Resonances, G. C. Schatz, *Science*, **288**, 1599–1600 (2000).
286. A New Potential Surface and Quasiclassical Trajectory Study of $H+H_2O \rightarrow OH+H_2$, G.-S. Wu, G. C. Schatz, G. Lendvay, D.-C. Fang, and L. B. Harding, *J. Chem. Phys.* **113**, 3150–61 (2000).
287. Probing the H₂ rotational state in $O(^1D) + H_2 \rightarrow OH + H$: Theoretical dynamics including nonadiabatic effects and a crossed molecular beam study, Gray, S. K.; Balint-Kurti, G. G.; Schatz, G. C.; Lin, J. J.; Liu, X.; Harich, S.; Yang, X. *J. Chem. Phys.* **113**, 7330–44 (2000).
288. A model for simulating dynamics of DNA Denaturation, Karen Drukker and G. C. Schatz, *J. Phys. Chem.* **104**, 6108–11 (2000).
289. A benchmark system for insertion chemistry: quantum state resolved differential cross sections for $O(^2D) + H_2(J=0) \rightarrow OH(^2\Pi, v, N) + H(^2S)$, J. J. Lin, X. Liu, S. Harich, G. C. Schatz, and X. Yang, *Science*, **289**, 1536–38 (2000).
290. Theoretical Studies of Intersystem Crossing Effects in the $O + H_2$ Reaction, Mark R. Hoffmann and George C. Schatz, *J. Chem. Phys.*, **113**, 9456–9465 (2000).
291. A Quasiclassical Trajectory study of the $H + HCN \rightarrow H_2 + CN$ reaction dynamics, Diego Troya, Irene Banos, Miguel Gonzales, Guosheng Wu, Marc ter Horst and George C. Schatz, *J. Chem. Phys.*, **113**, 6253–63 (2000).
292. Nanosphere Lithography: Effect of the Substrate on the Localized Surface Plasmon Resonance Spectrum of Silver Nanoparticles, M. D. Malinsky, K. L. Kelly, G. C. Schatz and R. P. Van Duyne, *J. Phys. Chem.* **105**, 2343–50 (2001).
293. Chain Length Dependence and Sensing Capabilities of the Localized Surface Plasmon Resonance of Silver Nanoparticles Chemically Modified with Alkanethiol Self-Assembled Monolayers, M. D. Malinsky, K. L. Kelly, G. C. Schatz and R. P. Van Duyne, *J. Am. Chem. Soc.* **123**, 1471–1482 (2001).

294. Reactive and Nonreactive Quenching of OH(A $^2\Sigma^+$) in Collisions with H atoms, George C. Schatz, Brent Fisher, Will Grande, Ken Kumayama and Lisa A. Pederson, *J. Phys. Chem.* **105**, 2515–21 (2001).
295. A QCT study of the Cl + HCN \rightarrow HCl + CN reaction dynamics. The microscopic reaction mechanism of the H(Cl) + HCN \rightarrow H₂(HCl) + CN reactions, Diego Troya, Miguel Gonzalez, Guosheng Wu and George C. Schatz, *J. Phys. Chem.* **105**, 2285–97 (2001).
296. The dynamics of the N(2D)+D₂ reaction from crossed beam and quasiclassical trajectory studies, N. Balucani, M. Alagia, L. Cartechini, P. Casavecchia, G. G. Volpi, L. A. Pederson and G. C. Schatz, *J. Phys. Chem.* **105**, 2414–22 (2001).
297. Model simulations of DNA denaturation dynamics, Karen Drukker, Guosheng Wu and George C. Schatz, *J. Chem. Phys.* **114**, 579–590 (2001).
298. Stretched Water is More Reactive, George C. Schatz, *Science*, **290**, 950–1 (2000).
299. Effective Medium Theory of DNA-linked Gold Nanoparticle Aggregates: Effect of Aggregate Shape, A. A. Lazarides, K. L. Kelly and G. C. Schatz, *Mater. Res. Soc. Symp. Proc.* **635**, C6.5.1–10 (2001).
300. Finite Element Method for Two-dimension Vibrational Wave Functions: Theory and Application to van der Waals Molecules, T. J. Dudley, R. R. Panday, P. E. Staffin, M. R. Hoffmann and G. C. Schatz, *J. Chem. Phys.* **114**, 6166–79 (2001).
301. Tribute to Aron Kuppermann, J. M. Bowman, J. A. Kaye, G. C. Schatz and D. G. Truhlar, *J. Phys. Chem. A* **105**, 2127–28 (2001).
302. Tribute to William H. Miller, N. Makri and G. C. Schatz, *J. Phys. Chem. A* **105**, 2485–86 (2001).
303. A Quasiclassical Trajectory Study of Reactivity and Product Energy Disposal in H + H₂O, H + D₂O and H + HOD, Diego Troya, Miguel Gonzalez, George C. Schatz, *J. Chem. Phys.* **114**, 8397–13 (2001).
304. Variation transition state theory and quasiclassical trajectory studies of the H₂ + OH \rightarrow H + H₂O reaction and some isotopic variants, D. Troya, M. J. Lakin, G. C. Schatz, and M. Gonzalez, *J. Chem. Phys.* **115**, 1828–42 (2001).
305. A Quasiclassical Trajectory Study of Angular and Internal State Distributions in H + H₂O and H + D₂O at E_T = 1.4 eV, D. Troya, G. Lendvay, M. Gonzalez and G. C. Schatz, *Chem. Phys. Lett.*, **343**, 420–28 (2001).
306. A quasiclassical trajectory study of product energy and angular distributions for the OH + D₂ reaction. Matthew J. Lakin, Diego Troya, György Lendvay, Miguel González and George C. Schatz, *J. Chem. Phys.*, **115**, 5160–69 (2001).
307. Model Studies of Intersystem Crossing Effects in the O + H₂ Reaction, Mark. R. Hoffmann and George. C. Schatz, In *Low-Lying Potential Energy Surfaces*, ACS Symposium Series No. 828, M. R. Hoffmann and K. G. Dyall, Eds., American Chemical Society, Washington, DC, 2002, pp 329–345.
308. Computational Electromagnetics of Metal Nanoparticles and Nanoparticle Aggregates, K. L. Kelly, A. A. Lazarides and G. C. Schatz, *Comput. Sci. Eng.* **3**, 67–73 (2001).
309. Electrodynamics of Nonspherical Noble Metal Nanoparticles and Nanoparticle Aggregates, George C. Schatz, *THEOCHEM*, **573**, 73–80 (2001).
310. Self Assembly of Ink Molecules in Dip-Pen Nanolithography: A Diffusion Model, Joonkyung Jang, Seunghun Hong, George C. Schatz and Mark A. Ratner, *J. Chem. Phys.* **115**, 2721–29 (2001).
311. The Branching Ratio between Reaction and Relaxation in the Removal of H₂O from its 104^- Vibrational State in Collisions with H Atoms, Peter W. Barnes, Ian R. Sims, Ian W. M. Smith, Gyorgy Lendvay and George. C. Schatz, *J. Chem. Phys.* **115**, 4586–92 (2001).
312. Synthesis and linear extinction properties of gold-core/silver-shell nanoparticles: comparisons of theory and experiment, Y. Kim, J. Li, R. C. Johnson, J. T. Hupp and G. C. Schatz, *Chem. Phys. Lett.*, **35**, 421–8 (2002).
313. Quasiclassical Trajectory Studies of the N(4S) + H₂ \rightarrow NH(X $^3\Sigma^-$) + H Reaction, Ronald Z. Pascual, George C. Schatz, György Lendvay, Diego Troya, *J. Phys. Chem.*, **106**, 4125–36 (2002).
314. Liquid meniscus condensation in dip pen nanolithography, J. K. Jang, G. C. Schatz and M. A. Ratner, *J. Chem. Phys.* **116**, 3875–86 (2002).
315. Photoinduced Conversion of Silver Nanospheres to Nanoprisms, R. Jin, Y. Cao, C. A. Mirkin, K. L. Kelly, G. C. Schatz, J.-G. Zheng, *Science*, **294**, 1901–1903 (2001).
316. Atomistic Simulations of Nanotube Fracture, T. Belytschko, S. P. Xiao, G. C. Schatz and R. Ruoff, *Phys. Rev. B* **65**, 235430/1–/8 (2002).
317. Hyper-Rayleigh Scattering Studies of Silver, Copper, and Platinum Nanoparticle Suspensions, Robert C. Johnson, Jiangtian Li, Joseph T. Hupp, and George C. Schatz, *Chem. Phys. Lett.*, **356**, 534–540 (2002).
318. A Comparative Classical-Quantum Study of the Photodissociation of Water in the B Band, Rob van Harreveld, Marc C. van Hemert and George C. Schatz, *J. Phys. Chem. A* **105**, 11480–87 (2001).
319. A Quasiclassical Trajectory Study of Energy and Angular Distributions for the H + CO₂ \rightarrow OH + CO Reaction, D. Troya, M. J. Lakin, G. C. Schatz, L. B. Harding, M. Gonzalez, *J. Phys. Chem. B* **106**, 8148–60 (2002).
320. Quasiclassical Trajectory Studies of Four Atom Reactions, D. Troya, M. J. Lakin, and G. C. Schatz, In *Modern Trends in Chemical Reaction Dynamics*, Advanced Series in Physical Chemistry, 14, X. M. Yang and K. Liu, Eds., World Scientific, Singapore, 2004, pp 249–90.
321. A Direct Trajectory Dynamics Investigation of Fast O + Alkane Reactions, R. Z. Pascual, D. J. Garton, and G. C. Schatz, In *Proceedings of sixth International Conference on Protection of Materials and Structures from Space Environment (ICPMSE-6)*, Toronto, May 1–3, 2002, Space Technology Proceedings, 5, J. Kleiman, Ed., Kluwer, Dordrecht, The Netherlands, 2003, pp 537–41.
322. Trajectory-Surface-Hopping Study of the Renner-Teller Effect in the N($2D$) + H₂ Reaction, F. Santoro, C. Petrongolo, G. C. Schatz, *J. Phys. Chem. A* **106**, 8276–84 (2002).
323. The CH + H reaction studied with quantum-mechanical and classical trajectory calculations, Rob van Harreveld, M. C. van Hemert, G. C. Schatz, *J. Chem. Phys.* **116**, 6002–11 (2002).
324. The Optical Properties of Metal Nanoparticles: The Influence of Size, Shape and Dielectric Environment, Lance Kelly, Eduardo Coronado, Lin Lin Zhao, George C. Schatz, *J. Phys. Chem. B*, **107**, 668–77 (2003).
325. Hyper-Rayleigh scattering (HRS) from silver nanoparticles, E. Hao, G. C. Schatz, R. C. Johnson and J. T. Hupp, *J. Chem. Phys.* **117**, 5963–5 (2002).
326. Synthesis of Silver Nanodiscs Using Polystyrene Mesospheres as Templates, E. Hao, K. L. Kelly, J. T. Hupp and G. C. Schatz, *J. Am. Chem. Soc.*, **124**, 15182–3 (2002).
327. What Controls the Melting Properties of DNA-Linked Gold Nanoparticle Assemblies? Rongchao Jin, Guosheng Wu,

Zhi Li, Chad A. Mirkin, and George C. Schatz, *J. Am. Chem. Soc.*, **125**, 1643–1654 (2003).

328. Geometric Packing Considerations for Hydrophobically Driven Self-Assembly of Cone-Shaped Nanoparticles, Stefan Tsonchev, Mark A. Ratner and George C. Schatz, *Nano. Lett.*, **3**, 623–626 (2003).

329. Anomalous Surface Diffusion in Nanoscale Direct Deposition Processes, Pradeep Manandhar, Seunghun Hong, Joonkyung Jang, George C. Schatz and Mark A. Ratner, *Phys. Rev. Lett.*, **90**, 115505 (2003).

330. High Quality Optical Modes in Low-Dimensional Arrays of Nanoparticles: Application to Random Lasers, A. L. Burin, H. Cao, G. C. Schatz and M. A. Ratner, *J. Opt. Soc. Am. B: Opt. Phys.* **21**, 121–131 (2004).

331. Molecular Dynamics Studies of Ion Distributions around DNA Duplexes and Duplex Dimers: Salt Effects and the Connection to Cooperative DNA Melting, H. Long and G. C. Schatz, *Mater. Res. Soc. Symp. Proc.* **735**, C10.1.1–C10.1.9 (2003).

332. A crossed molecular beams study of the $O(^3P) + H_2$ reaction: comparison of excitation function with accurate quantum reactive scattering calculations, D. J. Garton, T. K. Minton, B. Maiti, D. Troya and G. C. Schatz, *J. Chem. Phys.*, **118**, 1585–8 (2003).

333. A local interpolation scheme using no derivatives in potential sampling: Application to $O(^1D) + H_2$ system, Toshimasa Ishida, and George C. Schatz, *J. Comput. Chem.*, **24**, 1077–86 (2003).

334. Hyperthermal reactions of $O(^3P)$ with alkanes: observations of novel reaction pathways in crossed-beams and theoretical studies, D. J. Garton, T. K. Minton, D. Troya, R. Pascual and G. C. Schatz, *J. Phys. Chem. A*, **107**, 4583–4587 (2003).

335. Theoretical Studies of the $O(^3P) + Methane$ Reaction, D. Troya, R. Z. Pascual and G. C. Schatz, *J. Phys. Chem. A*, **107**, 10497–506 (2003).

336. Theoretical Studies of the $O(^3P) + Ethane$ Reaction, D. Troya, R. Z. Pascual, D. J. Garton, T. J. Minton and G. C. Schatz, *J. Phys. Chem. A*, **107**, 7161–69 (2003).

337. The extinction spectra of silver nanoparticle arrays: influence of array structure on plasmon resonance wavelength and widths, LinLin Zhao, K. Lance Kelly and George C. Schatz, *J. Phys. Chem. B*, **107**, 7343–7350 (2003).

338. Nanoparticle Optics: The Importance of Radiative Dipole Coupling in Two-Dimensional Nanoparticle Arrays, Christy L. Haynes, Adam D. McFarland, Lin Lin Zhao, George C. Schatz, Richard P. Van Duyne, Linda Gunnarsson, Juris Prikulis, Bengt Kasemo, and Mikael Käll, *J. Phys. Chem. B*, **107**, 7337–7342 (2003).

339. Capillary Force on a Nanoscale Tip in Dip-Pen Nanolithography, J. K. Jang, G. C. Schatz and M. A. Ratner, *Phys. Rev. Lett.*, **90**, 156104 (2003).

340. Can Plasmon Excitation be Used to Control Nanoparticle Growth? R. Jin, Y. C. Cao, E. Hao, G. S. Métraux, G. C. Schatz, and C. A. Mirkin, *Nature*, **425**, 478–90 (2003).

341. Surface Plasmon Broadening for Arbitrary Shape Nanoparticles: A Geometrical Probability Approach, E. A. Coronado and G. C. Schatz, *J. Chem. Phys.*, **119**, 3926–34 (2003).

342. Influence of Spin–Orbit Effects on Chemical Reactions: Quantum Scattering Studies for the $Cl(^2P) + HCl \rightarrow ClH + Cl(^2P)$ Reaction using Coupled ab initio Potential Energy Surfaces, G. C. Schatz, M. Hankel, T. Whiteley and J. N. L. Connor, *J. Phys. Chem. A*, **107**, 7278–89 (2003).

343. Electromagnetic Fields Around Silver Nanoparticles and Dimers, E. Hao and G. C. Schatz, *J. Chem. Phys.* **120**, 357–66 (2004).

344. A Quasiclassical Trajectory Study of the Reaction $OH + CO \rightarrow H + CO_2$, M. J. Lakin, D. Troya, G. C. Schatz and L. B. Harding, *J. Chem. Phys.* **119**, 5848–59 (2003).

345. How Narrow Can A Meniscus Be?, J. K. Jang, G. C. Schatz and M. A. Ratner, *Phys. Rev. Lett.*, **92**, 085504 (2004).

346. Capillary Force in Atomic Force Microscopy, J. K. Jang, G. C. Schatz and M. A. Ratner, *J. Chem. Phys.*, **120**, 1157–60 (2004).

347. A QM/MM Model for Hyperthermal $O(^3P)$ Collisions with Hydrocarbon Self-Assembled Monolayers, D. Troya and G. C. Schatz, *Proceedings of the ninth International Symposium on Materials in a Space Environment*, June 16–20, 2003, Noordwijk, The Netherlands, ESA SP-540, Sept 2003, pp 121–128.

348. Model atomic oxygen reactions: detailed experimental and theoretical studies of the reactions of ground-state $O(^3P)$ with H_2 , CH_4 , CH_3CH_3 and $CH_3CH_2CH_3$ at hyperthermal collision energies, T. K. Minton, D. J. Garton, D. Troya, B. Maiti, R. Pascual and G. C. Schatz, *Proceedings of the ninth International Symposium on Materials in a Space Environment*, June 16–20, 2003, Noordwijk, The Netherlands, ESA SP-540, Sept 2003, pp 129–136.

349. Dynamics Studies of $O(^3P) + CH_4$, C_2H_6 , C_3H_8 Reactions, Diego Troya and G. C. Schatz, In *Proceedings of NATO Advanced Research Workshop on the Theory of Chemical Reaction Dynamics*, Balatonfoldvar, Hungary, June 7–12, 2003, A. Lagana and G. Lendvay, Eds., Kluwer, Dordrecht, The Netherlands, 2004, pp 329–48.

350. Nonadiabatic Dynamics in the $O + H_2$ Reaction: A Time-Independent Quantum Mechanical Study, B. Maiti and G. C. Schatz, In *Proceedings of NATO Advanced Research Workshop on the Theory of Chemical Reaction Dynamics*, Balatonfoldvar, Hungary, June 7–12, 2003, A. Lagana and G. Lendvay, Eds., Kluwer, Dordrecht, The Netherlands, 2004, pp 89–103.

351. Theoretical studies of intersystem crossing effects in the $O(^3P) + H_2$ reaction, B. Maiti and G. C. Schatz, *J. Chem. Phys.*, **119**, 12360–71 (2003).

352. Extinction spectra of silver nanoparticle arrays, Shengli Zou, Linlin Zhao, George C. Schatz, *Proc. SPIE*, **5221** (Plasmonics: Metallic Nanostructures and Their Optical Properties), 174–181 (2003).

353. A Nanoscale Optical Biosensor: The Long Range Distance Dependence of the Localized Surface Plasmon Resonance of Noble Metal Nanoparticles, Amanda J. Haes, Shengli Zou, George C. Schatz, and Richard P. Van Duyne, *J. Phys. Chem. B*, **108**, 109–116 (2004).

354. A Nanoscale Optical Biosensor: The Short Range Distance Dependence of the Localized Surface Plasmon Resonance of Noble Metal Nanoparticles, Amanda J. Haes, Shengli Zou, George C. Schatz, and Richard P. Van Duyne, *J. Phys. Chem. B*, **108**, 6961–68 (2004).

355. Crossed-Beams and Theoretical Studies of the $O(^3P) + CH_4 \rightarrow H + OCH_3$ Reaction Excitation Function, Diego Troya, George C. Schatz, Donna J. Garton, Amy L. Brunsvold, and Timothy K. Minton, *J. Chem. Phys.*, **120**, 731–9 (2004).

356. Quantum and Classical Studies of the $O(^3P) + H_2(v=0-3, j=0) \rightarrow OH + H$ Reaction Using Benchmark Potential Surfaces, M. Braunstein, S. Adler-Golden, B. Maiti and G. C. Schatz, *J. Chem. Phys.*, **120**, 4316–23 (2004).

357. The Optical Properties of Metal Nanoshells, Encai Hao, Shuyou Li, Ryan C. Bailey, Shengli Zou, George C. Schatz, and Joseph T. Hupp, *J. Phys. Chem. B*, **108**, 1224–1229 (2004).
358. Carbon nanotube fracture—differences between quantum mechanical mechanisms and those of empirical potentials, Diego Troya, Steven L. Mielke, and George C. Schatz, *Chem. Phys. Lett.*, **382**, 133–41 (2003).
359. Influence of van der Waals wells on the quantum scattering dynamics of the $\text{Cl}(^2\text{P})+\text{HCl} \rightarrow \text{ClH} + \text{Cl}(^2\text{P})$ reaction, M. Hankel, J. N. L. Connor and G. C. Schatz, *Chem. Phys.*, **308**, 225–36 (2004).
360. Theoretical Studies of Hyperthermal $\text{O}(^3\text{P})$ Collisions with Hydrocarbon Self-Assembled Monolayers, Diego Troya and George C. Schatz, *J. Chem. Phys.*, **120**, 7696–7707 (2004).
361. Silver nanoparticle array structures that produce remarkably narrow plasmon lineshapes, Shengli Zou, Nicolas Janel, and George C. Schatz, *J. Chem. Phys.*, **120**, 10871–10875 (2004).
362. Electrostatically Directed Self-Assembly of Cylindrical Peptide Amphiphile Nanostructures, S. Tsonchev, G. C. Schatz and M. A. Ratner, *J. Phys. Chem. B*, **108**, 8817–22 (2004).
363. On the Structure and Stability of Self-Assembled Zwitterionic Peptide Amphiphiles: A Theoretical Study, S. Tsonchev, A. Troisi, G. C. Schatz and M. A. Ratner, *Nano Lett.*, **4**, 427–431 (2004).
364. Synthesis and Optical Properties of “Branched” Gold Nanocrystals, E. Hao, R. C. Bailey, G. C. Schatz, J. T. Hupp and S. Li, *Nano Lett.*, **4**, 327–330 (2004).
365. Synthesis and Optical Properties of Anisotropic Metal Nanoparticles, Encai Hao, George C. Schatz, Joseph T. Hupp, *J. Fluorescence*, **14**, 331–41 (2004).
366. The importance of intersystem crossing in the $\text{S}(^3\text{P}, ^1\text{D}) + \text{H}_2 \rightarrow \text{SH} + \text{H}$ reaction, Biswajit Maiti, G. C. Schatz and G. Lendvay, *J. Phys. Chem. A*, **108**, 8772–8781 (2004).
367. Quantum wave packet and quasiclassical trajectory studies of $\text{OH}+\text{CO}$: Influence of the reactant channel well on thermal rate constants. Dmitry M. Medvedev, Stephen K. Gray, Evelyn M. Goldfield, Matthew J. Lakin, Diego Troya, George C. Schatz, *J. Chem. Phys.*, **120**, 1231–38 (2004).
368. Surface plasmons at single nanoholes in Au-films. L. Yin, V. K. Vlasko-Vlasov, A. Rydh, J. Pearson, U. Welp, S.-H. Chang, S. K. Gray, G. C. Schatz, D. E. Brown, C. W. Kimball, *Appl. Phys. Lett.*, **85** 467–469 (2004).
369. The role of vacancy defects and holes in the fracture of carbon nanotubes, Steven L. Mielke, Diego Troya, Sulin Zhang, Je-Luen Li, Shaoping Xiao, Roberto Car, Rodney S. Ruoff, George C. Schatz, and Ted Belytschko, *Chem. Phys. Lett.*, **390**, 413–20 (2004).
370. Cooperative DNA Melting in DNA Linked Gold Nanoparticle Aggregates, H. Long, M. Chen and G. C. Schatz, *Proceedings of the Conference on Foundations of Nanoscience*, Snowbird, UT, April 24–27, 2004, Foundations of Nanoscience, Self-Assembled Architectures and Devices, J. Reif, Ed., Science Technica, Washington, DC, 2004, pp 90–103.
371. Hyperthermal Chemistry in the Gas phase and on Surfaces: Theoretical Studies, Diego Troya and George C. Schatz, *Int. Rev. Phys. Chem.*, **23**(3), 341–373 (2004).
372. Theoretical Study of Reactions of Hyperthermal $\text{O}(^3\text{P})$ with Perfluorinated Hydrocarbons, Diego Troya and George C. Schatz, *Proceedings of seventh ICPMSE*, Toronto, May 10–13, 2004, Space Technology Proceedings, Vol. 6, Springer, Berlin, 2006, pp 365–375.
373. A Comparative analysis of Localized and Propagating Surface Plasmon Resonance Sensors: The Binding of Con-
- canavalin A to a Monosaccharide Functionalized Self-Assembled Monolayer, Chanda Ranjit Yonzon, Eunhee Jeoung, Shengli Zou, George C. Schatz, Milan Mrksich and Richard P. Van Duyne, *J. Am. Chem. Soc.*, **126**, 12669–76 (2004).
374. Confined plasmons in nanofabricated single silver particle pairs – experimental observations of strong interparticle interactions, Linda Gunnarsson, Tomas Rindzevicius, Juris Prikulis, Bengt Kasemo, Mikael Kall, Shengli Zou and George C. Schatz, *J. Phys. Chem. B*, **109**, 1079–1087 (2005).
375. Electrodynamics in Computational Chemistry, Linlin Zhao, Shengli Zou, Encai Hou and G. C. Schatz, *Theory and Applications of Computational Chemistry: The First 40 Years, A Volume of Technical and Historical Perspectives*, Clifford E. Dykstra, Gernot Frenking, Kwang S. Kim, and Gustavo Scuseria, Eds., Elsevier, Amsterdam, 2005, pp 47–66.
376. Electronic structure studies of surface enhanced Raman scattering, L. Zhao and G. C. Schatz, *Proc. SPIE*, **5512**, 10–19; Plasmonics: Metallic nanostructures and Their Optical Properties II, N. J. Halas and T. R. Huser, Eds., 2004.
377. Generating narrow plasmon resonances from silver nanoparticle arrays: influence of array pattern and particle spacing, Shengli Zou, George C. Schatz, *Proc. SPIE*, **5513**, 22–29; Physical Chemistry of Interfaces and Nanomaterials III, G. V. Hartland and X.-Y. Zhu, Eds., 2004.
378. Crossed-Beams and Theoretical Studies of the Dynamics of Hyperthermal Collisions between Ar and Ethane, Amy L. Brunsvold, Donna J. Garton, Timothy K. Minton, Diego Troya and George C. Schatz, *J. Chem. Phys.*, **121**, 11702–14 (2004).
379. Hyperthermal reactions of $\text{O}^+(^4\text{S}_{3/2})$ with CD_4 and CH_4 : theory and experiment, Dale J. Levandier, Yu-hui Chiu, Rainer A. Dressler, Lipeng Sun and George C. Schatz, *J. Phys. Chem. A*, **108**, 9794–9804 (2004).
380. Near-field photochemical imaging of noble metal nanostructures, C. Hubert. A. Remyantseva, G. Lerondel, J. Grand, S. Kostchev, A. Vial, R. Bachelot, P. Royer, S.-H. Chang, S. K. Gray, G. P. Wiederrecht, and G. C. Schatz, *Science, Nano Lett.*, **5**, 615–19 (2005).
381. Multi-Walled Carbon Nanotubes Experiencing Electrical Breakdown as Gas Sensors Jaehyun Chung, Kyong-Hoon Lee, Junghoon Lee, Diego Troya, George C. Schatz, *Nanotechnology*, **15**, 1–7 (2004).
382. All-atom numerical studies of self-assembly of zwitterionic peptide amphiphiles, S. Tsonchev, A. Troisi, G. C. Schatz, M. A. Ratner, *J. Phys. Chem. B*, **108**, 15278–15284 (2004).
383. Biography of Gert D. Billing. Michael Baer, Cecilia Coletti, George C. Schatz, Soren Toxvaerd, and Lichang Wang, *J. Phys. Chem. A*, **108**, 8553 (2004).
384. Mechanics of defects in carbon nanotubes: Atomistic and multiscale simulations, Sulin Zhang, Steven L. Mielke, Roopam Khare, Diego Troya, Rodney S. Ruoff, George C. Schatz and Ted Belytschko, *Phys. Rev. B*, **71**, 115403/1-12 (2005).
385. Narrow plasmonic/photonic extinction and scattering lineshapes for one and two-dimensional silver nanoparticle arrays, Shengli Zou and George C. Schatz, *J. Chem. Phys.*, **121**, 12606–12612 (2004).
386. Silver nanoparticle array structures that produce giant enhancements in electromagnetic fields, Shengli Zou and George C. Schatz, *Chem. Phys. Lett.*, **403**, 62–67 (2005).
387. Reply to “Silver nanoparticle array structures that produce remarkable narrow plasmon lineshapes” [*J. Chem. Phys.* **130**, 10871 (2004)], Shengli Zou and George C. Schatz, *J. Chem. Phys.*, **122**, 097102/1–097102/2 (2005).

388. Screened multipole electrostatic interactions at the Debye–Hueckel level, Stefan Tsonchev, George C. Schatz, and Mark A. Ratner, *Chem. Phys. Lett.*, **400**, 221–5 (2004).
389. Optical properties of one-dimensional metal nanostructures. Encai Hao, Shengli Zou, George C. Schatz, *Mater. Res. Soc. Symp. Proc.*, **818**, 53–58 (2004).
390. Fracture Paths and Ultrananocrystalline Diamond, Jeffrey T. Paci, Lipeng Sun, T. Belytschko, and George C. Schatz, *Chem. Phys. Lett.*, **403**, 16–21 (2005).
391. Observation of the Quadrupole Plasmon Mode for a Colloidal Solution of Gold Nanoprisms, J. E. Millstone, S. Park, K. L. Shuford, L. Qin, G. C. Schatz and C. A. Mirkin, *J. Am. Chem. Soc.*, **127**, 5312–5313 (2005).
392. Review of: Modern Problems in Classical Electrodynamics, Gilbert Chang and George C. Schatz, Edited by Charles A. Brau, *ChemPhysChem*, **6**(2), 374 (2005).
393. Direct Dynamics Classical Trajectory Simulations of the $O^+ + CH_4$ Reaction at Hyperthermal Energies, Lipeng Sun and George C. Schatz, *J. Phys. Chem. B*, **109**, 8431–8 (2005).
394. Surface plasmon generation and light transmission by isolated nanoholes and arrays of nanoholes in thin metal films, S-H. Chang, S. K. Gray and G. C. Schatz, *Opt. Express*, **13**, 3150–65 (2005).
395. Finite lifetime effects on the polarizability within time-dependent density functional theory, L. Jensen, J. Autschbach and G. C. Schatz, *J. Chem. Phys.* **122**, 224115/1–/11 (2005).
396. Plasmonic Materials for Surface-Enhanced Sensing and Spectroscopy, A. J. Haes, C. L. Haynes, A. D. McFarland, S. Zou, G. C. Schatz, and R. P. Van Duyne, *MRS Bull.*, **30**, 368–375 (2005).
397. Hyperthermal collisions of $O^+(^4S_{3/2})$ with Methane at 5 eV, LiPeng Sun and George C. Schatz, *J. Spacecraft Rockets*, **43**, 436–438 (2006).
398. Time-dependent density functional calculations of optical rotatory dispersion including resonance wavelengths as a potentially useful tool for determining absolute configurations of chiral molecules, Jochen Autschbach, Lasse Jensen, George C. Schatz, Y. C. Electra Tse and Mykhaylo Krykunov, *J. Phys. Chem. A*, **110**, 2461–73 (2006).
399. Controlling plasmon line-shapes through diffractive coupling in linear arrays of cylindrical nanoparticles fabricated by electron beam lithography, E. M. Hicks, S. Zou, G. C. Schatz, K. G. Spears, R. P. Van Duyne, L. Gunnarsson, T. Rindzevicius, B. Kasemo, M. Kall, *Nano Lett.*, **5**, 1065–70 (2005).
400. Solution-phase triangular Ag nanotriangles fabricated by nanosphere lithography, A. J. Haes, J. Zhao, S. Zou, C. S. Own, L. D. Marks, G. C. Schatz, R. P. Van Duyne, *J. Phys. Chem. B*, **109**, 11158–62 (2005).
401. Electrochemical tuning of silver nanoparticles fabricated by nanosphere lithography, X. Zhang, E. M. Hicks, J. Zhao, G. C. Schatz, and R. P. Van Duyne, *Nano Lett.*, **5**, 1503–7 (2005).
402. Sandra J. Tomczak, Darrell Marchant, Steve Svejda, Timothy K. Minton, Amy L. Brunsvold, Irina Gouzman, Eitan Grossman, George C. Schatz, Diego Troya, Diego, LiPeng Sun, Rene I. Gonzalez, *Properties and improved space survivability of POSS (polyhedral oligomeric silsesquioxane) polyimides*. Materials Research Society Symposium Proceedings No. 851 (Materials for Space Applications), Materials Research Society, Warrendale, PA, 2005, pp 395–406.
403. Anisotropic polarizability tensor of a dimer of nanospheres in the vicinity of a plane substrate, Anatoliy Pinchuk and George C. Schatz, *Nanotechnology*, **16**, 2209–17 (2005).
404. A Reinterpretation of the Mechanism of the Simplest Reaction at an sp^3 Hybridized Carbon Atom: $H + CD_4 \rightarrow CD_3 + HD$, Jon P. Camden, Hans A. Bechtel, Davida J. Ankeny Brown, Marion R. Martin, Richard N. Zare, Wenfang Hu, György Lendvay, Diego Troya, George C. Schatz, *J. Am. Chem. Soc.*, **127**(34), 11898–11899 (2005).
405. $H + CD_4$ Abstraction Reaction Dynamics: Excitation Function, and Angular and Translational Energy Distributions, Jon P. Camden, Wenfang Hu, Hans A. Bechtel, Davida J. Ankeny Brown, Marion R. Martin, Richard N. Zare, György Lendvay, Diego Troya, and George C. Schatz, *J. Phys. Chem. A*, **110**, 677–686 (2006).
406. $H + CD_4$ Abstraction Reaction Dynamics: Product Energy Partitioning, Wenfang Hu, György Lendvay, Diego Troya and George C. Schatz, Jon P. Camden, Hans A. Bechtel, Davida J. A. Brown, Marion R. Martin, and Richard N. Zare, *J. Phys. Chem. A*, **110**, 3017–27 (2006).
407. The mechanical properties of single-crystal and ultrananocrystalline diamond: a theoretical study, Jeffrey T. Paci, Ted Belytschko and George C. Schatz, *Chem. Phys. Lett.*, **414**(4–6), 351–358 (2005).
408. Multipolar Excitation in Triangular Nanoprisms, Kevin L. Shuford, Mark. A. Ratner and George C. Schatz, *J. Chem. Phys.*, **123**(11), 114713/1–114713/9 (2005).
409. Surface Plasmon Standing Waves in Large-Area Sub-wavelength Hole Arrays, Eun-Soo Kwak, Joel Henzie, Shih-Hui Chang, Stephen K. Gray, George C. Schatz, and Teri W. Odom, *Nano Lett.*, **5**(10), 1963–1967 (2005).
410. Atomic-scale roughness effect on capillary force in atomic force microscopy, J. K. Jang, M. A. Ratner, G. C. Schatz, *J. Phys. Chem. B*, **110**, 659–662 (2006).
411. Melting mechanisms of DNA-linked nanocomposite systems, Sung Yong Park and George C. Schatz, *Proceedings of the Conference on Foundations of Nanoscience*, Snowbird, UT, April 24–28, 2005, Foundations of Nanoscience, Self-Assembled Architectures and Devices, J. Reif, Ed., Science Technica, Washington, DC, 2005, pp 207–214.
412. Theory and method for calculating resonance Raman scattering from resonance polarizability derivatives, L. Jensen, L. Zhao, J. Autschbach and G. C. Schatz, *J. Chem. Phys.*, **123**, 174110/1–174110/11 (2005).
413. DNA as Helical Ruler: Exciton-Coupled Circular Dichroism in DNA Conjugates, Frederick D. Lewis, Ligang Zhang, Xiaoyang Liu, Xiaobing Zuo, David M. Tiede, Hai Long, and George C. Schatz, *J. Am. Chem. Soc.*, **127**, 14445–53 (2005).
414. Duplex and hairpin dimer structures for perylene diimide-oligonucleotide conjugates, Yan Zheng, Hai Long, George Schatz, and Frederick D. Lewis, *Chem. Commun.*, **38**, 4795–97 (2005).
415. Experimental and theoretical investigations of the inelastic and reactive scattering dynamics of $O(^3P) + D_2$, D. J. Garton, A. L. Brunsvold, T. K. Minton, D. Troya, B. Maiti and G. C. Schatz, *J. Phys. Chem. A*, **110**, 1327–1341 (2006).
416. Intersystem crossing effects in reactions of O and S with small molecules, B. Maiti, D. Troya, G. Lendvay and G. C. Schatz, In *Semiclassical and Other Methods for Understanding Molecular Collisions and Chemical Reactions*, D. Sokolovski, J. N. L. Connor and S. Sen, Eds., Collaborative Computational Project on Molecular Quantum Dynamics (CCP6), Daresbury Laboratory, Daresbury, Warrington WA4 4AD, United Kingdom, 2005, pp 9–14.
417. Localized Surface Plasmon Resonance Spectroscopy of Single Silver Nanocubes, Leif J. Sherry, Shih-Hui Chang,

George C. Schatz, Richard P. Van Duyne, Benjamin J. Wiley and Younan Xia, *Nano Lett.*, **5**, 2034–38 (2005).

418. Electrodynamics simulations of surface plasmon behavior in metallic nanostructures, S. K. Gray, T.-W. Lee, S.-H. Chang and G. C. Schatz, In *SPIE Proceedings (Plasmonics: Metallic Nanostructures and Their Optical Properties III)*, M. I. Stockman, Ed., SPIE: Bellingham, WA, 2005, No. 5927, pp 96–101.

419. Controlling the Shape, Orientation and Pitch of Carbon Nanotube Features Using Nano Affinity Templates, Yuhuang Wang, Daniel Maspoch, Shengli Zou, George C. Schatz, Richard E. Smalley, Chad A. Mirkin, *Proc. Natl. Acad. Sci. U.S.A.*, **103**, 2026–2031 (2006).

420. Localized Surface Plasmon Resonance Nanosensor: A High-Resolution Distance-Dependence Study Using Atomic Layer Deposition, Alyson V. Whitney, Jeffrey W. Elam, Shengli Zou, Alex. V. Zinovev, Peter C. Stair, George C. Schatz and Richard P. Van Duyne, *J. Phys. Chem B*, **109**, 20522–28 (2005).

421. Semiclassical nonadiabatic dynamics using mixed wave function representation, Sophia Garashchuk, Vitaly A. Rassolov, and George C. Schatz, *J. Chem. Phys.*, **123**, 174108/1–10 (2005).

422. Plasmonic Properties of Film over Nanowell Surfaces Fabricated by Nanosphere Lithography. Hicks, Erin M.; Zhang, Xiaoyu; Zou, Shengli; Lyandres, Olga; Spears, Kenneth G.; Schatz, George C.; Van Duyne, Richard P. *J. Phys. Chem. B*, **109**(47), 22351–22358 (2005).

423. Pyridine-Ag₂₀ Cluster: A model system for studying surface enhanced Raman scattering, L. Zhao, L. Jensen and G. C. Schatz, *J. Am. Chem. Soc.*, **128**, 2911–19 (2006).

424. Alkanethiol mediated release of surface bound nanoparticles fabricated by nanosphere lithography, J. Zhao, A. J. Haes, X. Zhang, S. Zou, E. M. Hicks, and G. C. Schatz, *Mater. Res. Soc. Symp. Proc.*, **900E**, O13–O8.1 (2006).

425. Multipole plasmon resonances in gold nanorods, Emma K. Payne, Kevin L. Shuford, Sungho Park, George C. Schatz and Chad A. Mirkin, *J. Phys. Chem. B*, **110**(5), 2150–2154. (2006).

426. New Editor in Chief of *The Journal of Physical Chemistry*, George C. Schatz, *J. Phys. Chem. A/B* **109**, 1 (2005).

427. Editorial, George C. Schatz, *J. Phys. Chem. A/B*, **110**, 1 (2006).

428. α - and β -Stilbenosides as base-pair surrogates in DNA hairpins, Ligang Zhang, Hai Long, Grant E. Boldt, Kim D. Janda, George C. Schatz, and Frederick D. Lewis, *Org. Biomol. Chem.*, **4**, 314–322 (2006).

429. Molecular Dynamics Studies of Ion Distributions for DNA Duplexes and DNA Clusters: Salt Effects and Connection to DNA Melting, H. Long, A. Kudlay and G. C. Schatz, *J. Phys. Chem. B*, **110**, 2918–26 (2006).

430. Phase of molecular ink in nanoscale direct deposition processes, Narae Cho, Seol Ryu, Byeongui Kim, George C. Schatz, and Seunghun Hong, *J. Chem. Phys.*, **124**, 024714/1–/6 (2006).

431. Coupled plasmon/photonic resonance effects in SERS, Shengli Zou and George C. Schatz, In *Surface Enhanced Raman Scattering: Physics and Applications*, K. Kneipp, M. Moskovits and H. Kneipp, Eds., Springer Topics in Applied Physics, Vol. 103, Springer, Berlin, 2006, pp 67–86.

432. Electromagnetic mechanism of SERS, George C. Schatz, Matthew Young and Richard P. Van Duyne, In *Surface Enhanced Raman Scattering: Physics and Applications*, K. Kneipp, M. Moskovits and H. Kneipp, Eds., Springer Topics in Applied Physics, Vol. 103, Springer, Berlin, 2006, pp 19–46.

433. Transition states and minimum energy pathways for the collapse of carbon nanotubes, Sulin Zhang, Roopam Khare, Ted Belytschko, K. Jimmy Hsia, Steven L. Mielke and George C. Schatz, *Phys. Rev. B*, **73**, 075423 (2006).

434. Finite-difference time-domain studies of light transmission through nanohole structures, K. L. Shuford, Mark A. Ratner, Stephen K. Gray and George C. Schatz, *Appl. Phys. B*, **84**, 11–18 (2006).

435 Focusing a beam of light with left-handed metamaterials, A. O. Pinchuk and G. C. Schatz, *Solid-State Electron.*, **51**, 1381–86 (2007).

436. Melting behavior of DNA-linked polymers, A. Kudlay and G. C. Schatz, Proceedings of Foundations of Nanoscience Conference, Snowbird, Utah, April, 2006, Science Technica, 264–272 (2006).

437. Ion current calculations based on three-dimensional Poisson-Nernst-Planck theory for a cyclic peptide nanotube, Hyonseok Hwang, George C. Schatz and Mark A. Ratner, *J. Phys. Chem. B*, **110**, 6999–7008 (2006).

438. Resonance Raman scattering of Rhodamine 6G as calculated using time-dependent density functional theory, Lasse Jensen and George C. Schatz, *J. Phys. Chem. A*, **110**, 5973–77 (2006).

439. Quantum trajectory dynamics in arbitrary coordinates, Vitaly A. Rassolov, S. Garashchuk and G. C. Schatz, *J. Phys. Chem. A*, **110**, 5530–36 (2006).

440. Theoretical studies of plasmon resonances in one-dimensional nanoparticle chains: narrow lineshapes with tunable widths, Shengli Zou and George C. Schatz, *Nanotechnology*, **17**, 2813–20 (2006).

441. Combining micron size glass spheres with silver nanoparticles to produce extraordinary field enhancements for surface enhanced Raman scattering applications, S. Zou and G. C. Schatz, *Isr. J. Chem.*, **46**, 293–97 (2006).

442. Surface-enhanced Raman scattering of pyrazine at the junction between two Ag₂₀ nanoclusters, Linlin Zhao, Lasse Jensen and George C. Schatz, *Nano Lett.*, **6**, 1229–1234 (2006).

443. Electric Field Enhancement and Light Transmission in Cylindrical Nanoholes, Kevin Shuford, Mark A. Ratner, Stephen K. Gray, and George C. Schatz, *J. Comput. Theor. Nanosci.*, **4**, 1–8 (2007).

444. Optics of Nanoparticles: Substrate, Size and Interface Effects, Anatoliy O. Pinchuk, George C. Schatz, Alexander Reinholdt and Uwe Kreibig, In *Progress in Nanotechnology Research*, A. O. Pinchuk, Ed., NOVA Publishing, Inc., New York, *Nanotechnol. Res. J.*, **1**, 3/4, 1 (2007).

445. Electrostatic Aggregation and Formation of Core–Shell Suprastructures in Binary Mixtures of Charged Metal Nanoparticles, Alexander M. Kalsin, Maciej Paszewski, Anatoliy O. Pinchuk, George C. Schatz and Bartosz A. Grzybowski, *Nano Lett.*, **6**, 1896–1903 (2006).

446. Structures of DNA-linked nanoparticle aggregates, Sung Yong Park, Jae-Seung Lee, Dimitra Georganopoulou, Chad A. Mirkin and George C. Schatz, *J. Phys. Chem. B*, **110**, 12673–81 (2006).

447. Semiclassical nonadiabatic dynamics based on quantum trajectories for the O(³P, ¹D) + H₂ system, Sophia Garashchuk, Vitaly Rassolov and George C. Schatz, *J. Chem. Phys.*, **124**, 244307/1–/8 (2006).

448. Manipulating the optical properties of pyramidal nanoparticle arrays, J. Henzie, K. L. Shuford, E.-S. Kwak, G. C. Schatz and T. W. Odom, *J. Phys. Chem. B*, **110**, 14028–31 (2006).

449. Designing, fabricating, and imaging Raman hot spots, Lidong Qin, Shengli Zou, Can Xue, Ariel Atkinson, George C. Schatz and Chad A. Mirkin, *Proc. Natl. Acad. Sci. U.S.A.*, **103**, 13300–3 (2006).
450. Ultrafast pulse excitation of a metallic nanosystem containing a Kerr nonlinear material, Xiwen Wang, George C. Schatz, and Stephen K. Gray, *Phys. Rev. B*, **74**, 195439/1–/5 (2006).
451. Sharp melting transition in DNA-linked polymer nanocomposites, S. Y. Park, J. M. Gibbs, S. B. Nguyen, and G. C. Schatz, *J. Phys. Chem. B*, **111**, 8785–91 (2007).
452. Sharp melting of polymer-DNA hybrids: an associative phase separation approach, A. Kudlay, J. M. Gibbs, G. C. Schatz, S. T. Nguyen and G. C. Schatz, *J. Phys. Chem. B*, **111**, 1610–19 (2007).
453. Metal nanoparticle array waveguides: Proposed structures for subwavelength devices, S. Zou and G. C. Schatz, *Phys. Rev. B*, **74**, 125111/1–/15 (2006).
454. Localized Surface Plasmon Resonance Spectroscopy of Single Silver Triangular Nanoprisms. Leif J. Sherry, Rongchao Jin, Chad A. Mirkin, George C. Schatz and Richard P. Van Duyne, *Nano Lett.*, **6**, 2060–2065 (2006).
455. Localized Surface Plasmon Resonance Spectroscopy near Molecular Resonances. Amanda J. Haes, Shengli, Zou, Jing Zhao, George C. Schatz, and Richard P. Van Duyne, *J. Am. Chem. Soc.*, **128**, 10905–14 (2006).
456. Resonance Surface Plasmon Spectroscopy: Low Molecular Weight Substrate Binding to Cytochrome P450. Jing Zhao, Aditya Das, Xiaoyu Zhang, George C. Schatz, Stephen G. Sligar and Richard P. Van Duyne, *J. Am. Chem. Soc.*, **128**, 11004–11005 (2006).
457. Nanografting: Modeling and Simulation. Seol Ryu and George C. Schatz, *J. Am. Chem. Soc.*, **128**, 11563–11573 (2006).
458. Microscopic mechanisms and dynamics simulations of $O^+(^4S_{3/2})$ reacting with methane; L. P. Sun and G. C. Schatz, Proceedings of seventh ICPMSE, Toronto, May 10–13 (2004), Springer, Space Technology Proceedings, Vol. 6, 359–364 (2006).
459. Reorganization of *The Journal of Physical Chemistry*, George C. Schatz, *J. Phys. Chem. A*, **110**, 10655 (2006); *J. Phys. Chem. B*, **110**, 18073 (2006).
460. A cooperative beads-on-a-string approach to exceptionally stable DNA triplexes. Yan Zheng, Hai Long, George C. Schatz and Frederick D. Lewis, *Chem. Commun.*, **36**, 3830–3832 (2006).
461. Theories of reactive scattering, Wenfang Hu, George C. Schatz, *J. Chem. Phys.*, **125**(13), 132301/1–132301/15 (2006).
462. Localized surface plasmon and molecular resonance: fundamental study and application. Jing Zhao, Xiaoyu Zhang, Amanda J. Haes, Shengli Zou, George C. Schatz, Richard P. Van Duyne, *Proc. SPIE*, **6323** (Plasmonics: Metallic Nanostructures and Their Optical Properties IV), 63231B (2006).
463. FDTD/TDSE study on surface-enhanced infrared absorption by metal nanoparticles. Shih-Hui Chang, George C. Schatz, Stephen K. Gray, *Proc. SPIE*, **6323** (Plasmonics: Metallic Nanostructures and Their Optical Properties IV), 632321 (2006).
464. TDDFT studies of absorption and SERS spectra of pyridine interacting with Au_{20} , Christine M. Aikens and George C. Schatz, *J. Phys. Chem. A*, **110**, 13317–24 (2006).
465. Synthesis and properties of nicked dumbbell and dumbbell DNA conjugates, Ligang Zhang, Hai Long, George C. Schatz and Frederick D. Lewis, *Org. Biomol. Chem.*, **5**, 450–456 (2007).
466. Substrate effects on Surface Plasmons in Single Nanoholes, Kevin L. Shuford, Stephen K. Gray, Mark A. Ratner and George C. Schatz, *Chem. Phys. Lett.*, **435**, 123–6 (2007).
467. Rings of single-walled carbon nanotubes: molecular-template directed assembly and Monte Carlo modeling, Shengli Zou, Daniel Maspoeh, Yuhuang Wang, Chad A. Mirkin and George C. Schatz, *Nano Lett.*, **7**, 276–80 (2007).
468. Mechanical properties of ultrananocrystalline diamond prepared in a nitrogen-rich plasma: A theoretical study, Jeffrey T. Paci, Ted Belytschko, George C. Schatz, *Phys. Rev. B*, **74**, 184112/1–1/9 (2006).
469. Steered molecular dynamics studies of the potential of mean force of a Na^+ or K^+ ion in a cyclic peptide nanotube, Hyonseok Hwang, George C. Schatz and Mark A. Ratner, *J. Phys. Chem. B*, **110**, 26448–60 (2006).
470. New Journals in a New Year, G. C. Schatz, *J. Phys. Chem. A/B/C*, **111**, 1 (2007).
471. Direct dynamic simulations of $O(^3P) + HCl$ at hyperthermal energies, Jon P. Camden and George C. Schatz, *J. Phys. Chem. A*, **110**, 13681–13685 (2006).
472. George H. Chan, Jing Zhao, Erin M. Hicks, George C. Schatz, Richard P. Van Duyne, Plasmonic properties of copper nanoparticles fabricated by nanosphere lithography, *Nano Lett.*, **7**, 1947–52 (2007).
473. Coupled quantum mechanical/molecular mechanical modeling of the fracture of defective carbon nanotubes and graphene sheets, R. Khare, S. L. Mielke, J. T. Paci, S. Zhang, G. C. Schatz, T. Belytschko, *Phys. Rev. B*, **75**, 075412/1–075412/12 (2007).
474. A. O. Pinchuk and G. C. Schatz, Metamaterials with Gradient of the Negative Index of Refraction, *J. Opt. Soc. A*, **24**, 39–44 (2007).
475. Influence of surface roughness on the pull-off force in atomic force microscopy, J. K. Jang, J. Y. Sung and G. C. Schatz, *J. Phys. Chem. C*, **111**, 4648–4654 (2007).
476. Size-dependence of the enhanced Raman scattering of pyridine adsorbed on Ag_n ($n = 2–8, 20$) clusters, Lasse Jensen, Linlin Zhao, George C. Schatz, *J. Phys. Chem. C*, **111**, 4756–4764 (2007).
477. Quantitative evaluation of plasmon enhanced Raman scattering from nanoaperture arrays, Thomas Reilly III, Shih-Hui Chang, Jordan D. Corbman, George C. Schatz, Kathy L. Rowlen, *J. Phys. Chem. C*, **111**, 1689–94 (2007).
478. Structure and electronic spectra of DNA mini-hairpins with $G_n:C_n$ stems, Jennifer Tuma, Stefano Tonzani, George C. Schatz, Andrew H. Karaba and Frederick D. Lewis, *J. Phys. Chem. B*, **111**, 13101–106 (2007).
479. Synthesis and Properties of Hairpin and Dumbbell DNA Conjugates Having Oligo(ethylene glycol) Linkers and Short A-Tract Base Pair Domains, Ligang Zhang, Andrew H. Karaba, Huihe Zhu, Martin McCullagh, George C. Schatz and Frederick D. Lewis, *J. Phys. Chem. B*, **112**, 11415–21 (2008).
480. Theoretical investigation of hyperthermal reactions at the gas–liquid interface: $O(^3P)$ and squalane, Dongwook Kim and George C. Schatz, *J. Phys. Chem. A*, **111**, 5019–31 (2007).
481. Using theory and computation to model nanoscale properties, G. C. Schatz, *Proc. Natl. Acad. Sci. U.S.A.*, **104**, 6885–92 (2007).
482. Size-dependent angular distributions of low energy photoelectrons emitted from NaCl nanoparticles, Kevin R. Wilson, Shengli Zou, Eckart Rühl, Stephen R. Leone, George C. Schatz and Musahid Ahmed, *Nano Lett.*, **7**, 2014–9 (2007).

483. Interaction of plasmon and molecular resonances for rhodamine 6G adsorbed on silver nanoparticles, J. Zhao, L. Jensen, J. Sung, S. Zou, G. C. Schatz, R. P. Van Duyne, *J. Am. Chem. Soc.*, **129**, 7647–56 (2007).
484. Nanoscale fracture mechanics, Steven L. Mielke, Ted Belytschko and George C. Schatz, *Annu. Rev. Phys. Chem.*, **58**, 185–209 (2007).
485. Microscopic origin of the humidity dependence of the adhesion force in atomic force microscopy, Joonkyung Jang, Mino Yang, George Schatz, *J. Chem. Phys.* **126**, 174705/1–174705/6 (2007).
486. Kinetic lattice grand canonical Monte Carlo simulation for ion current calculations in a model ion channel system, Hyonseok Hwang, Mark A. Ratner, and George C. Schatz, *J. Chem. Phys.*, **127**, 024706/1–/10 (2007).
487. Time-dependent density functional theory examination of the effects of ligand adsorption on metal nanoparticles, Christine M. Aikens and George C. Schatz, In *Nanoparticles: synthesis, stabilization, passivation and functionalization*, R. Nagarajan and T. A. Hatton, Eds., ACS Books Symposium Series 996, American Chemical Society, Washington, DC, 2008, pp 108–121.
488. Modeling of electrodynamic interactions between metal nanoparticles aggregated by electrostatic interactions into closely packed clusters, A. O. Pinchuk, A. M. Kalsin, B. Kowalczyk, G. C. Schatz and B. A. Grzybowski, *J. Phys. Chem. C*, **111**, 11816–22 (2007).
489. Resonance vibrational Raman optical activity: a time-dependent density functional theory approach, L. Jensen, J. Autschbach, M. Krykunov and G. C. Schatz, *J. Chem. Phys.*, **127**, 134101/1–/11 (2007).
490. Modeling Ion Channels using Poisson-Nernst-Planck Theory as an Integrated Approach to Introducing Nanotechnology Concepts: The PNP Cyclic Peptide Ion Channel Model, Brian Radak, Hyonseok Hwang, George C. Schatz, *J. Chem. Educ.*, **85**, 744–48 (2008).
491. The effects of extensive pitting on the mechanical properties of carbon nanotubes, Steven L. Mielke, Sulin Zhang, Roopam, Khare, Rodney S. Ruoff, Ted Belytschko and George C. Schatz, *Chem. Phys. Lett.*, **446**, 128–132 (2007).
492. Significant nonadiabatic effects in the S(¹D) + HD reaction, Tian-Shu Chu, Ke-Li Han and George C. Schatz, *J. Phys. Chem. A*, **111**, 8286–90 (2007).
493. Near-field spectroscopy of surface plasmons in flat gold nanoparticles, M. Achermann, K. L. Shuford, G. C. Schatz, D. H. Dahanayaka, L. A. Bumm and V. I. Klimov, *Opt. Lett.*, **32**, 2254–6 (2007).
494. Crossed-Beams and Theoretical Studies of the O(³P) + H₂O → HO₂ + H Reaction Excitation Function, A. L. Brunsvold, Jianming Zhang, Hari P. Upadhyaya, Timothy K. Minton, Jon P. Camden, Jeffrey T. Paci and George C. Schatz, *J. Phys. Chem. A*, **111**, 10907–13 (2007).
495. Sharp Melting Transitions in DNA Hybrids Without Aggregate Dissolution: Proof of Nearest-Neighbor Cooperativity, Julianne M. Gibbs-Davis, George C. Schatz, Son Binh T. Nguyen, *J. Am. Chem. Soc.*, **129**, 15535–40 (2007).
496. Optical near-fields of triangular nanostructures, J. Boneberg, J. König-Birk, H.-J. Münzer, P. Leiderer, K. L. Shuford and G. C. Schatz, *Appl. Phys.*, **A89**, 299–303 (2007).
497. Ethical Responsibilities for Authors in *The Journal of Physical Chemistry*, G. C. Schatz, *J. Phys. Chem. A/B/C*, **111**, 8281 (2007).
498. Incorporation of inhomogeneous diffusion coefficients of ions into kinetic lattice grand canonical Monte Carlo simulations and its application to ion current calculations in a simple model ion channel, Hyonseok Hwang, George C. Schatz, and Mark A. Ratner, *J. Phys. Chem. A*, **111**, 12506–12 (2007).
499. Nanoparticle optical properties: Far- and near-field electrodynamic coupling in a chain of silver nanoparticles, A. O. Pinchuk and G. C. Schatz, *Mater. Sci. Eng. B*, **149**, 251–258 (2008).
500. Synthesis of heterodimeric sphere-prism nanostructures via metastable gold supraspheres, Rafal Klajn, Anatoliy O. Pinchuk, George C. Schatz and Bartosz A. Grzybowski, *Angew. Chem. Int. Ed.*, **46**, 8363–67 (2007).
501. Tailoring the parameters of nanohole arrays in gold films for sensing applications, George C. Schatz, Jeffrey M. McMahon and Stephen K. Gray, *Proc. SPIE* **6641**, 664103-1,3-8 (2007); Plasmonics: metallic Nanostructures and Their Optical Properties, V, Mark I. Stockman, Ed.
502. Nanoscale fracture of tetrahedral amorphous carbon by molecular dynamics: Flaw size insensitivity, Qiang Lu, Nigel Marks, George C. Schatz, Ted Belytschko, *Phys Rev. B*, **77**, 014109/1–/9 (2008).
503. Multiscale coupling schemes spanning the quantum mechanical, atomistic forcefield, and continuum regimes, Roopam Khare, Steven L. Mielke, George C. Schatz, Ted Belytschko, *Comput. Methods Appl. Mech. Eng.*, **197**, 3190–3202 (2008).
504. Phase diagram for assembly of biologically active peptide amphiphiles, Stefan Tsonchev, Krista L. Niece, George C. Schatz, Mark A. Ratner and Samuel I. Stupp, *J. Phys. Chem.*, **112**, 441–47 (2008).
505. Tailoring the sensing capabilities of nanohole arrays in gold films with Rayleigh anomaly surface plasmon polaritons, Jeffrey McMahon, Joel Henzie, Teri W. Odom, George C. Schatz and Stephen K. Gray, *Opt. Express*, **15**, 18119–29 (2007).
506. Trajectory surface hopping study of the O(³P) + ethylene reaction dynamics, Wenfang Hu, Gyorgi Lendvay, Biswajit Maiti and George C. Schatz, *J. Phys. Chem. A*, **112**, 2093–2103 (2008).
507. DNA-programmable nanoparticle crystallization, Sung Yong Park, Abigail K. R. Lytton-Jean, Byeongdu Lee, Steven Weigand, George C. Schatz, Chad A. Mirkin, *Nature*, **451**, 553–6 (2008).
508. Near-field polarization effects in molecular-motion-induced photochemical imaging, Christophe Hubert, Renaud Bachelot, Jérôme Plain, Sergei Kostechkov, Gilles Lerondel, Juan Mathieu, Pascal Royer, Shengli Zou, George C. Schatz, Gary Wiederrecht and Stephen Gray, *J. Phys. Chem. C*, **112**, 4111–6 (2008).
509. Editorial for January 2008, G. C. Schatz, *J. Phys. Chem. A/B/C*, **112**, 1–2 (2008).
510. Computational studies of the structure, behavior upon heating, and mechanical properties of graphite oxide, Jeffrey T. Paci, Ted Belytschko, George C. Schatz, *J. Phys. Chem. C*, **111**, 18099–111 (2007).
511. Electronic structure methods for studying surface-enhanced Raman scattering, L. Jensen, C. M. Aikens and G. C. Schatz, *Chem. Soc. Rev.*, **37**, 1061–73 (2008).
512. Effect of structural dynamics on charge transfer in DNA hairpins, Ferdinand C. Grozema, Stefano Tonzani, Yuri A. Berlin, George C. Schatz, Laurens D. A. Siebbeles, and Mark A. Ratner, *J. Am. Chem. Soc.*, **130**, 5157–66 (2008).
513. Molecular Plasmonics: Chromophore-Plasmon Coupling and Single Particle Nanosensors, Jing Zhao, Leif J. Sherry,

George C. Schatz, and Richard P. Van Duyne, *IEEE J. Selected Top. Quantum Electron.*, **14**, 1418–29 (2008).

514. A simple energy-scaling scheme for fine-tuning empirical potentials for coupled quantum mechanical/molecular mechanical studies, Roopam Khare, Steven L. Mielke, Jeffrey T. Paci, George C. Schatz, Ted. Belytschko, *Chem. Phys. Lett.*, **460**, 311–314 (2008).

515. Electronic excitations and spectra in single stranded DNA, S. Tonzani and G. C. Schatz, *J. Am. Chem. Soc.*, **130**, 7607–7612 (2008).

516. Correlating the crystal structure of a thiol-protected Au₂₅ cluster and optical properties, Manzhou Zhu, Christine M. Aikens, Frederick J. Hollander, George C. Schatz, Rongchao Jin, *J. Am. Chem. Soc.*, **130**, 5883–5 (2008).

517. Methods for describing the electromagnetic properties of anisotropic silver and gold nanoparticles, Jing Zhao, Anatoliy O. Pinchuk, Jeffrey M. McMahon, Shuzhou Li, Logan K. Ausman, Ariel L. Atkinson, George C. Schatz, *Acc. Chem. Res.*, **41**, 1710–1720 (2008).

518. Resonance localized surface plasmon spectroscopy: sensing substrate and inhibitor binding to cytochrome P450, Jing Zhao, Aditi Das, George C. Schatz, Stephen G. Sligar and Richard P. Van Duyne, *J. Phys. Chem. C*, **112**, 13084–88 (2008).

519. The effect of surface roughness on the extinction spectra and electromagnetic fields around gold nanoparticles, Shuzhou Li and George C. Schatz, *Mater. Res. Soc. Proc.*, **1087E**, V01–08 (2008).

520. Optical properties of gold pyramidal shape nanoshells, Kevin L. Shuford, Jeunghoon Lee, Teri W. Odom and George C. Schatz, *J. Phys. Chem. C*, **112**, 6662–6 (2008).

521. Toward Plasmonic Solar Cells: Protection of Silver Nanoparticles via Atomic Layer Deposition of TiO₂, Stacey Standridge, George C. Schatz and Joseph T. Hupp, *Langmuir*, **25**, 2596–2600 (2009).

522. Modeling self-assembly processes driven by nonbonded interactions in soft materials, Martin McCullagh, Tatiana Prytkova, Stefano Tonzani, Nicolas D. Winter and George C. Schatz, *J. Phys. Chem. B*, **112**, 10388–10398 (2008).

523. Localized surface plasmon resonance spectroscopy of triangular aluminum nanoparticles, George H. Chan, Jing Zhao, George C. Schatz and Richard P. Van Duyne, *J. Phys. Chem. C*, **112**, 13958–63 (2008).

524. Highly accurate first-principles benchmark data sets for the parametrization and validation of density functional and other approximate methods. Derivation of a robust, generally applicable, double-hybrid functional for thermochemistry and thermochemical kinetics, Amir Karton, Alex Tarnopolsky, Jean-Francois Lamere, George C. Schatz, and J. M. L. Martin, *J. Phys. Chem. A.*, **112**, 12868–12886 (2009).

525. From discrete electronic states to plasmons: TDDFT optical absorption properties of Ag_n ($n = 10, 20, 35, 56, 84, 120$) tetrahedral clusters, Christine M. Aikens, Shuzhou Li and George C. Schatz, *J. Phys. Chem. C*, **112**, 11272–11279 (2008).

526. Surface plasmon-mediated energy transfer in heterogap Au–Ag Nanowires, Wei Wei, Shuzhou Li, Lidong Qin, Can Xue, Jill E. Millstone, Xiaoyang Xu, George C. Schatz and Chad A. Mirkin, *Nano Lett.*, **8**, 3446–9 (2008).

527. Many-body theory of surface-enhanced Raman scattering, David J. Masiello and George C. Schatz, *Phys. Rev. A*, **78**, 042505/1–/24 (2008).

528. A discrete action principle for electrodynamics and the construction of explicit symplectic integrators, Jeffrey M.

McMahon, Stephen K. Gray and George C. Schatz, *J. Comput. Phys.*, in press, 2009.

529. Unusual mechanisms can dominate reactions at hyperthermal energies: an example from O(3P) + HCl → ClO + H, Jianming Zhang, Jon P. Camden, Amy L. Brunsvold, Hari P. Upadhyaya, Timothy K. Minton, George C. Schatz, *J. Am. Chem. Soc.*, **130**, 8896–7 (2008).

530. Highly cooperative behavior of peptide nucleic acid-linked DNA-modified gold nanoparticle and comb polymer aggregates, Abigail K. R. Lytton-Jean, Julianne M. Gibbs-Davis, Hai Long, George C. Schatz, Chad A. Mirkin and SonBinh T. Nguyen, *Adv. Mater.*, **21**, 706–9 (2008).

531. An electrochemical approach to and the physical consequences of preparing nanostructures from gold nanorods with smooth ends, Matthew Banholzer, Shuzhou Li, Jacob Ketter, Dorta Rozkiewica, George C. Schatz and Chad Mirkin, *J. Phys. Chem. C*, **112**, 15729–34 (2008).

532. An atomistic-continuum Cosserat rod model of carbon nanotubes, Karthick Chandraseker, Subrata Mukherjee, Jeffrey T. Paci and George C. Schatz, *J. Mech. Phys. Solids*, in press (2009).

533. Measurements of near-ultimate strength for multiwalled carbon nanotubes and irradiation-induced cross-linking improvements, Bei Peng, Mark Locascio, Peter Zapol, Shuyou Li, Steven L. Mielke, George C. Schatz and Horacio D. Espinosa, *Nat. Nanotechnol.*, **3**, 626–631 (2008).

534. Whispering-gallery mode resonators: surface enhanced Raman scattering without plasmons, Logan K. Ausman and George C. Schatz, *J. Chem. Phys.*, **129**, 054704/1–/10 (2008).

535. Optical absorption spectra and monomer interaction in polymers: investigation of exciton coupling in DNA hairpins, A. L. Burin, J. A. Dickman, D. B. Uskov, C. F. F. Hebbard, and G. C. Schatz, *J. Chem. Phys.*, **129**, 091102/1–/4 (2008).

536. Probing the structure of single molecule surface-enhanced Raman scattering hot spots, Jon P. Camden, Jon A. Dieringer, Yingmin Wang, David J. Masiello, Lawrence D. Marks, George C. Schatz and Richard P. Van Duyne, *J. Am. Chem. Soc.*, **130**, 12616–7 (2008).

537. Collective surface plasmon resonance coupling in silver nanoshell arrays. A. O. Pinchuk and G. C. Schatz, *Appl. Phys. B*, **93**, 31–38 (2008).

538. Dephasing of electromagnetic fields in scattering from an isolated slit in a gold film, Jeffrey M. McMahon, Stephen K. Gray and George C. Schatz, *Proc. SPIE*, **7033**, 703311, 1–6 (2008); Plasmonics: Nanoimaging, Nanofabrication, and Their Applications IV, Satoshi Kawata, Vladimir M. Shalaev, Din Ping Tsai, Eds.

539. Wavelength-scanned surface-enhanced resonance Raman excitation spectroscopy, Jing Zhao, Jon A. Dieringer, Xiaoyu Zhang, George C. Schatz, Richard P. Van Duyne, *J. Phys. Chem. C*, **112**, 19302–10 (2008).

540. Modeling reactive scattering of F(2P) at a liquid squalane interface: A hybrid QM/MM molecular dynamics study, Brian K. Radak, Scott Yockel, Dongwook Kim and George C. Schatz, *J. Phys. Chem. A*, in press (2009).

541. Plasmonic focusing in rod-sheath heteronanostructures, Xiaodong Chen, Shuzhou Li, Can Xue, Matthew J. Banholzer, George C. Schatz, Chad A. Mirkin, *ACS Nano*, **3**, 87–92 (2009).

542. Surface-enhanced Raman excitation spectroscopy of a single rhodamine 6G molecules, J. A. Dieringer, K. L. Wustholz, D. J. Masiello, J. P. Camden, S. L. Kleinman, G. C. Schatz and R. P. Van Duyne, *J. Am. Chem. Soc.*, **131**, 849–854 (2009).

543. Molecular dynamics simulation of DNA-functionalized gold nanoparticles, One Sun Lee and George C. Schatz, *J. Phys. Chem. C*, **113**, 2316–21 (2009).

544. Correlating the structure, optical spectra and electro-dynamics of single silver nanocubes, Jeffrey M. McMahon, Yingmin Wang, Leif J. Sherry, Richard P. Van Duyne, Laurence D. Marks, Stephen K. Gray, and George C. Schatz, *J. Phys. Chem. C*, **113**, 2731–35 (2009).

545. Coarse-grained molecular dynamics study of cyclic peptide nanotube insertion into a lipid bilayer, Hyonseok Hwang, George C. Schatz and Mark A. Ratner, *J. Phys. Chem. A*, **113**, 4780–87 (2009).

546. Editorial for 2009, George C. Schatz, *J. Phys. Chem. A/B/C*, **113**, 1 (2009).

547. Theoretical and experimental studies of the reactions between hyperthermal O(³P) and graphite: Graphene-based direct-dynamic and beam-surface scattering approaches, Jeffrey T. Paci, Hari P. Upadhyaya, Jianming Zhang, George C. Schatz and Timothy K. Minton, *J. Phys. Chem. A*, **113**, 4677–85 (2009).

548. Core–shell triangular bifrustrums, Hyojong Yoo, Jill E. Millstone, Shuzhou Li, Jae-Wong Jang, Wei Wei, Jinsong Wu, George C. Schatz and Chad A. Mirkin, *Angew. Chem.*, submitted (2009).

549. Experimental and theoretical investigations of the inelastic and reactive scattering dynamics of O(³P) collisions with ethane, Donna J. Garton, Timothy K. Minton, Wenfang Hu, George C. Schatz, *J. Phys. Chem. A*, **113**, 4722–38 (2009).

550. Hydrophobic dimerization and thermal dissociation of perylenediimide-linked DNA hairpins, Mahesh Hariharan, Yan Zheng, Hai Long, Tarek A. Zeidan, George C. Schatz, Josh Vura-Weis, Michael R. Wasielewski, Xiaobing Zuo, David M. Tiede, and Frederick D. Lewis, *J. Am. Chem. Soc.*, submitted (2009).

551. Reversible switching of magnetism in thiol-protected Au₂₅ superatoms, Manzhou Zhu, Christine M. Aikens, Michael P. Hendrich, Rupal Gupta, Huifeng Qian, George C. Schatz, and Rongchao Jin, *J. Am. Chem. Soc.*, **131**, 2490–2492 (2009).

552. Rayleigh anomaly surface plasmon polariton resonances in palladium and gold subwavelength hole arrays, H. Gao, J. M. McMahon, M. H. Lee, J. Henzie, S. K. Gray, G. C. Schatz and T. W. Odom, *Opt. Express*, **17**, 2334–40 (2009).

553. Gold nanoparticle dimer plasmonics: Finite element method calculations of the electromagnetic enhancement to surface-enhanced Raman spectroscopy, Jeffrey M. McMahon, Anne-Isabelle Henry, Kristin L. Wustholz, Michael J. Natan, R. Griffith Freeman, Richard P. Van Duyne and George C. Schatz, *Anal. Biochem.*, in press (2009).

554. Confining standing waves in optical corrals, Yelizaveta Babayan, Jeffrey M. McMahon, Shuzhou Li, Stephen K. Gray, George C. Schatz, and Teri W. Odom, *ACS Nano*, ASAP (2009).

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