

George C. Schatz
List of Publications

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, D. C., 1997, xii+330 pages. ISBN13: 9780841235342
3. **Introduction to Quantum Mechanics in Chemistry**, M. A. Ratner and G. C. Schatz, Prentice Hall, Upper Saddle River, NJ, 2001, x+296 pages. ISBN 0-13-895491-7
4. **Frontiers of Plasmon Enhanced Spectroscopy**, Volume 1 and Volume 2, Y. Ozaki, G. C. Schatz, D. Graham and T. Itoh, ACS Symposium Series Vols. 1245 and 1246, American Chemical Society, Washington, D. C., 210 and 271 pp (2016) ISBN13: 9780841232013, ISBN13: 9780841232037

Patent application and Patents:

Nanoparticulate Nanosensors, NU application 22078/23008/25033, filed May 2005 based on provisional patents 10/784,129 filed Feb. 20, 2004 and 60/448,592 filed Feb. 20, 2003.

Immobilized Nano Rod Assembly (INRA): Multi-scale Fabrication Technique for Plasmonic Substrates, NU application 2012-143, filed Oct. 26, 2012

Broadband plasmonic absorber with hotspot generating gapped nanoantennas, NU application 2012-136, filed Nov. 5, 2012. Provisional application serial number 61/722,319.

Compositions, devices and methods for SERS and LSPR, Van Duyne, Richard P.; Zhang, Xiaoyu; Zhao, Jing; Whitney, Alyson V.; Elam, Jeffrey W.; Schatz, George C.; Stair, Peter C.; Zou, Shengli; Young, Matthew; Lyandres, Olga, Patent No. US 8,628,727 B2, dated Jan. 14, 2014

Conical pore ion pump for desalination, Yu Zhang and George C. Schatz, NU application NU2017-086, filed May 5, 2017

Photonic crystal built with nanoparticles and spacer groups, NU application 2017-130, ChadA. Mirkin, George C. Schatz, Haixing Lin and Lin Sun, filed July 14, 2017

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).
Doi: 10.1063/1.1676413
2. Chemiluminescence Excited by Atomic Fluorine, G.C. Schatz and M. Kaufman, *J. Phys. Chem.*, **76**, 3586-90 (1972).
Doi: 10.1021/j100668a015

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).
Doi: 10.1016/0009-2614(73)87052-6
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).
Doi: 10.1063/1.1679760
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).
Doi: 10.1063/1.1680122
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).
Doi: 10.1016/0009-2614(74)85282-6
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).
Doi: 10.1063/1.1681746
8. Quantum Mechanical Reactive Scattering: An Accurate Three-Dimensional Calculation, Aron Kuppermann and G.C. Schatz, *J. Chem. Phys.*, **62**, 2502-4 (1975).
Doi: 10.1063/1.430733
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).
Doi: 10.1063/1.431390
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).
Doi: 10.1063/1.431391
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).
Doi: 10.1103/PhysRevLett.35.1266
12. The Quantum Dynamics of Atom Plus Diatom Chemical Reactions, G.C. Schatz, Ph.D. Thesis, California Institute of Technology, 1975.
<http://de.scientificcommons.org/15473309>
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).
Doi: 10.1063/1.432916

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).
Doi: 10.1063/1.432917
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).
Doi: 10.1063/1.432918
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).
Doi: 10.1063/1.432919
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).
Doi: 10.1063/1.434059
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).
Doi: 10.1063/1.434060
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).
Doi: 10.1016/0009-2614(77)85211-1
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).
Doi: 10.1063/1.434363
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).
Doi: 10.1063/1.434395
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).
Doi: 10.1063/1.433785
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).
Doi: 10.1016/0301-0104(77)85233-6
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).

Doi: 10.1016/0009-2614(78)80111-0

25. A Direct Method for Determining Moments of Final State Distributions in Molecular Collisions, G.C. Schatz, *Mol. Phys.*, **35**, 477-500 (1978).
Doi: 10.1080/00268977800100351
26. The Importance of Anharmonicity on the Rates of Energy Transfer in Rare Gas/CO₂ Systems, G.C. Schatz and M.D. Moser, *J. Chem. Phys.*, **68**, 1992-1993 (1978).
Doi: 10.1063/1.435877
27. A Generalized Langevin Equation Approach to Molecular Collision Dynamics, G.C. Schatz, *Chem. Phys.*, **31**, 295-307 (1978).
Doi: 10.1016/0301-0104(78)87044-X
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).
Doi: 10.1016/0009-2614(78)85055-6
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).
Doi: 10.1063/1.436436
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).
Doi: 10.1016/0301-0104(78)85209-4
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).
Doi: 10.1016/0301-0104(79)85068-5
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).
Doi: 10.1063/1.437752
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).
Doi: 10.1063/1.437783
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).
Doi: 10.1080/00268977900101641
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).
Doi: 10.1021/j100471a021

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).
Doi: 10.1063/1.438336
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).
Doi: 10.1063/1.439518
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).
Doi: 10.1063/1.438130
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).
Doi: 10.1063/1.439399
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).
Doi: 10.1063/1.439421
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).
Doi: 10.1016/0301-0104(80)85069-5
42. Collisional Energy Transfer as a Probe of Ergodicity in Molecular Vibrational Motions, G.C. Schatz, *Chem. Phys. Lett.* **67**, 248-251 (1979).
Doi: 10.1016/0009-2614(79)85156-8
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).
Doi: 10.1063/1.438920
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).
Doi: 10.1063/1.440448
45. A Quasiclassical Trajectory Study of Collisional Excitation in Li⁺ + CO₂, G.C. Schatz, *J. Chem. Phys.*, **72**, 3929-3938 (1980).
Doi: 10.1063/1.439662
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).
Doi: 10.1016/0039-6028(80)90639-1

47. A Quasi-Classical Trajectory Study of Product Vibrational Distributions in the $\text{OH} + \text{H}_2 \rightarrow \text{H}_2\text{O} + \text{H}$ Reaction, G.C. Schatz and H. Elgersma, *Chem. Phys. Phys. Lett.*, **73**, 21-24 (1980).
Doi: 10.1016/0009-2614(80)85193-1
48. On the Mode Specificity of Reaction Rate Enhancements, G.C. Schatz, *J. Chem. Soc. Far. Disc.* **67**, 140-141 (1979).
49. On the Use of Mass Scaled Cluster Coordinates to Describe Polyatomic Molecule Reaction Dynamics: Application to $\text{O} + \text{CS}_2 \rightarrow \text{SO} + \text{CS}$, Henry Elgersma and George C. Schatz, *Chem. Phys.*, **54**, 201-216 (1981).
Doi: 10.1016/0301-0104(81)80235-2
50. *Ab initio* Calculation of Transition State Normal Mode Properties and Rate Constants for the $\text{H}(\text{T}) + \text{CH}_4(\text{CD}_4)$ Abstraction and Exchange Reactions, George C. Schatz, Stephen P. Walch and Albert F. Wagner, *J. Chem. Phys.*, **73**, 4536-4547 (1980).
Doi: 10.1063/1.440692
51. A Quasiclassical Trajectory Study of Reagent Vibrational Excitation Effects in the $\text{OH} + \text{H}_2 \rightarrow \text{H}_2\text{O} + \text{H}$ Reaction, George C. Schatz, *J. Chem. Phys.*, **74**, 1133-1139 (1981).
Doi: 10.1063/1.441220
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).
Doi: 10.1016/0009-2614(80)80496-9
53. An Analytical Fit to an Accurate *ab initio* ($^1\text{A}_1$) Potential Surface of H_2O . Michael J. Redmon and George C. Schatz, *Chem. Phys.*, **54**, 365-374 (1981).
Doi: 10.1016/0301-0104(81)85112-9
54. A Quasiclassical Trajectory Study of Product Rotational, Angular and Projection Distributions in the $\text{OH} + \text{H}_2 \rightarrow \text{H}_2\text{O} + \text{H}$ Reaction, G.C. Schatz and H. Elgersma, in: **Potential Energy Surfaces and Dynamics Calculations**, D.G. Truhlar, ed., Plenum, New York, 1981, 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, 287-310.
56. The Evaluation of Fitting Functions for the Representation of an $\text{O} + \text{H}_2$ Potential Energy Surface, A.F. Wagner, G.C. Schatz and J. M. Bowman, *J. Chem. Phys.*, **74**, 4960-4983 (1981).
Doi: 10.1063/1.441749
57. A Comparative Study of the Reaction Dynamics of Several Potential Energy Surfaces of $\text{O} (^3\text{P}) + \text{H}_2 \rightarrow \text{OH} + \text{H}$, I, G.C. Schatz, A.F. Wagner, S.P. Walch and J.M. Bowman, *J. Chem. Phys.*, **74**, 4984-4996 (1981).
Doi: 10.1063/1.441750
58. Collisional Excitation of H_2O 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. Saatz, G.C.

- Schatz, and I. Shavitt, in: **Potential Energy Surfaces and Dynamics Calculations**, D. G. Truhlar, ed., Plenum, New York, 1981, 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), p. 25-60.
 60. Quasiclassical Trajectory Study of Collisional Excitation in $O(^3P) + CO_2$, G.C. Schatz and M.J. Redmon, *Chem. Phys.*, **58**, 195-202 (1981).
Doi: 10.1016/0301-0104(81)80056-0
 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).
Doi: 10.1063/1.441815
 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).
Doi: 10.1021/j150625a019
 63. A Quasiclassical Trajectory Study of Mode Specific Reaction Rate Enhancements in $H + H_2O$ (v_1, v_2, v_3) $\rightarrow OH + H_2$, H. Elgersma and G.C. Schatz, *Int. J. Quant. Chem. Symp.*, **15**, 611-619 (1981).
Doi: 10.1002/qua.560200864
 64. A Comparative Study of the Reaction Dynamics of the $O(^3P) + H_2 \rightarrow OH + H$ 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).
Doi:10.1063/1.443394
 65. A Comparative Study of the Reaction Dynamics of the $O(^3P) + H_2 \rightarrow OH + H$ 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).
Doi: 10.1063/1.443395
 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).
Doi: 10.1016/0009-2614(81)85442-5
 67. The Image Field Effect: How Important Is It? G.C. Schatz, in: **Surface Enhanced Raman Scattering**, R.K. Chang and T.E. Furtak, ed., Plenum, New York, 1982, pages 35-50.
<http://stinet.dtic.mil/oai/oai?&verb=getRecord&metadataPrefix=html&identifier=ADA099606>
 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).

Doi: 10.1063/1.443370

69. Energy Transfer, Stabilization and Dissociation in Collisions of He with Highly Excited HO₂, C.R. Gallucci and G.C. Schatz, *J. Phys. Chem.*, **86**, 2352-2358 (1982).
Doi: 10.1021/j100210a022
70. An **ab initio** Determination of the Rate Constant for H₂ + C₂H → H + C₂H₂, L.B. Harding, G.C. Schatz and R.A. Chiles, *J. Chem. Phys.*, **76**, 5172-5173 (1982).
Doi: 10.1063/1.442821
71. An **ab initio** Determination of the Rate Constant for H + H₂CO → H₂ + HCO, L.B. Harding and G.C. Schatz, *J. Chem. Phys.*, **76**, 4296-4297 (1982).
Doi: 10.1063/1.443472
72. Time Dependent Hartree-Fock Calculations of Surface Enhanced Raman Intensities: I. H₂ Adsorbed on a Model Li Cluster, P.K.K. Pandey and G.C. Schatz, *Chem. Phys. Lett.*, **88**, 193-197 (1982).
Doi: 10.1016/0009-2614(82)83366-6
73. **Ab initio** Calculation of the Transition State Properties and Addition Rate Constants for H + C₂H₂ 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).
Doi: 10.1021/j100219a009
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).
Doi: 10.1063/1.444776
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).
Doi: 10.1016/0009-2614(82)80157-7
76. Orientation Dependence of Surface Enhanced Raman Intensities: Results from *Ab Initio* Calculations, P.K.K. Pandey and G.C. Schatz, *J. Electron Spectroscopy and Related Phenomena*, **29**, 351-355 (1983).
Doi: 10.1016/0368-2048(83)80087-5
77. The Quantum Dynamics of H + H₂ (v = 1): A Coupled States Study of Cross Sections and Rate Constants, G.C. Schatz, *Chem. Phys. Lett.*, **94**, 183-187 (1983).
Doi: 10.1016/0009-2614(83)87570-8
78. A Theoretical Study of Deuterium Isotope Effects in the Reactions H₂ + CH₃ and H + CH₄, G.C. Schatz, A.F. Wagner and T.H. Dunning, *J. Phys. Chem.*, **88**, 221-232 (1984).
Doi: 10.1021/j150646a013
79. Analytical Potential Energy Surfaces for Ethynyl (C₂H), Acetylene (C₂H₂) and Vinyl (C₂H₃), K.A. White and G.C. Schatz, *J. Phys. Chem.*, **88**, 2049-2057 (1984).

Doi: 10.1021/j150654a023

80. Dynamical Instabilities and Structural Changes in Molecules, B. Barboy, G.C. Schatz, M.A. Ratner and R.B. Gerber, *Mol. Phys.*, **50**, 353 (1983).
Doi: 10.1080/00268978300102401
81. Dissociation Dynamics of Vibrationally Excited Van der Waals Clusters: $I_2XY \rightarrow X + Y$ ($X, Y = \text{He, Ne}$); G.C. Schatz, V. Buch, M.A. Ratner and R.B. Gerber, *J. Chem. Phys.*, **79**, 1808-1822 (1983).
Doi: 10.1063/1.446026
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).
Doi: 10.1063/1.445702
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).
Doi: 10.1063/1.446107
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).
Doi: 10.1016/0301-0104(83)85266-5
85. Plasmon Resonance Broadening in Spheroidal Metal Particles, W.A. Kraus and G.C. Schatz, *Chem. Phys. Lett.*, **99**, 353-357 (1983).
Doi: 10.1016/0009-2614(83)87555-1
86. Plasmon Resonance Broadening in Small Metal Particles, W.A. Kraus and G.C. Schatz, *J. Chem. Phys.*, **79**, 6130-6139 (1983).
Doi: 10.1063/1.445794
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).
Doi: 10.1063/1.447045
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).
Doi: 10.1021/j150646a012
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).
Doi: 10.1021/j150658a011
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).

Doi: 10.1063/1.447367

91. Theoretical Studies of Surface Enhanced Raman Scattering, G.C. Schatz, *Accounts of Chemical Research*, **17**, 370-376 (1984).
Doi: 10.1021/ar00106a005
92. Semiclassical Vibrational Eigenvalues of Triatomic Molecules: Application of the FFT Method to SO₂, H₂O, H₃⁺ and CO₂, C.W. Eaker and G.C. Schatz, *J. Chem. Phys.*, **81**, 2394-2399 (1984).
Doi: 10.1063/1.447939
93. A Coupled States Quantum Reactive Scattering Study of H + D₂ → HD + D at E_{rel} (v = j = 0) = 0.55 eV, G.C. Schatz, *Chem. Phys. Lett.*, **108**, 532-534 (1984).
Doi: 10.1016/0009-2614(84)85048-4
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, editor (American Chemical Society, Washington D.C., 1984), p. 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, **Dynamics on Surfaces**, edited by B. Pullman, *Proceedings of the 17th Jerusalem Symposium on Quantum Chemistry and Biochemistry* (Reidel, Dordrecht, Holland, 1984), p. 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).
Doi: 10.1063/1.447592
97. Theories of Time Dependent Chemical Phenomena, G.C. Schatz, in *The Register of Phi Lambda Upsilon*, Vol. 69, p. 13-16, 1984.
98. A Quasiclassical Trajectory Study of the H₂⁺ + H₂ → H₃⁺ + H Reaction, C.W. Eaker and G.C. Schatz, *J. Phys. Chem.*, **89**, 2612-2620 (1985).
Doi: 10.1021/j100258a036
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).
Doi: 10.1016/0009-2614(85)85133-2
100. Theoretical Studies of Fast H Atom Collisions with NO, M.C. Colton and G.C. Schatz, *J. Chem. Phys.*, **83**, 3413-3425 (1985).
Doi: 10.1063/1.449146
101. A Quantum Reactive Scattering Study of Mu + H₂ → MuH + H, G.C. Schatz, *J. Chem. Phys.*, **83**, 3441-3448 (1985).
Doi: 10.1063/1.449845

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).
Doi: 10.1063/1.449148
103. Recent Quantum Scattering Calculations on the H + H₂ Reaction and Its Isotopic Counterparts, G.C. Schatz, in **Theory of Chemical Reaction Dynamics**, D.C. Clary, editor, Proceedings of NATO Workshop, Orsay, France, 1986 (D. Reidel, Dordrecht, 1986) p. 1-26.
104. A Coupled States Distorted Wave Study of the O(³P) + H₂ (D₂, HD, DH) Reaction, G. C. Schatz, *J. Chem. Phys.*, **83**, 5677-5686 (1985).
Doi: 10.1063/1.449862
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).
Doi: 10.1063/1.450386
106. Test of Variational Transition State Theory and Multidimensional Semiclassical Transmission Coefficients Methods Against Accurate Quantal Rate Constants for H + H₂/HD, D + H₂ and O + H₂/D₂/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).
Doi: 10.1021/ja00271a015
107. Future Directions for Supercomputer Use in Chemistry, by G.C. Schatz (Proceedings of Workshop on Supercomputers in Chemistry, Evanston, IL 1984), National Science Foundation, 1985.
108. Theoretical Studies of Chemical Reactions, T. H. Dunning, Jr., L. B. Harding, A. F. Wagner, R. A. Bair, R. L. Shephard, M. J. Davis, J. M. Bowman and G. C. Schatz, in **Proceedings of Workshop on Theory and Modelling for Materials Design (Texas A&M University, College Station, TX, 1984)** published by U.S. Department of Energy, 1985.
Simulation in Materials Science, George C. Schatz, Information and Communications, The National Academies Press, Washington, D. C., 2003, pp. 146-151.
109. Theoretical Studies of Vibrational Excitation in Collisions of O(³P) with H₂O(¹A₁), M. J. Redmon, B. C. Garrett and G. C. Schatz, *J. Chem. Phys.*, **84**, 764-773 (1986).
Doi: 10.1063/1.450574
110. A Coupled States Reactive Scattering Study of Bending Excited Resonances in Three Dimensional H + H₂, M. C. Colton and G. C. Schatz, *Chem. Phys. Lett.*, **124**, 256-9 (1986).
Doi: 10.1016/0009-2614(86)87041-5
111. A Coupled States Calculation of Accurate Quantum Rate Constants for H + H₂, M. C. Colton and G. C. Schatz, *Int. J. of Chem. Kinetics*, **18**, 961-975 (1986).
Doi: 10.1002/kin.550180907
112. A Theoretical Study of Complex Formation, Isotope Effects and Energy Partitioning in the O(¹D) + H₂(D₂, HD) Reaction, M. S. Fitzcharles and G. C. Schatz, *J. Phys. Chem.*, **90**, 3634-3644 (1986).

Doi: 10.1021/j100407a034

113. Tunnelling in Bimolecular Collisions, G. C. Schatz, *Chemical Reviews*, **87**, 81-89 (1987).
Doi: 10.1021/cr00077a004
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).
Doi: 10.1063/1.451148
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. Badenhop and C. W. Eaker, *Int. J. Quant. Chem. Symp.*, **31**, 57-63 (1987).
Doi: 10.1002/qua.560310107
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).
Doi: 10.1016/0009-2614(86)80293-7
117. The Rate Constants for the $H + H_2$ Reaction and Its Isotopic Analogs at Low Temperatures: Wigner Threshold Low Temperature Behavior, T. Takayanagi, N. Masaki, K. Nakamura, M. Okamoto, S. Sato and G. C. Schatz, *J. Chem. Phys.*, **86**, 6133-9 (1987).
Doi: 10.1063/1.452453
118. Superminicomputer Accelerates Combustion Research, G. C. Schatz, *Research & Development*, **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).
Doi: 10.1021/j100287a028
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).
Doi: 10.1016/0009-2614(86)80683-2
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).
Doi: 10.1063/1.451985
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).
Doi: 10.1063/1.452373
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, *Comp. Phys. Comm.*, **47**, 45-53 (1987).
Doi : 10.1016/0010-4655(87)90065-8

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).
Doi: 10.1063/1.452923
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).
Doi: 10.1063/1.453649
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, *Far. Disc. Chem. Soc.*, **84**, 359-369 (1987).
Doi: 10.1039/DC9878400359
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, *Far. Disc. Chem. Soc.*, **84**, 387-403 (1987).
Doi: 10.1039/DC9878400387
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).
Doi: 10.1021/j100322a030
129. Spatially Resolved Surface Enhanced Second Harmonic Generation: Theoretical and Experimental Evidence for Electrodynamical 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).
Doi: 10.1063/1.456129
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).
Doi: 10.1063/1.454251
131. A Theoretical Study of the Oriented Reaction $HBr + CO_2 + hv \rightarrow OH + CO + Br$, G. C. Schatz and M. S. Fitzcharles, in **Selectivity in Chemical Reactions**, edited by J. C. Whitehead (NATO ASI C245), Kluwer, Dordrecht, 1988, p. 353-364.
132. Energies and Lifetimes of Predissociative States of van der Waals Molecules: Self-Consistent Field Calculations for $I_2(v)He$, $I_2(v)Ne$, G. C. Schatz, R. B. Gerber and M. A. Ratner, *J. Chem. Phys.*, **88**, 3709-3714 (1988).
Doi: 10.1063/1.453870
133. State-Selective Studies of $T \rightarrow R, V$ Energy Transfer: The $H + CO$ System, G. K. Chawla, G. C. McBane, P. L. Houston and G. C. Schatz, *J. Chem. Phys.*, **88**, 5481-5488 (1988).
Doi: 10.1063/1.454559

134. A Program for Determining Primitive Semiclassical Eigenvalues for Vibrating/Rotating Nonlinear Triatomic Molecules, G. C. Schatz, *Comp. Phys. Comm.*, **51**, 135-147 (1988).
Doi : 10.1016/0010-4655(88)90067-7
135. Quantum Effects in Gas Phase Bimolecular Chemical Reactions, G. C. Schatz, *Annu. Rev. Phys. Chem.*, **39**, 317-340 (1988).
Doi: 10.1146/annurev.pc.39.100188.001533
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).
<http://www.jstor.org/stable/1701183>
137. Theoretical Studies of Collisional Energy Transfer in Highly Excited Molecules: The Importance of Intramolecular Vibrational Redistribution in Successive Collision Modelling of He + CS₂, M. Bruehl and G. C. Schatz, *J. Chem. Phys.*, **89**, 770-779 (1988).
Doi: 10.1063/1.455200
138. Quantum Reactive Scattering Using Hyperspherical Coordinates: Results for H + H₂ and Cl + HCl, G. C. Schatz, *Chem. Phys. Lett.*, **150**, 92-98 (1988).
Doi: 10.1016/0009-2614(88)80402-0
139. Oscillating Reactivity and Resonances in the Three Dimensional Cl + HCl Reaction, G. C. Schatz, *Chem. Phys. Lett.*, **151**, 409-14 (1988).
Doi: 10.1016/0009-2614(88)85158-3
140. Theoretical Studies of Collisional Energy Transfer in Highly Excited Molecules: Temperature and Potential Surface Dependence of Relaxation in He, Ne, Ar + CS₂, M. Bruehl and G. C. Schatz, *J. Phys. Chem.*, **92**, 3190-95 (1988).
Doi: 10.1021/j100337a013
141. Collision Induced Dissociation of H₂⁺ and D₂⁺ with H₂ using a Surface Hopping Trajectory Method, C. W. Eaker and G. C. Schatz, *J. Chem. Phys.*, **89**, 6713-6718 (1988).
Doi: 10.1063/1.455344
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**, edited by T. H. Dunning, Jr. (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).
Doi: 10.1103/RevModPhys.61.669
144. A Three Dimensional Reactive Scattering Study of the Photodetachment Spectrum of ClHCl, G. C. Schatz, *J. Chem. Phys.*, **90**, 3582-9 (1989).
Doi: 10.1063/1.455817

145. Spectroscopy of High Vibrational Levels of the N–N Stretching Mode of N–N-¹⁶O and N–N-¹⁸O, N. L. S. Yamasaki, C. Manzanares, L. C. Baylor, G. C. Schatz, and E. Weitz, *J. Phys. Chem.*, **93**, 2204-9 (1989).
Doi: 10.1021/j100343a007
146. A Three Dimensional Quantum Reactive Scattering Study of the I + HI Reaction and of the IHI⁻ Photodetachment Spectrum, G. C. Schatz, *J. Chem. Phys.*, **90**, 4847-4854 (1989).
Doi: 10.1063/1.456578
147. A Reduced Dimensionality Quantum Reactive Scattering Study of the Insertion Reaction O(¹D) + H₂ → OH + H, J. K. Badenhop, H. Koizumi and G. C. Schatz, *J. Chem. Phys.*, **91**, 142-9 (1989).
Doi: 10.1063/1.457502
148. Rotational Distributions in the Photodetachment of IHI⁻ and in the I + HI Reaction: The influence of IHI Transition State Resonances, G. C. Schatz, *Is. J. Chem.*, **29**, 361-7 (1989).
149. A Coupled Channel Quantum Scattering Study of Alignment Effects in Na(²P_{3/2}) + He → Na(²P_{1/2}) + He Collisions, G. C. Schatz, L. J. Kovalenko and S. R. Leone, *J. Chem. Phys.*, **91**, 6961-72 (1989).
Doi: 10.1063/1.457313
150. Transition State Resonances in Collinear O(³P) + HCl → OH + Cl, H. Koizumi and G. C. Schatz, *Int. J. Quant. Chem.*, **23**, 137-45 (1989).
Doi: 10.1002/qua.560360817
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).
Doi: 10.1063/1.458097
152. A Centrifugal Sudden Distorted Wave Study of the Cl + HCl → ClH + 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).
Doi: 10.1063/1.457706
153. Reduced-Dimensionality Quantum Calculations of the Thermal Rate Coefficient for the Cl + HCl → ClH + 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).
Doi: 10.1063/1.457706
154. A Three-Dimensional Quantum Reactive Scattering Study of the I + DI Reaction and of the IDI⁻ Photodetachment Spectrum, G. C. Schatz, *J. Chem. Soc. Faraday Trans.*, **86**, 1729-35 (1990).
Doi: 10.1039/FT9908601729
155. Three Dimensional Quantum Scattering Studies of Transition State Resonances: Results for O + HCl → OH + Cl, H. Koizumi and G. C. Schatz, in **Molecular Vibrations (Vol. IA)**, edited by J. M. Bowman and M. A. Ratner (JAI Press, Greenwich, CT, 1990), pp. 139-164.

156. The Evolution of Vibrational Phase Space During the Collisional Relaxation of Highly Excited CS₂, M. Bruehl and G. C. Schatz, *J. Chem. Phys.*, **92**, 6561-6573 (1990).
Doi: 10.1063/1.458292
157. Quantum Theory of Photodetachment Spectra of Transition States, G. C. Schatz, *J. Phys. Chem.*, **94**, 6157-6164 (1990).
Doi: 10.1021/j100379a005
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).
Doi: 10.1063/1.459538
159. A Centrifugal Sudden Distorted Wave Study of Isotope Effects for the Reactions Cl + HCl → ClH + Cl and Cl + DCl → ClD + Cl, G. C. Schatz, B. Amaee and J. N. L. Connor, *J. Chem. Phys.*, **93**, 5544 (1990).
Doi: 10.1063/1.459624
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).
Doi: 10.1063/1.460353
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).
Doi: 10.1021/j100389a003
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).
Doi: 10.1021/j100161a026
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).
Doi: 10.1063/1.460020
164. Influence of Transition State Resonances on Integral Cross Sections and Product Rovibrational Distributions for the Cl + HCl → ClH + Cl Reaction, G. C. Schatz, D. Sokolovski, and J. N. L. Connor, *J. Chem. Phys.*, **94**, 4311-19 (1991).
Doi: 10.1063/1.460617
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, *Far. Disc. Chem. Soc.*, **91**, 17-30 (1991).
Doi: 10.1039/DC9919100017
166. A Quasiclassical Trajectory Study of H + CO₂ → OH + 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).

Doi: 10.1021/j100174a047

167. Quantum Non-adiabatic Effects in the Photodissociation of Vibrationally Excited CH₃I, H. Guo, K. Q. Lao, G. C. Schatz and A. D. Hammerich, *J. Chem. Phys.*, **94**, 6562-8 (1991).
Doi: 10.1063/1.460283
168. A Quasiclassical Trajectory Study of the OH + CO Reaction, K. Kudla, G. C. Schatz, and A. F. Wagner, *J. Chem. Phys.*, **95**, 1635-47 (1991).
Doi: 10.1063/1.461076
169. A Coupled Channel Study of HN₂ 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).
Doi: 10.1063/1.460768
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).
Doi: 10.1016/0009-2614(91)87195-H
171. HN₂ and DN₂ Resonance Spectra: Scattering and Stabilization Calculations, H. Koizumi, G. C. Schatz, and J. M. Bowman, in **Isotope Effects in Gas-Phase Chemistry**, edited by J. A. Kaye, ACS Symp. Series, No. 502, 1992, pp. 37-47.
172. Energy Dependence of Energy Transfer in Collisional Relaxation of Vibrationally Highly Excited CS₂, G. Lendvay and G. C. Schatz, *J. Phys. Chem.* **95**, 8748-53 (1991).
Doi: 10.1021/j100175a061
173. An Analytical Representation of the Lowest Potential Energy Surface for the Reaction O(³P) + HCl(X¹Σ) → OH(X²Π) + Cl(²P), H. Koizumi, G. C. Schatz, and M. S. Gordon, *J. Chem. Phys.* **95**, 6421-28 (1991).
Doi: 10.1021/j100175a061
174. A Reduced Dimension Quantum Reactive Scattering Study of OH + CO → H + CO₂, G. C. Schatz and J. Dyck, *Chem. Phys. Lett.*, **188**, 11-15 (1992).
Doi: 10.1016/0009-2614(92)85080-T
175. Trajectory Studies of Collisional Relaxation of Highly Excited CS₂ by H₂, CO, HCl, CS₂ and CH₄, G. Lendvay and G. C. Schatz, *J. Chem. Phys.*, **96**, 4356-65 (1992).
Doi: 10.1063/1.462827
176. A Quasiclassical Trajectory Study of OH Rotational Excitation in OH + 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).
Doi: 10.1063/1.462397
177. A Quantum Scattering Study of the Cl + HCl → ClH + 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).
Doi: 10.1063/1.463703
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).
Doi: 10.1021/j100188a035
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).
Doi: 10.1016/0009-2614(92)85840-7
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).
Doi: 10.1063/1.463511
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).
Doi: 10.1063/1.462965
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).
Doi: 10.1063/1.463460
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).
10.1063/1.463502
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, Volume 1, pp. 759-774 (2002).
http://chemgroups.northwestern.edu/vanduyne/pdf/Sersreview_0601_o.pdf
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).
Doi: 10.1016/0009-2614(93)85591-B
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).
Doi: 10.1016/0009-2614(93)90037-2
188. Collisional Energy Transfer from Highly Excited SF_6 , G. Lendvay and G. C. Schatz, *J. Chem. Phys.*, **98**, 1034-41 (1993).
Doi: 10.1063/1.464328

189. Theoretical Studies of Energy Transfer and Reaction in $H + H_2O$ and $H + D_2O$ Collisions, K. Kudla and G. C. Schatz, *J. Chem. Phys.*, **98**, 4644-51 (1993).
Doi: 10.1063/1.464992
190. Theoretical Studies of the Reactions $H + CH \rightarrow C + H_2$ and $C + H_2 \rightarrow CH_2$ 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).
Doi: 10.1021/j100123a005
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).
Doi: 10.1016/0009-2614(93)85527-U
192. A Quasiclassical Trajectory Study of Mode Specific Reaction Dynamics in the $Cl + HOD$ and $H + HOD$ Reactions, K. Kudla and G. C. Schatz, *Chem. Phys.*, **175**, 71-82 (1993).
Doi: 10.1016/0301-0104(93)80229-3
193. Quantum and Quasiclassical Calculations on the $OH + CO \rightarrow CO_2 + H$ Reaction, D. C. Clary and G. C. Schatz, *J. Chem. Phys.*, **99**, 4578-89 (1993).
Doi: 10.1063/1.466057
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).
Doi: 10.1063/1.466149
195. A Coupled Channel Hyperspherical Scattering Study of the $Cl + HCl \rightarrow ClH + Cl$ 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).
Doi: 10.1139/v94-117
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**, J. A. Barker, ed., *Advances in Chemical Kinetics and Dynamics*, Vol. 2B (JAI Press, 1995), pp. 481-513.
197. Product State Distributions in Chemical Reactions: The Reaction $OH + CO \rightarrow H + CO_2$. K. Kudla and G. C. Schatz, In **The Chemical Dynamics and Kinetics of Small Radicals** edited by K. Liu and A. F. Wagner (World Scientific, 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).
Doi: 10.1103/PhysRevB.49.8320
199. Transition States of Chemical Reactions, G. C. Schatz, *Science*, **262**, 1828-9 (1993)
<http://www.jstor.org/stable/2882816>

200. A Quasiclassical Trajectory Study of Product Energy and Angular Distributions in OH + H₂(D₂), K. S. Bradley and G. C. Schatz, *J. Phys. Chem.*, **98**, 3788-95 (1994).
Doi: 10.1021/j100065a039
201. Differential Cross Sections for Fine Structure Transitions in O(³P₂) + Ar Collisions, Z. Ma, K. Liu, L. B. Harding, M. Komotos, and G. C. Schatz, *J. Chem. Phys.*, **100**, 8026-39 (1994).
Doi: 10.1063/1.466796
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).
Doi: 10.1364/JOSAB.11.002036
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).
Doi: 10.1021/j100077a018
204. Experimental and Theoretical Study of the O + 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).
Doi: 10.1063/1.468463
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).
Doi: 10.1063/1.468352
206. Global Potential Energy Surfaces for the Lowest ¹A', ³A'' and ²A'' States of HNO, R. Guadagnini, G. C. Schatz and S. P. Walch, *J. Chem. Phys.*, **102**, 774-83 (1995).
Doi: 10.1063/1.469191
207. Quasiclassical Trajectory Studies of N + OH, O + NH and H + 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).
Doi: 10.1063/1.469192
208. Quasiclassical Trajectory Studies of State Resolved Bimolecular Reactions: Vibrational Distributions in Triatomic Products, G. C. Schatz, *J. Phys. Chem.*, **99**, 516-24 (1995).
Doi: 10.1021/j100002a012
209. The Influence of Atomic Fine-Structure on Bimolecular Rate Constants: The Cl(²P) + HCl Reaction, G. C. Schatz, *J. Phys. Chem.*, **99**, 7522-29, 1995.
Doi: 10.1021/j100019a038
210. Quantum Dynamics of a Planar Model for the Complex Forming OH + CO → H + CO₂ Reaction, E.M. Goldfield, S. K. Gray and G. C. Schatz, *J. Chem. Phys.*, **102**, 8807-17 (1995).
Doi: 10.1063/1.468934
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).

Doi: 10.1016/0009-2614(95)00397-5

212. A Theoretical Study of the NH + NO Reaction, K. S. Bradley, P. McCabe, G. C. Schatz, and S. P. Walch, *J. Chem. Phys.*, **102**, 6696-705 (1995).
Doi: 10.1063/1.469143
213. Theoretical Studies of Polyatomic Bimolecular Reaction Dynamics, J. M. Bowman and G. C. Schatz, *Annu. Rev. Phys. Chem.* **46**, 169-95 (1995).
Doi: 10.1146/annurev.pc.46.100195.001125
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.
Doi: 10.1016/0009-2614(95)00278-C
215. Complex Angular Momentum Analysis of Resonance Scattering in the Cl + HCl \rightarrow ClH + Cl Reaction, D. Sokolovski, J. N. L. Connor and G. C. Schatz, *J. Chem. Phys.*, **103**, 5979-98 (1995).
Doi: 10.1063/1.470427
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).
Doi: 10.1063/1.469787
217. RRKM Studies of Product Branching in the NH + NO Reaction, M. Simonson, K. S. Bradley and G. C. Schatz, *Chem. Phys. Lett.* **244**, 19-26 (1995).
Doi: 10.1016/0009-2614(95)00881-4
218. Scattering Theory and Dynamics: Time-Dependent and Time-Independent Methods, G. C. Schatz, *J. Phys. Chem.* **100**, 12839-47 (1996).
Doi: 10.1021/jp953344y
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).
Doi: 10.1103/PhysRevB.53.4162
220. Potential Energy Surface and Quasiclassical Trajectory Studies of the H₂ + CN Reaction, M. ter Horst, G. C. Schatz, and L. B. Harding, *J. Chem. Phys.*, **105**, 558-71 (1996).
Doi: 10.1063/1.471909
221. Mode-Specific Chemistry in the H + HCN and H + N₂O Reactions, M. ter Horst, K. S. Bradley and G. C. Schatz, in *Gas Phase Chemical Reaction Systems* (Springer Series in Chemical Physics 61), Ed. J. Wolfrum, H. -R. Volpp, R. Rannacher, and J. Warnatz, 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, *SPIE Proceedings* **2622**, 254-61 (1995).
Doi: 10.1117/12.216816

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).
Doi: 10.1063/1.471241
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).
Doi: 10.1016/0301-0104(96)00023-7
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).
Doi: 10.1063/1.472099
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).
Doi: 10.1063/1.472576
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).
Doi: 10.1021/jp960530a
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).
Doi: 10.1021/jp961164y
229. Theoretical Studies of Collisional Relaxation of Highly Excited SO_2 in an Ar Bath, G. Lendvay, G. C. Schatz and L. B. Harding, *Far. Disc. Chem. Soc.*, **102**, 389-403 (1995) (published in 1997).
Doi: 10.1039/FD9950200389
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).
Doi: 10.1021/jp961623v
231. A Global H_2O Potential Energy Surface for the Reaction $\text{O}({}^1\text{D}) + \text{H}_2 \rightarrow \text{OH} + \text{H}$, T. -S. Ho, T. Hollebeek, H Rabitz, L. B. Harding and G. C. Schatz, *J. Chem. Phys.*, **105**, 10472-86 (1996).
Doi: 10.1063/1.472977
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. Far. Trans.*, **93**, 755-64 (1997).
Doi: 10.1039/A606673I

233. Coupled Potential Energy Surfaces and Quantum Reactive Scattering for the $\text{Cl}(^2\text{P}) + \text{HCl} \rightarrow \text{ClH} + \text{Cl}(^2\text{P})$ Reaction, C. S. Maierle, G. C. Schatz, M. S. Gordon, P. M. McCabe, and J. N. L. Connor, *J. Chem. Soc. Far. Trans.*, **93**, 709-20 (1997).
Doi: 10.1039/A606570H
234. Quantum Scattering Studies of Collisional Energy Transfer from Highly Excited Polyatomic Molecules: Classical/Quantum Comparisons for Collinear $\text{He} + \text{CS}_2$, G. C. Schatz and G. Lendvay, *J. Chem. Phys.*, **106**, 3548-57 (1997).
Doi: 10.1063/1.473451
235. Quantum reactive scattering studies of the $\text{CN} + \text{H}_2 \rightarrow \text{HCN} + \text{H}$ reaction: the role of the nonreactive CN bond, T. Takayanagi and G. C. Schatz, *Chem. Phys. Lett.*, **265**, 410-417 (1997).
Doi: 10.1016/S0009-2614(96)01444-3
236. Reaction Dynamics Calculations for the Reaction $\text{CN} + \text{H}_2 \rightarrow \text{HCN} + \text{H}$: Applications of the Rotating-Bond Approximation, T. Takayanagi and G. C. Schatz, *J. Chem. Phys.*, **106**, 3227-36 (1997).
Doi: 10.1063/1.473061
237. A Quasiclassical Trajectory Study of Product State Distributions from the $\text{CN} + \text{H}_2 \rightarrow \text{HCN} + \text{H}$ Reaction, G. A. Bethardy, A. F. Wagner, G. C. Schatz and M. A. ter Horst, *J. Chem. Phys.*, **106**, 6001-15 (1997).
Doi: 10.1063/1.473264
238. Quantum Scattering Studies of Collisional Energy Transfer from Highly Excited Polyatomic Molecules: A Bend-Stretch Model of $\text{He} + \text{CS}_2$, G. Lendvay and G. C. Schatz, *Ber. Bunsenges. Phys. Chem.*, **101**, 587-94 (1997).
Doi: 10.1002/bbpc.19971010335
239. Quasiclassical Trajectory Studies of $\text{H}(\text{D}) + \text{HF}(\text{DF})$ Collisions at 2eV, G. C. Schatz, *J. Chem. Phys.* **106**, 2277 (1997).
Doi: 10.1063/1.473088
240. A Quasiclassical Trajectory Study of $\text{H} + \text{CO}_2$: Angular and Translational Distributions, and OH angular momentum alignment, K. S. Bradley and G. C. Schatz, *J. Chem. Phys.* **106**, 8464-72 (1997).
Doi: 10.1063/1.473923
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).
Doi: 10.1063/1.475625
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**, ed. A. S. Mullin and G. C. Schatz, ACS Symp Series 678, 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**, ed. A. S. Mullin and G. C. Schatz, ACS Symp Series 678, 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).
Doi: 10.1063/1.475099
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).
Doi: 10.1021/jp970178g
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. Hollebeck, T. -S. Ho, and H. Rabitz, *J. Chem. Phys.* **107**, 2340-50 (1997).
Doi: 10.1063/1.474614
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**, ed. D. L. Thompson, 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).
Doi: 10.1063/1.474695
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**, Ed. W. L. Hase, Adv. In Classical Trajectory Methods, Vol. III, 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, *Far. Disc. Chem. Soc.* **108**, 357-74, (1997)
Doi: 10.1039/A705888H
251. A further theoretical exploration of the surface-aligned photo-initiated 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).
Doi: 10.1063/1.475209
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).
Doi: 10.1021/jp982069n

253. Quantum Scattering Studies of Spin-Orbit Effects in the $\text{Cl}(^2\text{P}) + \text{HCl} \rightarrow \text{ClH} + \text{Cl}(^2\text{P})$ Reaction, G. C. Schatz, P. McCabe and J. N. L. Connor, *Far. Disc. Chem. Soc.*, **110**, 139-157 (1998).
Doi: 10.1039/A801825A
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).
Doi: 10.1021/jp9812132
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).
Doi: 10.1021/jp9811070
256. A Quasiclassical Trajectory Study of $\text{H} + \text{H}_2\text{O} \rightarrow \text{OH} + \text{H}_2$: Angular Distributions and OH Angular Momentum Alignment, Kimberly S. Bradley and George C. Schatz, *J. Chem. Phys.*, **108**, 7994-8003 (1998).
Doi: 10.1063/1.476234
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. BS. Ho, H. Rabitz, *J. Chem. Phys.*, **110**, 8857-60 (1999).
Doi: 10.1063/1.478806
258. Calculating Dipole and Quadrupole Polarizabilities Relevant to Surface Enhanced Raman Spectroscopy, Gary S. Kedziora and George C. Schatz, *Spectrochimica Acta*, **A55**, 625-638, (1999).
Doi: 10.1016/S1386-1425(98)00266-2
259. Monte Carlo sampling methods for determining potential energy surfaces using Shepard interpolation. The $\text{O}(^1\text{D}) + \text{H}_2$ system. T. Ishida and G. C. Schatz, *Chem. Phys. Lett.*, **298**, 285-92 (1998).
Doi: 10.1016/S0009-2614(98)01202-0
260. Coupled *ab initio* potential energy surfaces for the reaction $\text{Cl}(^2\text{P}) + \text{HCl} \rightarrow \text{ClH} + \text{Cl}(^2\text{P})$ 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).
Doi: 10.1039/A808183B
261. Nanosphere lithography: Surface plasmon resonance spectrum of a periodic array of silver nanoparticles by UV-vis extinction spectroscopy and electrodynamic modelling, T. R. Jensen, G. C. Schatz and R. P. Van Duyne, *J. Phys. Chem.*, **B103**, 2394-2401 (1999)
Doi: 10.1021/jp984406y
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).
Doi: 10.1063/1.477939

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).
Doi: 10.1039/A809325C
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. B* **103**, 9846-53 (1999).
Doi: 10.1021/jp9926802
265. Perspective on "Exchange Reactions with Activation Energy. I. Simple Barrier Potential for (H, H₂)" by M. Karplus, R. N. Porter and R. D. Sharma [*J. Chem. Phys.* 43, 3259-87 (1965)], George C. Schatz, *Theoretical Chemistry Accounts*, **103**, 270-272 (2000).
Doi: 10.1007/s002140050032
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).
Doi: 10.1021/jp9839347
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).
Doi: 10.1063/1.478830
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, *Far. Disc. Chem. Soc.*, **113**, 151-66(1999)
Doi: 10.1039/A901950B
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).
Doi: 10.1063/1.479522
270. Electrodynamics of Noble Metal Nanoparticles and Nanoparticle Clusters, T. Jensen, L. Kelly, A. Lazarides and G. C. Schatz, *J. Cluster Science*, **10**, 295-317 (1999).
Doi: 10.1023/A:1021977613319
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).
Doi: 10.1063/1.480127
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).
Doi: 10.1063/1.480128
273. Potential energy surface of the A state of NH_2 , 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).

- Doi: 10.1021/jp9924575
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).
Doi: 10.1016/S0009-2614(99)00881-7
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).
Doi: 10.1021/jp991601j
276. Fitting potential energy surfaces, G. C. Schatz, in **Reaction and Molecular Dynamics**, Lecture Notes in Chemistry, Vol. 14, ed. A. Lagana and A. Riganelli, 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, Ed. J. H. Moore and N. D. Spencer, Institute of Physics Publ, Bristol, 2001, 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).
Doi: 10.1021/jp992179+
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).
Doi: 10.1063/1.480873
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).
Doi: 10.1039/A908614E
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, 89-118.
http://www.sciencedirect.com/science?_ob=ArticleListURL&_method=list&_ArticleListID=596869654&_sort=d&_view=c&_acct=C000049540&_version=1&_urlVersion=0&_userid=965532&md5=74ed0b89c6d2ca73a7ddd657a2cc5467
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. Amer. Chem. Soc.*, **122**, 4640-50 (2000).
Doi: 10.1021/ja9938251
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).
Doi: 10.1016/S0166-1280(00)00532-7
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).
Doi: 10.1063/1.481142

285. Detecting Resonances, G. C. Schatz, *Science*, **288**, 1599-1600 (2000).
Doi: 10.1126/science.288.5471.1599
286. A New Potential Surface and Quasiclassical Trajectory Study of $\text{H}+\text{H}_2\text{O} \rightarrow \text{OH}+\text{H}_2$, G.-S. Wu, G. C. Schatz, G. Lendvay, D. -C. Fang, and L. B. Harding, *J. Chem. Phys.* **113**, 3150-61 (2000).
Doi: 10.1063/1.1287329
287. Probing the H_2 rotational state in $\text{O}(^1\text{D}) + \text{H}_2 \rightarrow \text{OH} + \text{H}$: 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).
Doi: 10.1063/1.1313785
288. A model for simulating dynamics of DNA Denaturation, Karen Drukker and G. C. Schatz, *J. Phys. Chem.* **104**, 6108-11 (2000).
Doi: 10.1021/jp000550j
289. A benchmark system for insertion chemistry: quantum state resolved differential cross sections for $\text{O}(^2\text{D})+\text{H}_2(\text{J}=0) \rightarrow \text{OH}(^2\Pi, \nu, \text{N})+\text{H}(^2\text{S})$, J. J. Lin, X. Liu, S. Harich, G. C. Schatz, and X. Yang, *Science*, **289**, 1536-38 (2000).
Doi: 10.1126/science.289.5484.1536
290. Theoretical Studies of Intersystem Crossing Effects in the $\text{O} + \text{H}_2$ Reaction, Mark R. Hoffmann and George C. Schatz, *J. Chem. Phys.*, **113**, 9456-9465, (2000).
Doi: 10.1063/1.1319937
291. A Quasiclassical Trajectory study of the $\text{H} + \text{HCN} \rightarrow \text{H}_2 + \text{CN}$ reaction dynamics, Diego Troya, Irene Banos, Miguel Gonzales, Guosheng Wu, Marc ter Horst and George C. Schatz, *J. Chem. Phys.*, **113**, 6253-63 (2000).
Doi: 10.1063/1.1308090
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).
Doi: 10.1021/jp002906x
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).
Doi: 10.1021/ja003312a
294. Reactive and Nonreactive Quenching of $\text{OH}(\text{A } ^2\Sigma^+)$ 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).
Doi: 10.1021/jp003092n
295. A QCT study of the $\text{Cl} + \text{HCN} \rightarrow \text{HCl} + \text{CN}$ reaction dynamics. The microscopic reaction mechanism of the $\text{H}(\text{Cl})+\text{HCN} \rightarrow \text{H}_2(\text{HCl}) + \text{CN}$ reactions, Diego Troya, Miguel Gonzalez, Guosheng Wu and George C. Schatz, *J. Phys. Chem.* **105**, 2285-97 (2001).
Doi: 10.1021/jp003371a

296. The dynamics of the $N(^2D)+D_2$ 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).
Doi: 10.1021/jp0036238
297. Model simulations of DNA denaturation dynamics, Karen Drukker, Guosheng Wu and George C. Schatz, *J. Chem. Phys.* **114**, 579-590 (2001).
Doi: 10.1063/1.1329137
298. Stretched Water is More Reactive, George C. Schatz, *Science*, **290**, 950-1 (2000).
Doi: 10.1126/science.290.5493.950
299. Effective Medium Theory of DNA-linked Gold Nanoparticle Aggregates: Effect of Aggregate Shape, A. A. Lazarides, K. L. Kelly and G. C. Schatz, *Mat. Res. Soc. Symp. Proc.* **635**, C6.5.1-10 (2001).
Doi: 10.1557/PROC-635-C6.5
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).
Doi: 10.1063/1.1355310
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).
Doi: 10.1021/jp010296a
302. Tribute to William H. Miller, N. Makri and G. C. Schatz, *J. Phys. Chem. A* **105**, 2485-86 (2001).
Doi: 10.1021/jp0103981
303. A Quasiclassical Trajectory Study of Reactivity and Product Energy Disposal in $H + H_2O$, $H + D_2O$ and $H + HOD$, Diego Troya, Miguel Gonzalez, George C. Schatz, *J. Chem. Phys.* **114**, 8397-13 (2001).
Doi: 10.1063/1.1366334
304. Variation transition state theory and quasiclassical trajectory studies of the $H_2 + OH \rightarrow H + H_2O$ reaction and some isotopic variants, D. Troya, M. J. Lakin, G. C. Schatz, and M. Gonzalez, *J. Chem. Phys.* **115**, 1828-42 (2001).
Doi: 10.1063/1.1382646
305. A Quasiclassical Trajectory Study of Angular and Internal State Distributions in $H + H_2O$ and $H + D_2O$ at $E_T=1.4$ eV, D. Troya, G. Lendvay, M. Gonzalez and G. C. Schatz, *Chem. Phys. Lett.*, **343**, 420-28 (2001).
Doi: 10.1016/S0009-2614(01)00697-2
306. A quasiclassical trajectory study of product energy and angular distributions for the $OH + D_2$ reaction. Matthew J. Lakin, Diego Troya, György Lendvay, Miguel González and George C. Schatz, *J. Chem. Phys.*, **115**, 5160-69 (2001).
Doi: 10.1063/1.1394218

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**, M.R. Hoffmann and K.G. Dyall eds., ACS Symposium Series 828, 329-345 (2002).
308. Computational Electromagnetics of Metal Nanoparticles and Nanoparticle Aggregates, K. L. Kelly, A. A. Lazarides and G. C. Schatz, *Computing in Science & Engineering* **3**, 67-73 (2001).
Doi: 10.1109/5992.931905
309. Electrodynamics of Nonspherical Noble Metal Nanoparticles and Nanoparticle Aggregates, George C. Schatz, *Theochem*, **573**, 73-80 (2001).
Doi: 10.1016/S0166-1280(01)00545-0
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).
Doi: 10.1063/1.1384550
311. The Branching Ratio between Reaction and Relaxation in the Removal of H₂O from its |04>-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).
Doi: 10.1063/1.1389304
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).
Doi: 10.1016/S0009-2614(01)01506-8
313. Quasiclassical Trajectory Studies of the N(⁴S) + H₂ → NH(X³Σ) + H Reaction, Ronald Z. Pascual, George C. Schatz, György Lendvay, Diego Troya, *J. Phys. Chem.*, **106**, 4125-36 (2002).
Doi: 10.1021/jp0133079
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).
Doi: 10.1063/1.1446429
315. Photo-induced 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).
DOI: 10.1126/science.1066541
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).
Doi: 10.1103/PhysRevB.65.235430
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).
Doi: 10.1016/S0009-2614(02)00407-4
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)
Doi: 10.1021/jp011871d

319. A Quasiclassical Trajectory Study of Energy and Angular Distributions for the $\text{H} + \text{CO}_2 \rightarrow \text{OH} + \text{CO}$ Reaction, D. Troya, M. J. Lakin, G. C. Schatz, L. B. Harding, M. Gonzalez, *J. Phys. Chem. B* **106**, 8148-60 (2002).
Doi: 10.1021/jp0256950
320. Quasiclassical Trajectory Studies of Four Atom Reactions, D. Troya, M. J. Lakin, and G. C. Schatz, in *Modern Trends in Chemical Reaction Dynamics*, Ed. X. M. Yang and K. Liu, World Scientific, Singapore, 2002, *Advanced Series in Physical Chemistry*, **14**, 249-90 (2004).
321. A Direct Trajectory Dynamics Investigation of Fast O + Alkane Reactions, R. Z. Pascual, D. J. Garton, and G. C. Schatz, in *Proceedings of 6th International Conference on Protection of Materials and Structures from Space Environment (ICPMSE-6)*, Toronto, May 1-3, 2002, Ed. J. Kleiman, Kluwer, Dordrecht, *Space Technology Proceedings*, **5**, 537-41 (2003).
Doi: 10.1007/1-4020-2595-5_49
322. F. Santoro, C. Petrongolo, G. C. Schatz, Trajectory-Surface-Hopping Study of the Renner-Teller Effect in the $\text{N}(^2\text{D}) + \text{H}_2$ Reaction. *J. Phys. Chem. A* **106**, 8276-84 (2002).
Doi: 10.1021/jp014312f
323. Rob van Harrevelt, M. C. van Hemert, G. C. Schatz, The CH + H reaction studied with quantum-mechanical and classical trajectory calculations. *J. Chem. Phys.* **116**, 6002-11, (2002).
Doi: 10.1063/1.1459416
324. Lance Kelly, Eduardo Coronado, Lin Lin Zhao, George C. Schatz, The Optical Properties of Metal Nanoparticles: The Influence of Size, Shape and Dielectric Environment. *J. Phys. Chem. B*, **107**, 668-77 (2003).
Doi: 10.1021/jp026731y
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).
Doi: 10.1063/1.1510439
326. Synthesis of Silver Nanodiscs Using Polystyrene Meso-spheres as Templates, E. Hao, K. L. Kelly, J. T. Hupp and G. C. Schatz, *J. Am. Chem. Soc.*, **124**, 15182-3 (2002).
Doi: 10.1021/ja028336r
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).
Doi: 10.1021/ja021096v
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)
Doi: 10.1021/nl0340531
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).
Doi: 10.1103/PhysRevLett.90.115505

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, *Journal of the Optical Society of America B: Optical Physics* **21**, 121-131 (2004).
Doi: 10.1364/JOSAB.21.000121
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, *Mat. Res. Soc. Symp. Proc.* 735, C10.1.1-C10.1.9 (2003).
Doi: 10.1557/PROC-735-C10.1
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).
Doi: 10.1063/1.1539043
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. Comp. Chem.*, **24**, 1077-86 (2003).
Doi: 10.1002/jcc.10252
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).
Doi: 10.1012/jp0226026
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).
Doi: 10.1021/jp034027r
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).
Doi: 10.1021/jp034028j
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, *Journal of Physical Chemistry B*, **107**, 7343-7350 (2003)
Doi: 10.1021/jp034235j
338. Nanoparticle Optics: The Importance of Radiative Dipole Coupling in Two-Dimensional Nanoparticle Arrays, Christy L. Haynes, Adam D. McFarland, LinLin Zhao, George C. Schatz, Richard P. Van Duyne, Linda Gunnarsson, Juris Prikulis, Bengt Kasemo, and Mikael Käll, *Journal of Physical Chemistry B*, **107**, 7337-7342 (2003).
Doi: 10.1021/jp034234r
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).
Doi: 10.1103/PhysRevLett.90.156104
340. Controlling anisotropic nanoparticle growth through plasmon excitation, R. Jin, Y. C. Cao, E. Hao, G. S. Métraux, G. C. Schatz, and C. A. Mirkin, *Nature*, **425**, 487-90 (2003).
Doi: 10.1038/nature02020

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)
Doi: 10.1063/1.1587686
342. Influence of Spin-Orbit Effects on Chemical Reactions: Quantum Scattering Studies for the $\text{Cl}(^2\text{P}) + \text{HCl} \rightarrow \text{ClH} + \text{Cl}(^2\text{P})$ 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).
Doi: 10.1021/jp034680e
343. Electromagnetic Fields Around Silver Nanoparticles and Dimers, E. Hao and G. C. Schatz, *J. Chem. Phys.* 120, 357-66 (2004).
Doi: 10.1063/1.1629280
344. A Quasiclassical Trajectory Study of the Reaction $\text{OH} + \text{CO} \rightarrow \text{H} + \text{CO}_2$, M. J. Lakin, D. Troya, G. C. Schatz and L. B. Harding, *J. Chem. Phys.* 119, 5848-59 (2003).
Doi: 10.1063/1.1602061
345. How Narrow Can A Meniscus Be?, J. K. Jang, G. C. Schatz and M. A. Ratner, *Physical Review Letters*, 92, 085504 (2004).
Doi: 10.1103/PhysRevLett.92.085504
346. Capillary Force in Atomic Force Microscopy, J. K. Jang, G. C. Schatz and M. A. Ratner, *J. Chem. Phys.*, 120, 1157-60 (2004).
Doi: 10.1063/1.1640332
347. A QM/MM Model for Hyperthermal $\text{O}(^3\text{P})$ Collisions with Hydrocarbon Self-Assembled Monolayers, D. Troya and G. C. Schatz, in *Proceedings of the 9th International Symposium on Materials in a Space Environment*, June 16-20, 2003, Noordwijk, The Netherlands, (ESA SP-540, Sept. 2003) p. 121-128.
348. Model atomic oxygen reactions: detailed experimental and theoretical studies of the reactions of ground-state $\text{O}(^3\text{P})$ with H_2 , CH_4 , CH_3CH_3 and $\text{CH}_3\text{CH}_2\text{CH}_3$ at hyperthermal collision energies, T. K. Minton, D. J. Garton, D. Troya, B. Maiti, R. Pascual and G. C. Schatz, in *Proceedings of the 9th International Symposium on Materials in a Space Environment*, June 16-20, 2003, Noordwijk, The Netherlands (ESA SP-540, Sept. 2003) p. 129- 136.
349. Dynamics Studies of $\text{O}(^3\text{P}) + \text{CH}_4$, C_2H_6 , C_3H_8 Reactions, Diego Troya and G. C. Schatz, *Proceedings of NATO Advanced Research Workshop on the Theory of Chemical Reaction Dynamics*, Balatonfoldvar, Hungary, June 7-12, 2003, A. Lagana and G. Lendvay, Kluwer, pp. 329-48 (2004).
350. Nonadiabatic Dynamics in the $\text{O} + \text{H}_2$ Reaction: A Time-Independent Quantum Mechanical Study, B. Maiti and G. C. Schatz, *Proceedings of NATO Advanced Research Workshop on the Theory of Chemical Reaction Dynamics*, Balatonfoldvar, Hungary, June 7-12, 2003, A. Lagana and G. Lendvay, Kluwer, pp 89-103 (2004).
351. Theoretical studies of intersystem crossing effects in the $\text{O}(^3\text{P}) + \text{H}_2$ reaction, B. Maiti and G. C. Schatz, *J. Chem. Phys.* 119, 12360-71 (2003).
Doi: 10.1063/1.1623481

352. Extinction spectra of silver nanoparticle arrays, Shengli Zou, Linlin Zhao, George C. Schatz, SPIE Proceedings, 5221(Plasmonics: Metallic Nanostructures and Their Optical Properties), 174-181 (2003).
Doi: 10.1117/12.503436
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).
Doi: 10.1021/jp0361327
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).
Doi: 10.1021/jp036261n
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).
Doi: 10.1063/1.1631254
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)
Doi: 10.1063/1.1642580
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)
Doi: 10.1021/jp036301n
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).
Doi: 10.1016/j.cplett.2003.10.068
359. Influence of van der waals wells on the quantum scattering dynamics of the $Cl(^2P)+HCl \rightarrow ClH + Cl(^2P)$ reaction, M. Hankel, J. N. L. Connor and G. C. Schatz, Chem. Phys., 308, 225-36 (2004).
Doi: 10.1016/j.chemphys.2004.03.026
360. Theoretical Studies of Hyperthermal $O(^3P)$ Collisions with Hydrocarbon Self-Assembled Monolayers, Diego Troya and George C. Schatz, J. Chem. Phys., 120, 7696-7707 (2004).
Doi: 10.1063/1.1688312
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).
Doi: 10.1063/1.1760740
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)
Doi: 10.1021/jp037731g
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, Nanoletters, 4, 427-431 (2004).

- Doi: 10.1021/nl0351439
364. Synthesis and Optical Properties of “Branched” Gold Nanocrystals, E. Hao, R. C. Bailey, G. C. Schatz, J. T. Hupp and S. Li, *Nano Letters*, **4**, 327-330 (2004).
Doi: 10.1021/nl0351542
365. Synthesis and Optical Properties of Anisotropic Metal Nanoparticles, Encai Hao, George C. Schatz, Joseph T. Hupp, *Journal of Fluorescence*, **14**, 331-41 (2004).
Doi: 10.1023/B:JOFL.0000031815.71450.74
366. The importance of intersystem crossing in the $S(^3P, ^1D) + H_2 \rightarrow SH + H$ reaction, Biswajit Maiti, G. C. Schatz and G. Lendvay, *J. Phys. Chem. A*, **108**, 8772-8781. (2004).
Doi: 10.1021/jp049143o
367. Quantum wave packet and quasiclassical trajectory studies of OH+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).
Doi: 10.1063/1.1632901
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, *Applied Phys. Lett.* **85** 467-469 (2004).
Doi: 10.1063/1.1773362
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).
Doi: 10.1016/j.cplett.2004.04.054
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*, Ed. J. Reif, Science Technica, 90-103 (2004).
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).
Doi: 10.1080/0144235042000298484
372. Theoretical Study of Reactions of Hyperthermal $O(^3P)$ with Perfluorinated Hydrocarbons, Diego Troya and George C. Schatz, *Proceedings of 7th ICPMSE*, Toronto, May 10-13 (2004), *Springer, Space Technology Proceedings*, Vol. 6, 365-375 (2006).
Doi: 10.1007/1-4020-4319-8
373. A Comparative analysis of Localized and Propagating Surface Plasmon Resonance Sensors: The Binding of Concanavalin 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).
Doi: 10.1021/ja047118q
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).
Doi: 10.1021/jp049084e
375. Electrodynamics in Computational Chemistry, Linlin Zhao, Shengli Zou, Encai Hao 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, editors, Elsevier, Amsterdam (2005) pp. 47-66.
Doi: 10.1016/B978-044451719-7/50047-0
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, T. R. Huser, Eds. (2004).
Doi: 10.1117/12.561878
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, X. -Y. Zhu, Eds. (2004).
Doi: 10.1117/12.556064
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).
Doi: 10.1063/1.1815271
379. Hyperthermal reactions of $O^+(^4S_{3/2})$ 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).
Doi: 10.1021/jp047993y
380. Near-field photochemical imaging of noble metal nanostructures, C. Hubert. A. Rumyantseva, G. Lerondel, J. Grand, S. Kostcheev, A. Vial, R. Bachelot, P. Royer, S. -H. Chang, S. K. Gray, G. P. Wiederrecht, and G. C. Schatz, *Science, Nano Letters*, 5, 615-19 2005.
Doi: 10.1021/nl047956i
381. Multi-Walled Carbon Nanotubes Experiencing Electrical Breakdown as Gas Sensors Jaehyun Chung, Kyong-Hoon Lee, Junghoon Lee, Diego Troya, George C. Schatz, *Nanotechnology*, 2004, 15, 1-7, 2004.
Doi: 10.1088/0957-4484/15/11/038
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.
Doi: 10.1021/jp047880e
383. Biography of Gert D. Billing. Michael Baer, Cecilia Coletti, George C. Schatz, Soren Toxvaerd, and Lichang Wang, *Journal of Physical Chemistry A* 108, 8553 (2004).
Doi: 10.1021/jp0404798
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) .
Doi: 10.1103/PhysRevB.71.115403

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).
Doi: 10.1063/1.1826036
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).
Doi: 10.1016/j.cplett.2004.12.107
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).
Doi: 10.1063/1.1859282
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).
Doi: 10.1016/j.cplett.2004.10.112
389. Optical properties of one-dimensional metal nanostructures. Encai Hao, Shengli Zou, George C. Schatz, *Materials Research Society Symposium Proceedings* 818, 53-58 (2004).
Doi: 10.1557/PROC-818-M3.8.1
390. Fracture Paths and Ultrananocrystalline Diamond, Jeffrey T. Paci, Lipeng Sun, T. Belytschko, and George C. Schatz, *Chem. Phys. Lett*, 403, 16-21 (2005).
Doi: 10.1016/j.cplett.2004.12.067
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).
Doi: 10.1021/ja043245a
392. Chang, Gilbert; Schatz, George C..Review of: Modern Problems in Classical Electrodynamics Edited by Charles A. Brau. *ChemPhysChem* (2005), 6(2), 374.
Doi: 10.1002/cphc.200400366
393. Sun, Lipeng; Schatz, George C.. Direct Dynamics Classical Trajectory Simulations of the $O^+ + CH_4$ Reaction at Hyperthermal Energies. *Journal of Physical Chemistry B* 109, 8431-8 (2005).
Doi: 10.1021/jp0454568
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, *Optics Express*, 13, 3150-65 (2005).
Doi: 10.1364/OPEX.13.003150
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).
Doi: 10.1063/1.1929740
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 Bulletin*, 30, 368-375 (2005).
Doi: 10.1557/mrs2005.100

397. Hyperthermal collisions of $O^+(^4S_{3/2})$ with Methane at 5 eV, LiPeng Sun and George C. Schatz, *J. Spacecraft and 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)
Doi: 10.1021/jp054847z
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 Letters*, 5, 1065-70 (2005).
Doi: 10.1021/nl0505492
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).
Doi: 10.1021/jp051178g
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 Letters*, 5, 1503-7 (2005).
Doi: 10.1021/nl050873x
402. Tomczak, Sandra J.; Marchant, Darrell; Svejda, Steve; Minton, Timothy K.; Brunsvold, Amy L.; Gouzman, Irina; Grossman, Eitan; Schatz, George C.; Troya, Diego; Sun, LiPeng; Gonzalez, Rene I. **Properties and improved space survivability of POSS (polyhedral oligomeric silsesquioxane) polyimides.** *Materials Research Society Symposium Proceedings* (2005), 851(Materials for Space Applications), 395-406.
Doi:10.1557/PROC-851-NN9.1
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).
Doi: 10.1088/0957-4484/16/10/039
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)
Doi: 10.1021/ja052684m
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).
Doi: 10.1021/jp053827u
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).
Doi: 10.1021/jp055017o

- 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).
Doi: 10.1016/j.cplett.2005.08.019
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).
Doi: 10.1063/1.2046633
409. Surface Plasmon Standing Waves in Large-Area Subwavelength Hole Arrays, Eun-Soo Kwak, Joel Henzie, Shih-Hui Chang, Stephen K. Gray, George C. Schatz, and Teri W. Odom, *Nano Letters*, 5(10), 1963-1967 (2005).
Doi: 10.1021/nl051339s
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.
Doi: 10.1021/jp056554b
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*, Ed. J. Reif, Science Technica, 207-214 (2005).
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).
Doi: 10.1063/1.2046670
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. Amer. Chem. Soc.* 127, 14445-53 (2005).
Doi: 10.1021/ja0539387
414. Duplex and hairpin dimer structures for perylene diimide-oligonucleotide conjugates, Yan Zheng, Hai Long, George Schatz, and Frederick D. Lewis, *Chem. Comm.* 38, 4795-97 (2005).
Doi : 10.1039/b509754a
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).
Doi: 10.1021/jp054053k
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", edited by D. Sokolovski, J. N. L. Connor and S. Sen, Collaborative Computational Project on Molecular Quantum Dynamics (CCP6) Daresbury Laboratory Daresbury Warrington WA4 4AD United Kingdom, 2005, 9-14.
http://www.ccp6.ac.uk/booklets/CCP6-2005_Belfast.pdf
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 Letters*, 5, 2034-38 (2005).

Doi: 10.1021/nl0515753

418. Electrodynamics simulations of surface plasmon behavior in metallic nanostructures, S. K. Gray. T. –W. Lee, S. –H. Chang and G. C. Schatz, SPIE Proceedings (Plasmonics: Metallic Nanostructures and Their Optical Properties III) Ed. M. I. Stockman, 5927, 96-101 (2005).
Doi: 10.1117/12.614120
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, PNAS, 103, 2026-2031 (2006).
Doi: 10.1073/pnas.0511022103 PMCID: PMC1413750
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).
Doi: 10.1021/jp0540656
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).
Doi: 10.1063/1.2099547
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 (2005), 109(47), 22351-22358.
Doi: 10.1021/jp0545400
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)
Doi: 10.1021/ja0556326
424. Alkanethiol mediated release of surface bound nanoparticles fabricated by nanosphere lithography, J. Zhao, A. J. Haes, X. Zhang, S. Zou, E. M. Hicks, G. C. Schatz and R. P. Van Duyne, Materials Research Society Symposium Proceedings, 900E, O13-08.1 (2006).
Doi: 10.1557/PROC-0900-O13-08
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).
Doi: 10.1021/jp056606x
426. New Editor in Chief of the Journal of Physical Chemistry, J. Phys. Chem. A/B 109, 1(2005).
Doi: 10.1021/jp040657x
427. Editorial, George C. Schatz, J. Phys. Chem. A/B, 110, 1 (2006).
Doi: 10.1021/jp058271p
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, Organic & Biomolecular Chemistry, 4, 314-322 (2006).
Doi: 10.1039/B513694F

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).
Doi: 10.1021/jp0556815
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).
Doi: 10.1063/1.2147139
431. Coupled plasmon/photonic resonance effects in SERS, Shengli Zou and George C. Schatz, in *Surface Enhanced Raman Scattering: Physics and Applications*, Ed. K. Kneipp, M. Moskovits and H. Kneipp, Springer Topics in Applied Physics, 103, 67-86, 2006
Doi: 10.1007/3-540-33567-6
432. Electromagnetic mechanism of SERS, George C. Schatz, Matthew Young and Richard P. Van Duyne, in *Surface Enhanced Raman Scattering: Physics and Applications*, Ed. K. Kneipp, M. Moskovits and H. Kneipp, Springer Topics in Applied Physics, 103, 19-46, 2006
Doi: 10.1007/3-540-33567-6
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, *Physical Review B* 73, 075423 (2006).
Doi: 10.1103/PhysRevB.73.075423
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).
Doi: 10.1007/s00340-006-2218-x
435. Focusing a beam of light with left-handed metamaterials, A. O. Pinchuk and G. C. Schatz, *Solid-State Electronics* 51, 1381-86 (2007).
Doi: 10.1016/j.sse.2007.06.008
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)
<http://64.233.167.104/search?q=cache:oMjEIKIP0xoJ:cohesion.rice.edu/Engineering/bioe/emplibray/Schatz.pdf+Melting+behavior+of+DNA-linked+polymers&hl=en&ct=clnk&cd=6&gl=us>
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).
Doi: 10.1021/jp055740e
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).
Doi: 10.1021/jp061086
439. Quantum trajectory dynamics in arbitrary coordinates, Vitaly A. Rassolov, S. Garashchuk and G. C. Schatz, *J. Phys. Chem. A*, 110, 5530-36 (2006).
Doi: 10.1021/jp056741+

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).
Doi: 10.1088/0957-4484/17/11/014
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, *Israel J. Chem.* 46, 293-97 (2006).
Doi: 10.1560/IJC_46_3_293
442. Surface-enhanced Raman scattering of pyrazine at the junction between two Ag₂₀ nanoclusters, Linlin Zhao, Lasse Jensen and George C. Schatz, *Nano Letters*, 6, 1229-1234 (2006).
Doi: 10.1021/nl0607378
443. Electric Field Enhancement and Light Transmission in Cylindrical Nanoholes, Kevin Shuford, Mark A. Ratner, Stephen K. Gray, and George C. Schatz, *Journal of Computational and Theoretical Nanoscience*, 4, 1-8 (2007).
Doi: 10.1166/jctn.2007.006
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", ed. A.O. Pinchuk, NOVA Publishing, Inc. NY, 2007 *Nanotechnology Research Journal* 1, 3/4 (published in 2008)
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 Letters* 6, 1896-1903 (2006).
Doi: 10.1021/nl060967m
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).
Doi: 10.1021/jp062212+
447. Semiclassical nonadiabatic dynamics based on quantum trajectories for the O(³P, ¹D) + H₂ system, Sophya Garashchuk, Vitaly Rassolov and George C. Schatz, *J. Chem. Phys.* 124, 244307/1-8 (2006).
Doi: 10.1063/1.2208615
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).
Doi: 10.1021/jp063226i
449. Designing, fabricating, and imaging Raman hot spots, Lidong Qin, Shengli Zou, Can Xue, Ariel Atkinson, George C. Schatz and Chad A. Mirkin, *PNAS*, 103, 13300-3 (2006).
Doi: 10.1073/pnas.0605889103 PMCID: PMC1569158
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).
Doi: 10.1103/PhysRevB.74.195439

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).
Doi: 10.1021/jp071985a
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).
Doi: 10.1021/jp0664667
453. Metal nanoparticle array waveguides: Proposed structures for subwavelength devices, S. Zou and G. C. Schatz, *Physical Review B* 74, 125111/1-/15 (2006).
Doi: 10.1103/PhysRevB.74.125111
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 Letters* 6, 2060-2065 (2006).
Doi: 10.1021/nl061286u
455. Localized Surface Plasmon Resonance Spectroscopy near Molecular Resonances. Amanda J. Haes, Shengli, Zou, Jing Zhao, George C. Schatz, and Richard P. Van Duyne, *Journal of the American Chemical Society* 128, 10905-14 (2006).
Doi: 10.1021/ja063575q
456. Resonance Surface Plasmon Spectroscopy: Low Molecular Weight Substrate Binding to Cytochrome P450. Jing Zhao, Aditj Das, Xiaoyu Zhang, George C. Schatz, Stephen G. Sligar and Richard P. Van Duyne, *Journal of the American Chemical Society* 128, 11004-11005 (2006).
Doi: 10.1021/ja0636082
457. Nanografting: Modeling and Simulation. Seol Ryu and George C. Schatz, *Journal of the American Chemical Society* 128, 11563-11573 (2006).
Doi: 10.1021/ja063138b
458. Microscopic mechanisms and dynamics simulations of $O^+(^4S_{3/2})$ reacting with methane; L. P. Sun and G. C. Schatz, *Proceedings of 7th ICPMSE, Toronto, May 10-13 (2004)*, Springer, *Space Technology Proceedings*, Vol. 6, 359-364 (2006).
Doi: 10.1007/1-4020-4319-8
459. Reorganization of The Journal of Physical Chemistry. George C. Schatz, *Journal of Physical Chemistry A* 110, 10655 (2006); B 18073 (2006).
Doi: 10.1021/jp068067h
460. A cooperative beads-on-a-string approach to exceptionally stable DNA triplexes. Yan Zheng, Hai Long, George C. Schatz and Frederick D. Lewis, *Chemical Communications* 36, 3830-3832 (2006).
Doi: 10.1039/B607941E
461. Hu, Wenfang; Schatz, George C.. Theories of reactive scattering. *Journal of Chemical Physics* (2006), 125(13), 132301/1-132301/15.
Doi: 10.1063/1.2213961

462. Zhao, Jing; Zhang, Xiaoyu; Haes, Amanda J.; Zou, Shengli; Schatz, George C.; Van Duyne, Richard P. Localized surface plasmon and molecular resonance: fundamental study and application. *Proceedings of SPIE-The International Society for Optical Engineering* (2006), 6323(Plasmonics: Metallic Nanostructures and Their Optical Properties IV), 63231B.
Doi: 10.1117/12.681423
463. Chang, Shih-Hui; Schatz, George C.; Gray, Stephen K. FDTD/TDSE study on surface-enhanced infrared absorption by metal nanoparticles. *Proceedings of SPIE-The International Society for Optical Engineering* (2006), 6323(Plasmonics: Metallic Nanostructures and Their Optical Properties IV), 632321.
Doi: 10.1117/12.681514
464. Christine M. Aikens and George C. Schatz, TDDFT studies of absorption and SERS spectra of pyridine interacting with Au₂₀, *J. Phys. Chem. A*, 110, 13317-24 (2006).
Doi: 10.1021/jp065206m
465. Ligang Zhang, Hai Long, George C. Schatz and Frederick D. Lewis, Synthesis and properties of nicked dumbbell and dumbbell DNA conjugates, *Organic & Biomolecular Chemistry*, 5, 450-456 (2007).
Doi: 10.1039/B614572H
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).
Doi: 10.1016/j.cplett.2006.12.062
467. Rings of single-walled carbon nanotubes: molecular-template directed assembly and Monte Carlo modeling, Shengli Zou, Daniel MasPOCH, Yuhuang Wang, Chad A. Mirkin and George C. Schatz, *Nano Letters*, 7, 276-80 (2007).
Doi: 10.1021/nl062258e
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).
Doi: 10.1103/PhysRevB.74.184112
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).
Doi: 10.1021/jp0657888
470. New Journals in a New Year, G. C. Schatz, *J. Phys. Chem A,B,C* 111, 1 (2007)
Doi: 10.1021/jp068106p
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).
Doi: 10.1021/jp0664162
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).
Doi: 10.1021/nl070648a

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)
Doi: 10.1103/PhysRevB.75.075412
474. A. O. Pinchuk and G. C. Schatz, *Metamaterials with Gradient of the Negative Index of Refraction*, *Journal of the Optical Society, A* 24, 39-44 (2007).
Doi: 10.1364/JOSAA.24.000A39
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).
Doi: 10.1021/jp066667a
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).
Doi: 10.1021/jp067634y
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).
Doi: 10.1021/jp066802j
478. Structure and electronic spectra of DNA mini-hairpins with Gn:Cn stems, Jennifer Tuma, Stefano Tonzani, George C. Schatz, Andrew H. Karaba and Frederick D. Lewis, *J. Phys. Chem. B* 111, 13101-106 (2007).
Doi: 10.1021/jp072303m
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).
Doi: 10.1021/jp802378a
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).
Doi: 10.1021/jp0700478
481. Using theory and computation to model nanoscale properties, G. C. Schatz, *PNAS* 104, 6885-92 (2007).
Doi: 10.1073/pnas.0702187104 PMID: PMC1855400
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 Letters*, 7, 2014-9 (2007).
Doi: 10.1021/nl070834g
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, *JACS*, 129, 7647-56 (2007)
Doi: 10.1021/ja0707106
484. Nanoscale fracture mechanics, Steven L. Mielke, Ted Belytschko and George C. Schatz, *Annu. Rev. Phys. Chem.*, 58, 185-209 (2007).

Doi: 10.1146/annurev.physchem.58.032806.104502

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).
Doi: 10.1063/1.2734548
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).
Doi: 10.1063/1.2748373
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*, ed. R. Nagarajan and T. A. Hatton, ACS Books Symp. Series 996, 108-121 (2008).
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).
Doi: 10.1021/jp073403v
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).
Doi: 10.1063/1.2768533
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. Ed.*, 85, 744-48 (2008).
Doi: 10.1021/ed085p744
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. Letter*, 446, 128-132 (2007).
Doi: 10.1016/j.cplett.2007.08.033
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).
Doi: 10.1021/jp075173q
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).
Doi: 10.1364/OL.32.002254
494. Crossed-Beams and Theoretical Studies of the $O(^3P) + H_2O \rightarrow HO_2 + H$ 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).
Doi: 10.1021/jp0744228

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)
Doi: 10.1021/ja073034g
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).
Doi: 10.1007/s00339-007-4138-y
497. Ethical Responsibilities for Authors in the Journal of Physical Chemistry, G. C. Schatz, *J. Phys. Chem. A/B/C* 111, 8281 (2007).
Doi: 10.1021/jp0795331
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).
Doi: 10.1021/jp075838o
499. Nanoparticle optical properties : Far-and near- field electrodynamic coupling in a chain of silver nanoparticles, A. O. Pinchuk and G. C. Schatz, *Materials Science and Engineering B*, 149, 251-258 (2008)
Doi: 10.1016/j.mseb.2007.09.078
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).
Doi: 10.1002/anie.200702570
501. Tailoring the parameters of nanohole arrays in gold films for sensing applications, George C. Schatz, Jeffrey M. McMahon and Stephen K. Gray, *Plasmonics: metallic Nanostructures and Their Optical Properties V*, ed. Mark I. Stockman, *Proc. SPIE* 6641, 664103-1,3-8 (2007).
Doi: 10.1117/12.731368
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).
Doi: 10.1103/PhysRevB.77.014109
503. Multiscale coupling schemes spanning the quantum mechanical, atomistic forcefield, and continuum regimes, Roopam Khare, Steven L. Mielke, George C. Schatz, Ted Belytschko, *Computer Methods in Applied Mechanics and Engineering*, 197, 3190-3202 (2008).
Doi: 10.1016/j.cma.2007.11.029
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).
Doi: 10.1021/jp076273z

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, *Optics Express*, 15, 18119-29 (2007).
Doi: 10.1364/OE.15.018119
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).
Doi: 10.1021/jp076716z
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).
Doi: 10.1038/nature06508
508. Near-field polarization effects in molecular-motion-induced photochemical imaging, Christophe Hubert, Renaud Bachelot, Jérôme Plain, Sergeï Kostcheev, Gilles Lerondel, Juan Mathieu, Pascal Royer, Shengli Zou, George C. Schatz, Gary Wiederrecht and Stephen Gray, *J. Phys. Chem. C*, 112, 4111-6 (2008).
Doi: 10.1021/jp7096263
509. Editorial for January 2008, G. C. Schatz, *J. Phys. Chem. A, B, C* 112, 1-2(2008).
Doi: 10.1021/jp7110567
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).
Doi: 10.1021/jp075799g
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).
Doi: 10.1039/B706023H
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).
Doi: 10.1021/ja078162j
513. Molecular Plasmonics: Chromophore-Plasmon Coupling and Single Particle Nanosensors, Jing Zhao, Leif J. Sherry, George C. Schatz, and Richard P. Van Duyne, *IEEE Journal of Selected Topics in Quantum Electronics*, 14, 1418-29 (2008).
Doi: 10.1109/JSTQE.2008.924840
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).
Doi: 10.1016/j.cplett.2008.05.041

515. Electronic excitations and spectra in single stranded DNA, S. Tonzani and G. C. Schatz, *JACS*, 130, 7607-7612 (2008).
Doi: 10.1021/ja7103894
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, *JACS*, 130, 5883-5 (2008). Doi: 10.1021/ja801173r
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, *Accounts of Chemical Research*, 41(12), 1710-1720 (2008).
Doi: 10.1021/ar800028j
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).
Doi: 10.1021/jp801719c
519. The effect of surface roughness on the extinction spectra and electromagnetic fields around gold nanoparticles, Shuzhou Li and George C. Schatz, *Materials Research Society Proceedings*, 1087E, V01-08 (2008).
Doi: 10.1557/PROC-1087-V01-08
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).
Doi: 10.1021/jp8004844
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).
Doi: 10.1021/la900113e
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)
Doi: 10.1021/jp803192u
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).
Doi: 10.1021/jp804088z
524. Highly accurate first-principles benchmark datasets 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, J. M. L. Martin, Amir Karton, Alex Tarnopolsky and George C. Schatz, *J. Phys. Chem. A* 112, 12868-12886 (2009).
Doi: 10.1021/jp801805p
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).
Doi: 10.1021/jp802707r

526. Surface plasmon-mediated energy transfer in hetero-gap 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)
Doi: 10.1021/nl8023164
527. Many-body theory of surface-enhanced Raman scattering, David J. Masiello and George C. Schatz, *Phys. Rev. A* 78, 042505/1-/24 (2008)
Doi: 10.1103/PhysRevA.78.042505
528. A discrete action principle for electrodynamics and the construction of explicit symplectic integrators for linear, non-dispersive media, Jeffrey M. McMahon, Stephen K. Gray and George C. Schatz, *J. Comp. Phys.* 228, 3421-32 (2009).
Doi: 10.1016/j.jcp.2009.01.019
529. Unusual mechanisms can dominate reactions at hyperthermal energies: an example from $O(3P) + HCl \rightarrow ClO + H$, 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).
Doi: 10.1021/ja803080q
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, *Advanced Materials*, 21, 706-9 (2009).
Doi: 10.1002/adma.200801724
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).
Doi: 10.1021/jp805215j
532. An atomistic-continuum Cosserat rod model of carbon nanotubes, Karthick Chandraseker, Subrata Mukherjee, Jeffrey T. Paci and George C. Schatz, *Journal of Mechanics and Physics of Solids*, 57, 932-958 (2009).
Doi: 10.1016/j.jmps.2009.02.005
533. Measurements of near-ultimate strength for multiwalled carbon nanotubes and irradiation-induced crosslinking improvements, Bei Peng, Mark Locascio, Peter Zapol, Shuyou Li, Steven L. Mielke, George C. Schatz and Horacio D. Espinosa, *Nature Nanotech*, 3, 626-631 (2008)
Doi: 10.1038/nnano.2008.211
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).
Doi: 10.1063/1.2961012
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).
Doi: 10.1063/1.2977727
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).
Doi: 10.1021/ja8051427

537. Collective surface plasmon resonance coupling in silver nanoshell arrays. A. O. Pinchuk and G. C. Schatz, *Appl. Phys. B* 93, 31-38 (2008).
Doi: 10.1007/s00340-008-3148-6
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, *Plasmonics: Nanoimaging, Nanofabrication, and Their Applications IV*, Ed. Satoshi Kawata, Vladimir M. Shalaev, Din Ping Tsai, *Proc. SPIE* 7033, 703311, 1-6 (2008).
Doi: 10.1117/12.790647
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, 19302-19310 (2008).
Doi: 10.1021/jp807837t
540. Modeling reactive scattering of F(²P) at a liquid squalane interface: A hybrid QM/MM molecular dynamics study, Brian Radak, Scott Yockel, Dongwook Kim and George C. Schatz, *J. Phys. Chem. A* 113, 7218-26 (2009).
Doi: 10.1021/jp809546r
541. Plasmonic focusing in rod-sheath hetero-nanostructures, Xiaodong Chen, Shuzhou Li, Can Xue, Matthew J. Banholzer, George C. Schatz, Chad A. Mirkin, *ACS Nano*, 3, 87-92 (2009).
Doi: 10.1021/nn800695u
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. Amer. Chem. Soc.* 131, 849-854 (2009).
Doi: 10.1021/ja8080154
543. Molecular dynamics simulation of DNA-functionalized gold nanoparticles, One-Sun Lee and George C. Schatz, *J. Phys. Chem. C*, 113, 2316-21 (2009).
Doi: 10.1021/jp8094165
544. Correlating the structure, optical spectra and electrodynamics 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).
Doi: 10.1021/jp8098736
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(16), 4780-4787 (2009).
Doi: 10.1021/jp8080657
546. Editorial for 2009, George C. Schatz, *J. Phys. Chem. A, B, C* 113, 1 (2009).
Doi: 10.1021/jp810598t
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, Jianming Zhang, George C. Schatz and Timothy K. Minton, *J. Phys. Chem. C*, 113, 4677-85 (2009).
Doi: 10.1021/jp9000412

548. Core-shell triangular bipyramids, Hyojong Yoo, Jill E. Millstone, Shuzhou Li, Jae-Wong Jang, Wei Wei, Jinsong Wu, George C. Schatz and Chad A. Mirkin, *Nano Lett* 9, 3038-41 (2009).
Doi: 10.1021/nl901513g
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).
10.1021/jp900412w
550. Hydrophobic dimerization and thermal dissociation of perylene diimide-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.* 131, 5920-5929 (2009).
Doi: 10.1021/ja900347t
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).
Doi: 10.1021/ja809157f
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, *Optics Express*, 17, 2334-2340 (2009).
Doi: 10.1364/OE.17.002334
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, *Analytical Biochemistry*, 394, 1819 (2009).
Doi: 10.1007/s00216-009-2738-4
554. Confining standing waves in optical corrals, Yelizaveta Babayan, Jeffrey M. McMahon, Shuzhou Li, Stephen K. Gray, George C. Schatz, Teri W. Odom, *ACS Nano*, 3, 615-620 (2009).
Doi: 10.1021/nn8008596
555. FDTD studies of metallic nanoparticle systems, Ariel L. Atkinson, Jeffrey M. McMahon and George C. Schatz, in *Self-Organization of Molecular Systems: From Molecules and Clusters to Nanotubes and Proteins*, N. Russo, ed., NATO Science for Peace of Security Series A: Chemistry and Biology, Springer, Berlin, 2009, pp.11-32.
556. Screening of type I and II drug binding to human cytochrome P450-3A4 in nanodiscs by localized surface plasmon resonance spectroscopy, Aditi Das, Jing Zhao, George C. Schatz, Stephen G. Sligar, and Richard P. Van Duyne, *Anal. Chem.*, 81, 3754-59 (2009).
Doi: 10.1021/ac802612z
557. Functional representation for the Born-Oppenheimer diagonal correction and Born-Huang adiabatic potential energy surfaces for isotopomers of H₃, Steven L. Mielke, David W. Schwenke, George C. Schatz, Bruce C. Garrett, and Kirk A. Peterson, *J. Phys. Chem. A* 113, 4479-88 (2009).
Doi: 10.1021/jp8110887

558. A method to correlate optical properties and structures of metallic nanoparticles, Y. Wang, S. K. Eswaramoorthy, L. J. Sherry, J. A. Dieringer, J. P. Camden, G. C. Schatz, R. P. Van Duyne, L. D. Marks, *Ultramicroscopy*, 109, 1110-1113 (2009).
Doi: 10.1016/j.ultramic.2009.04.003
559. A charge-dipole interaction model for the frequency-dependent polarizability of silver clusters, A. Mayer, A. L. Gonzalez, C. M. Aikens and G. C. Schatz, *Nanotechnology* 20, 19504/1-/10 (2009).
Doi: 10.1088/0957-4484/20/19/195204
560. Autobiography, George C. Schatz, *J. Phys. Chem. A* 113, 3711-16 (2009).
Doi: 10.1021/jp901789m
561. Surprisingly Long-Range Surface-Enhanced Raman Scattering (SERS) on Au-Ni Multisegmented Nanowires, Wei Wei, Shuzhou Li, Jill E. Millstone, Matthew J. Banholzer, Xiaodong, Chen, Xiaoyang, Xu, George C. Schatz and Chad A. Mirkin, *Ange. Chemie*, 48, 4210-4212 (2009).
Doi: 10.1002/anie.200806116
562. Inversion of product selectivity in an enzyme-inspired metallosupramolecular tweezer catalyzed epoxidation reaction, Pirmin A. Ulmann, Adam B. Braunschweig, One-Sun Lee, Michael J. Wiester, George C. Schatz and Chad A. Mirkin, *Chem. Comm.* 34, 5121-23 (2009).
Doi: 10.1039/b908852k
563. The Journal of Physical Chemistry Letters, George C. Schatz, *J. Phys. Chem. A* 113, 7983, *B* 113, 9351, *C* 113, 11975 (2009).
Doi: 10.1021/jp9052105
564. Distance dependence of plasmon-enhanced photocurrent in dye-sensitized solar cells, S. D. Standridge, G. C. Schatz, J. T. Hupp, *J. Am. Chem. Soc.* 131, 8407-9 (2009).
Doi: 10.1021/ja9022072
565. Enhanced polarizability of aromatic molecules placed in the vicinity of silver clusters, A. Mayer and G. C. Schatz, *J. Phys.: Condensed Matter* 21, 325301/1-/8 (2009).
Doi: 10.1088/0953-8984/21/32/325301
566. Silver nanoparticles with broad multiband linear optical absorption, Osman M. Bakr, Vincenzo Amendola, Christine M. Aikens, Wim Wenseleers, Rui Li, Luca Dal Negro, George C. Schatz, Francesco Stellacci, *Angewandte Chemie*, 48, 5921-26 (2009).
Doi: 10.1002/anie.200900298
567. Photoinduced electron transfer from rail to rung within a self-assembled oligomeric porphyrin ladder, Chunxing She, Suk Joong Lee, James E. McGarrah, Josh Vura-Weis, Michael R. Wasielewski, Hanning Chen, George C. Schatz, Mark A. Ratner and Joseph T. Hupp, *Chem. Comm.*, 46, 547-549 (2010).
Doi: 10.1039/b916392a
568. Plasmon-mediated synthesis of silver triangular bipyramids, Jian Zhang, Shuzhou Li, Jinson Wu, George C. Schatz, Chad A. Mirkin, *Angew. Chemie*, 48, 7787-91 (2009).
Doi: 10.1002/anie.200903380
569. Nonlocal optical response of metal nanostructures with arbitrary shape, Jeffrey M. McMahon, Stephen K. Gray and George C. Schatz, *Phys. Rev. Lett* 103, 097403/1-/4 (2009).
Doi: 10.1103/PhysRevLett.103.097403

570. On the importance of incorporating dipole reradiation in the modeling of surface enhanced Raman scattering from spheres, Logan K. Ausman and George C. Schatz, *J. Chem. Phys.*, 131, 084708/1-10 (2009).
Doi: 10.1063/1.3211969
571. Interaction between DNAs on a gold surface, One-Sun Lee and George C. Schatz, *J. Phys. Chem. C*, 113, 15941-47 (2009).
Doi: 10.1021/jp905469q
572. Nanotechnology for Next Generation Solar Cells, P. V. Kamat and G. C. Schatz, *J. Phys. Chem. C* 113, 15473-5 (2009).
Doi: 10.1021/jp905378n
573. Single-molecule pulling and the folding of donor-acceptor oligorotaxanes: phenomenology and interpretation, Ignacio Franco, George C. Schatz and Mark A. Ratner, *J. Chem. Phys.* 131, 124902/1-124903/13 (2009).
Doi: 10.1063/1.3223729
574. Effect of GC base pairs on charge transfer through DNA hairpins: the importance of electrostatic interactions, F. C. Grozema, S. Tonzani, Y. A. Berlin, G. C. Schatz, L. D. A. Siebbeles, and M. A. Ratner, *J. Am. Chem. Soc.* 131, 14204-5 (2009).
Doi: 10.1063/1.3223729
575. Hyperthermal O-atom exchange reaction $O_2 + CO_2$ through a CO_4 intermediate, L. Y. Yeung, M. Okumura, J. T. Paci, G. C. Schatz, J. Zhang and T. K. Minton, *J. Am. Chem. Soc.* 131, 13940-42 (2009). Doi: 10.1021/ja903944k
576. Quantum mechanical calculations of the $S(^1D) + HD$ reaction dynamics on the ground electronic state, H. Yang, K.-L. Han, G. C. Schatz, S. C. Smith and M. Hankel, *Journal of Physics: Conference Series* 185, 012056 (2009).
577. Chemical fabrication of heterometallic nanogaps for molecular transport junctions, Xiaodong Chen, Sina Yeganeh, Lidong Qin, Shuzhou Li, Can Xue, Adam B. Braunschweig, George C. Schatz, Mark A. Ratner, Chad A. Mirkin, *Nano Lett.* 9, 3974-3979 (2009). Doi: 10.1021/nl9018726
578. Editorial for 2010, George C. Schatz, *J. Phys. Chem. A/B/C* 114, 1, (2010)
Doi: 10.1021/jp911612h
579. Conformation of DNA between gold surfaces, One-Sun Lee and George C. Schatz, *Journal of Computational and Theoretical Nanoscience* 7, 2568-2573 (2010).
Doi: 10.1166/jctn.2010.1643
580. Electron-beam mapping of plasmon resonances in electromagnetically interacting rough gold nanorods, Moussa N'Gom, Shuzhou Li, George Schatz, Rolf Erni, Ashish Agarwal, Nicholas Kotov and Theodore B. Norris, *Phys. Rev. B* 80, 113411 (2009).
Doi: 10.1103/PhysRevB.80.113411
581. Plasmonic superlattices: Hierarchical subwavelength hole arrays, Teri W. Odom, Hanwei Gao, Jeffrey M. McMahon, Joel Henzie and George C. Schatz, *Chem. Phys. Lett.* 483, 187-192 (2009).
Doi: 10.1016/j.cplett.2009.10.084

582. Integral and differential cross sections for the $S(^1D) + HD$ reaction employing the ground adiabatic electronic state, H. Yan, K. -L. Han, G. C. Schatz, S.-H. Lee, K. Liu, S. C. Smith, and M. Hankel, *PCCP* 11, 11587-95 (2009).
Doi: 10.1039/b917972k
583. Direct dynamics simulations of the reaction $O^+(^4S) + HCN$ at hyperthermal collision energies, Lipeng Sun and George C. Schatz, *J. Phys. Chem. C* 114, 5263-75 (2010).
Doi: 10.1021/jp903177a
584. Periodic electric field enhancement along gold rods with nanogaps, Maria L. Pedano, Shuzhou Li, George C. Schatz and Chad A. Mirkin, *Angew. Chem. Int. Ed.* 49, 78-82 (2010).
Doi: 10.1002/anie.200904646
585. A New High-Profile Journal for Cutting -Edge Research across Physical Chemistry, George Schatz, Prashant Kamat, Sharon, Hammes-Schiffer, Tim Zwier, *J. Phys. Chem. Lett.* 1,1 (2010).
Doi: 10.1021/jz9001899
586. Simplistic model for the dendritic growth of a monolayer in dip pen nanolithography, Hyojeong Kim, George C. Schatz, Joonkyung Jang, *J. Phys. Chem. C*, 114, 1922-27 (2010)
Doi: 10.1021/jp909766p
587. Assembly of nanorods into designer superstructures: the role of templating, capillary forces, adhesion, and polymer hydration, Jacob Ciszek, Ling Huang, Stefan Tsonchev, Yu-Huang Wang, Kenneth R. Shull, Mark A. Ratner, George C. Schatz, Chad A. Mirkin, *ACS Nano* 4, 259-66 (2010).
Doi: 10.1021/nn901383d
588. Trajectory surface-hopping study of methane photodissociation dynamics, Maricris D. Lodriguito, Gyoergy Lendvay, George C. Schatz, *J. Chem. Phys.* 131, 224320/1-/9 (2009).
Doi: 10.1063/1.3271242
589. On the linear response and scattering of an interacting molecule-metal system, David Masiello and George C. Schatz, *J. Chem. Phys.*, 132, 064102 (2010).
Doi: 10.1063/1.3308624
590. Calculating the Raman and Hyper Raman Spectra of Large Molecules and Molecules Interacting with Nanoparticles, Nicholas Valley, Lasse Jensen, Jochen Autschbach and George C. Schatz, in: *Computational Methods for Large systems: Electronic Structure Approaches for Biotechnology and Nanotechnology*, Ed. Jeffrey R. Reimers (Wiley, New York, 2010), pp. 426-444.
591. Design of nanodiamond based drug delivery patch for cancer therapeutics and imaging applications, Wing Kam Liu, Ashfaq Adnan, Adrian M. Kopacz, Michelle Hallikainen, Dean Ho, Robert Lam, Jessica Lee, Ted Belytschko, George Schatz, Yonhua Tzeng, Young-Jin Kim, Seunghyun Baik, Moon Ki Kim, Taesung Kim, Hunghoon Lee, Eung-Soo Hwang, Seyoung Im, Eiji Osawa, Amanda Barnard, Huang-Cheng Chang, Hia-Ching Chang, and Eugenio Onate, in D. Ho ed., *Nanodiamonds: applications in biology and nanoscale medicine*, Springer Science+Business Media, 2010, Chap. 12, pp.249-284.
Doi: 10.1007/978-1-4419-0531-4_12.
592. A new high-profile journal for cutting-edge research across physical chemistry, George Schatz, Prashant Kamat, Sharon Hammes-Schiffer and Tim Zwier, *J. Phys. Chem. Lett.* 1,1 (2010).
Doi: 10.1021/jz9001899

593. Scattering dynamics of hyperthermal oxygen atoms on ionic liquid surfaces: [emin]NTf₂] and [C(12)min][NTf₂], Bohan Wu, Jianming, Zhang, Timothy K. Minton, Kenneth, G. McKendrick, John M. Slattery, Scott Yockel and George C. Schatz, *J. Phys. Chem. C* 114, 4015-27 (2010).
Doi: 10.1021/jp910641s
594. DNA Melting in small-molecule-DNA-hybrid dimer structures: experimental characterization and coarse-grained molecular dynamics simulations, Tatiana Prytkova, Ibrahim Eryazici, Brian Stepp, Son-Binh Nguyen and George C. Schatz, *J. Phys. Chem. B*, 114, 2627-34 (2010).
Doi: 10.1021/jp910395k
595. Abnormally large plasmonic shifts in silica-protected gold triangular nanoprisms, M. J. Banholzer, N. Harris, J. E. Millstone, G. C. Schatz and C. A. Mirkin, *J. Phys. Chem. C*, 114, 7521-26 (2010).
Doi: 10.1021/jp911889a
596. Conformational control of TT dimerization in DNA conjugates. A molecular dynamics study, Martin McCullagh, Mahesh Hariharan, Frederick D. Lewis, Dimitra Markovitsi, Thierry Douki and George C. Schatz, *J. Phys. Chem. B* 114, 5215-5221 (2010).
Doi: 10.1021/jp100983t
597. Coarse-grained molecular dynamics study of permeability enhancement in DPPC bilayers by incorporation of lysolipid, Nicolas D. Winter, George C. Schatz, *J. Phys. Chem. B* 114, 5053-5060 (2010). PMID: PMC2859970
Doi: 10.1021/jp911309s
598. Gap structure effects on surface-enhanced Raman scattering intensities for gold gapped rods, Shuzhou Li, Maria L. Pedano, Shih-Hui Chang, Chad A. Mirkin, George C. Schatz, *Nano Lett.* 10, 1722-27 (2010).
Doi: 10.1021/nl100099g
599. Crossed-beams and theoretical studies of hyperthermal reactions of O(³P) with HCl, J. Zhang, Amy L. Brunsvold, H. P. Upadhyaya, T. K. Minton, J. P. Camden, S. Garashchuk and G. C. Schatz, *J. Phys. Chem. A*, 114, 4905-4916 (2010).
Doi: 10.1021/jp101023y
600. Nonlocal dielectric effects in core-shell nanowires, J. M. McMahon, S. K. Gray and G. C. Schatz, *J. Phys. Chem. C* 114, 15903-15908 (2010).
Doi: 10.1021/jp910899b
601. Modeling O(³P) and Ar scattering from the ionic liquid [emim][NO₃] at 5 eV with hybrid QM/MM molecular dynamics, S. Yockel, and G. C. Schatz, *J. Phys. Chem. B*, 114, 14241-48 (2010).
Doi: 10.1021/jp910707v
602. Lattice gas Monte Carlo simulation of capillary forces in atomic force microscopy, Joonkyung Jang and George C. Schatz, *J. Adhesion Sci. and Tech.* 24, 2429-2451 (2010). Also in "Adhesion Aspects in MEMS/NEMS" edited by S.H.Kim, M.T. Dugger, and K.L.Mittal (Brill, Leiden, 2010)
Doi: 10.1163/016942410X508172
603. Molecular dynamics simulation of ds-DNA on a gold surface at low surface coverage, George C. Schatz and One-Sun Lee, *MRS Proceedings* 1177, Z09-33 (2009).
Doi: 10.1557/PROC-1177-Z09-33

604. Tailoring DNA Structure to Increase Target Hybridization Kinetics on Surfaces, A. E. Prigodich, O. -S. Lee, W. L. Daniel, D. S. Seferos, G. C. Schatz and C. A. Mirkin, *J. Amer. Chem. Soc.* 132, 10638-10641 (2010).
Doi: 10.1021/ja104859j
605. Development and modeling of arsenic-trioxide-loaded thermosensitive liposomes for anticancer drug delivery, Nicolas D. Winter, Ryan K. J. Murphy, Thomas V. O'Halloran and George C. Schatz, *J. Liposome Research*, 21, 106-115 (2011).DOI: 10.3109/08982104.2010.483597
PMCID: PMC3616413
606. Structure-Activity Relationships in Gold Nanoparticle Dimers and Trimers for Surface-Enhanced Raman Spectroscopy, Kristin L. Wustholz, Anne-Isabelle Henry, Jeffrey M. McMahon, R. Griffith Freeman, Nicholas Valley, Marcelo E. Piotti, Michael J. Natan, George C. Schatz, and Richard P. Van Duyne, *J. Am. Chem. Soc.* 132, 10903-10910 (2010).
Doi: 10.1021/ja104174m
- 607 Radial deformation of carbon nanotubes in supersonic collisions with a silicon surface, Leton C. Saha, George C. Schatz and Joonkyung Jang, *J. Phys. Chem. C* 114, 12565-72 (2010).
Doi: 10.1021/jp101686r
608. Unraveling the Effects of Size, Composition, and Substrate on the Localized Surface Plasmon Resonance Frequencies of Gold and Silver Nanocubes: A Systematic Single-Particle Approach, Emilie Ringe, Jeffrey M. McMahon, Kwonnam Sohn, Claire Cobley, Younan Xia, Jiaying Huang, George C. Schatz, Laurence D. Marks, and Richard P. Van Duyne, *J. Phys. Chem. C* 114, 12511-16 (2010)
Doi: 10.1021/jp104366r
- 609 Optical properties of nanowire dimers with a spatially nonlocal dielectric function, Jeffrey M. McMahon, Stephen K. Gray and George C. Schatz, *Nano Lett.* 10, 3473-81 (2010).
Doi: 10.1021/nl101606j
610. Correlating nanorod structure with experimentally measured and theoretically predicted surface plasmon resonance, Abrin L. Schmucker, Nadine Harris, Matthew J. Banholzer, Martin G. Blaber, Kyle D. Osberg, George C. Schatz and Chad A. Mirkin, *ACS Nano*, 4, 5453-63 (2010).
Doi: 10.1021/nn101493t E 5, 7685 (2011).
611. Reversing the size dependence of surface plasmon resonances, Sheng Peng, Jeffrey M. McMahon, George C. Schatz, Stephen K. Gray, Yugang Sun, *PNAS*, 107, 14530-34 (2010).
Doi: 10.1073/pnas.1007524107 PMCID: PMC2930473
612. Classical electrodynamics coupled to quantum mechanics for calculation of molecular optical properties: a RT-TDDFT/FDTD approach, Hanning Chen, Jeffrey M. McMahon, Mark A. Ratner and George C. Schatz, *J. Phys. Chem. C*, 114, 14384-392 (2010).
Doi: 10.1021/jp1043392
613. Silver-based nanodisk codes, Matthew J. Banholzer, Kyle D. Osberg, Shuzhou Li, Bryan F. Mangelson, George C. Schatz, Chad A. Mirkin, *ACS Nano*, 4, 5446-52 (2010)
Doi: 10.1021/nn101231u

614. Perylenediimide-linked DNA dumbbells: long-distance electronic interactions and hydrophobic assistance of base-pair melting, Mahesh Hariharan, Karsten Siegmund, Yan Zheng, Hai Long, George C. Schatz, Frederick D. Lewis, *J. Phys. Chem. C* 114, 20466-20471 (2010).
Doi: 10.1021/jp1048309
615. Theoretical studies of surface enhanced hyper-Raman spectroscopy: the chemical enhancement mechanism, Nicholas Valley, Lasse Jensen, Jochen Autschbach and George C. Schatz, *J. Chem. Phys.* 133, 054103/1-054103/8 (2010).
Doi: 10.1063/1.3456544
616. Calculating nonlocal optical properties of structures with arbitrary shape, Jeffrey M. McMahon, Stephen K. Gray and George C. Schatz, *Phys. Rev. B* 82, 035423/1-035423/12 (2010).
Doi: 10.1103/PhysRevB.82.035423
617. DNA structures and excited states, G. C. Schatz, *J. Phys. Chem. Lett.* 1, 2054 (2010).
Doi: 10.1021/jz100697q
618. Using DNA to link gold nanoparticles, polymers and molecules: a theoretical perspective, One-Sun Lee, Tatiana Prytkova, George C. Schatz, *J. Phys. Chem. Lett.* 1, 1781-1788 (2010).
Doi: 10.1021/jz100435a PMICD: PMC2893743
619. Oxidation and etching of CVD diamond by thermal and hyperthermal atomic oxygen, Zeev Shpilman, Irina, Gouzman, Eitan, Grossman, Linhan, Shen, Timothy K. Minton, Jeffrey T. Paci, George C. Schatz, Rozalia Akhvlediani, Alon Hoffman, *J. Phys. Chem. C*, 114, 18996-19003 (2010).
Doi: 10.1021/jp1073208
620. Exact and truncated Coriolis coupling calculations for the S(1D) + HD reaction employing the ground adiabatic electronic state, H. Yang, K. -L. Han, G. C. Schatz, S. C. Smith and M. Hankel, *PCCP*, 12, 12711 – 12718 (2010).
Doi: 10.1039/c0cp00850h
621. Conformational control of thymine photodimerization in single-stranded and duplex DNA containing locked nucleic acid TT steps, Mahesh Hariharan, Martin McCullagh, George C. Schatz, Frederick D. Lewis, *J. Am. Chem. Soc.* 132, 12856-58, E 15831 (2010).
Doi: 10.1021/ja108528q
622. Cooperative melting in caged dimers with only two DNA duplexes, Ibrahim Eryazici, Tatiana R. Prytkova, George C. Schatz, SonBinh T. Nguyen, *J. Amer. Chem. Soc.* 132, 17068-17070 (2010).
Doi: 10.1021/ja107232x
623. Free-standing bimetallic nanorings and nanoring arrays made by on-wire lithography, Cipto Liusman, Shuzhou Li, Xiaodong Chen, Wei Wei, Hua Zhang, George C. Schatz, Freddy Boey, Chad A. Mirkin, *ACS Nano*, 4, 7676-82 (2010).
Doi: 10.1021/nn102495f
624. Plasmonic nanoparticles, George Schatz, *J. Phys. Chem. Lett.* 1, 802 (2010).
Doi: 10.1021/jz100069x
625. Metal nanostructures, George Schatz, *J. Phys. Chem. Lett.* 1, 2980-81 (2010).
Doi: 10.1021/jz101284n

626. Editorial for January 2011 for JPC A/B/C, *J. Phys. Chem. A* 115, 1 (2011).
Doi: 10.1021/jp111532x
627. Looking beyond the first anniversary, George C. Schatz, Prashant V. Kamat, Sharon Hammes-Schiffer, Timothy S. Zwier, *J. Phys. Chem. Lett.* 2, 34-35 (2011).
Doi: 10.1021/jz101663p
628. Atomistic simulation and measurement of pH dependent cancer therapeutic interactions with nanodiamond carrier, Ashfaq Adnan, Hanning Chen, Jessica Lee, Daniel J. Schaffer, Amanda S. Barnard, George C. Schatz, Dean Ho, Wing-Kam Liu, *Molec. Pharmaceutics*, 8, 368-74 (2011).
Doi: 10.1021/mp1002398
629. Computational electrodynamics methods, N. Harris, L. K. Ausman, J. M. McMahon, D. J. Masiello and G. C. Schatz, in *Computational Nanoscience*, RSC theoretical and computational chemistry series no. 4, ed. E. Bichoutskaia, (Royal Society of Chemistry, 2011) Chapter 6, p. 148-179.
DOI:10.1039/9781849732680-00147
630. Computational simulations of the interaction of lipid membranes with DNA-functionalized gold nanoparticles, One-Sun Lee and George C. Schatz, in *Biomedical Nanotechnology: Methods and Protocols*, *Methods in Molecular Biology*, vol.726, edited by Sarah J. Hurst, Springer Science+Business Media, 2011, 283-298
631. Computational Nanomaterials Modeling, George C. Schatz, *J. Phys. Chem. Lett.* 2, 125-126 (2011).
Doi: 10.1021/jz1017152
632. DNA-based optomechanical molecular motor, Martin McCullagh, Ignacio Franco, Mark A. Ratner and George C. Schatz, *J. Am. Chem. Soc.* 133, 3452-59 (2011).
Doi: 10.1021/ja109071a
633. Fundamental behavior of electric field enhancements in the gaps between closely spaced nanostructures, Jeffrey M. McMahon, Stephen K. Gray and George C. Schatz, *Phys. Rev. B* 83, 115428/1-5 (2011).
Doi: 10.1103/PhysRevB.83.115428
634. Kinetic isotope effects for the reactions of muonic helium and muonium with H₂, Donald G. Fleming, Donald J. Arseneau, Oleksandr Sukhorukov, Jess H. Brewer, Steven L. Mielke, George C. Schatz, Bruce C. Garrett, Kirk A. Peterson and Donald G. Truhlar, *Science*, 331, 448-450 (2011).
Doi: 10.1126/science.1199421
635. Mechanically activated molecular switch through single-molecule pulling, Ignacio Franco, Christopher B. George, Gemma C. Solomon, George C. Schatz and Mark A. Ratner, *J. Am. Chem. Soc.* 133, 2242-49 (2011).
Doi: 10.1021/ja1095396
636. Ionic liquids virtual special issue, Joan F. Brennecke, George C. Schatz, Robin D. Rogers, *Crystal Growth & Design*, 11, 625-626 (2011).
637. Atomistic molecular dynamics simulations of peptide amphiphile self-assembly into cylindrical nanofibers, One-Sun Lee, Samuel I. Stupp and George C. Schatz, *J. Am. Chem. Soc.* 113, 3677-3683 (2011)

Doi: 10.1021/mp1002398

638. Coulombic interactions and crystal packing effects in the folding of donor-acceptor oligorotaxanes, Ignacio Franco, Mark A. Ratner and George C. Schatz, *J. Phys. Chem. B*, 115, 2477-84 (2011).
Doi: 10.1021/jp108913s
639. Optical Properties of Metal Nanoparticles, Nadine Harris, Martin G. Blaber and George C. Schatz, in *Encyclopedia of nanotechnology*, B. Bhushan (ed), Springer, 2012, pp. 1950-69 DOI 10.1007/978-90-481-9751-4.
640. Extending SERS into the infrared with gold nanosphere dimers, Martin G. Blaber and George C. Schatz, *Chem. Comm.* 47, 3769-71 (2011).
Doi: 10.1039/c0cc05089j
641. Single-molecule surface-enhanced Raman spectroscopy of crystal violet isotopologues: theory and experiment, Samuel L. Kleinman, Emilie Ringe, Nicholas Valley, Kristin L. Wustholz, Eric Phillips, Karl A. Scheidt, George C. Schatz, Richard P. Van Duyne, *J. Amer. Chem. Soc.* 133, 4115-22 (2011).
Doi: 10.1021/ja110964d
642. Correlated structure and optical property studies of plasmonic nanoparticles, Anne-Isabelle Henry, Julia Bingham, Emilie Ringe, Laurence Marks, George C. Schatz and Richard P. Van Duyne, *J. Phys. Chem C*, 115, 9291-9305 (2011).
Doi: 10.1021/jp2010309
643. Triggered release of pharmacophores from [Ni(HAsO₃)]-loaded polymer-caged nanobin enhances pro-apoptotic activity: a combined experimental and theoretical study, Sang-Min Lee, One-Sun Lee, Thomas V. O'Halloran, George C. Schatz and SonBinh T. Nguyen, *ACS Nano*, 5, 3961-69. (2011).
644. Mixing rules and the Casimir force between composite systems, R. Esquivel-Sirvent and George C. Schatz, *Phys. Rev. A* 83, 042512 (2011).
Doi: 10.1103/PhysRevA.83.042512
645. Synthesis and isolation of {110}-faceted bold bipyramids and rhombic dodecahedra, Michelle L. Personick, Mark R. Langille, Jian Zhang, Nadine Harris, George C. Schatz, Chad A. Mikrin, *J. Amer. Chem. Soc.* 133, 6170-73 (2011).
Doi: 10.1021/ja201826r
646. Conformational control of thymine photodimerization in purine-containing trinucleotides, Zhengzheng Pan, Martin McCullagh, George C. Schatz, Frederick D. Lewis, *J. Phys. Chem. Lett*, 2, 1432-38 (2011). DOI: 10.1021/jz200532w
647. Theoretical calculation of the photo-induced electron transfer rate between a gold atom and a gold cation solvated in CCl₄, Hanning Chen, Mark A. Ratner and George C. Schatz, *J. Photochem. Photobiol. A* 221, 143-7 (2011) Doi: 10.1016/j.jphotochem.2011.04.021
648. A rod model for three dimensional deformations of single-walled carbon nanotubes, Ajeet Kumar, Subrata Mukherjee, Jeffrey T. Paci, Kathick Chandraseker and George C. Schatz, *International Journal of Solids and Structures*, 48, 2849-58 (2011). DOI: 10.1016/j.ijsolstr.2011.06.004

649. Introduction to plasmonics, Teri W. Odom and George C. Schatz, *Chemical Reviews*, 111, 3667-8 (2011) Doi: 10.1021/cr2001349
650. Confined propagation of covalent chemical reactions on single-walled carbon nanotubes, Shunliu Deng, Yin Zhang, Alexandra H. Brozena, Maricris Lodriguito Mayes, Parag Banerjee, Wen-An Chiou, Gary W. Rubloff, George C. Schatz and YuHuang Wang, *Nature Comm.* 2, 382 (2011) DOI: 10.1038/ncomms1384
651. Modeling DNA-bending in the nucleosome: role of AA periodicity. Tatiana Prytkova, Xiao Zhu, Jonathan Widom and George C. Schatz, *J. Phys. Chem. B*, 115, 8638-44 (2011). DOI: 10.1021/jp203564q PMID: PMC3140867
652. Molecular Dynamics Study of the Formation of a Self Assembled Monolayer on Gold, Ahn, Y. H.; Saha, J. K.; Schatz, G. C.; Jang, J. K. *J. Phys. Chem. C* **2011**, *115*, 10668-74. DOI: 10.1021/jp200447k
653. Small size limit to self assembled monolayer formation on gold (111), Saha, J. K.; Ahn, Y. H.; Kim, H.-J.; Schatz, G. C.; Jang, J. K. *J. Phys. Chem. C* **2011**, *115*, 13193-99. DOI: 10.1021/jp202564m
654. Theoretical studies of thymine-thymine photodimerization: using ground state dynamics to model photoreaction, M. McCullagh and G. C. Schatz, in *Practical aspects of computational chemistry I: An overview of the last two decades and current trends*, Ed. J. Leszczynski, M. K. Shukla and H. de Rode, Springer, Berlin, 2012, pp385-414. DOI: 10.1007/978-94-007-0919-5
655. Northwestern University Initiative for Teaching NanoSciences (NUITNS): An Approach for Teaching Computational Chemistry to Engineering Undergraduate Students, Tomekia Simeon, Christine M. Aikens, Baudilio Tejerina, and George C. Schatz, *J. Chem. Ed.* 88, 1079-84 (2011) DOI: 10.1021/ed101015a
656. Amphiphilic Soft Materials, George C. Schatz, *J. Phys. Chem. Lett.*, 2, 1624-25 (2011). DOI: 10.1021/jz200693s
657. Correlated optical measurements and plasmon mapping of silver nanorods, Beth S. Guiton, Vighter Iberi, Shuzhou Li, Donovan N. Leonard, Chad. M Parish, Paul G. Kotula, Maia Varela, George C. Schatz, Stephen J. Pennycook and Jon. P. Camden, *Nano Lett.* 11, 3482-88 (2011) DOI: 10.1021/nl202027h
658. Editorial: new deputy editors for the Journal of Physical Chemistry A, B and C, *J. Phys. Chem. A, B, C, Lett.* 115, 6319-20, 7711-7712, 11889-11890, 1408, 1409 (2011).
659. Theoretical studies of the erosion of (100) and (111) diamond surfaces by hyperthermal O(3P), Jeffrey T. Paci, George C. Schatz and Timothy K. Minton, *J. Phys. Chem. C*, 115, 14770-14777 (2011). DOI: 10.1021/jp201563m
660. Optical and electrical properties of inner tubes in outer wall-selectively functionalized double-wall carbon nanotubes, Yanmei Piao, Chien-Fu Chen, Alexander A. Green, Hyejin Kwon, Mark C. Hersam, Cheng S. Lee, George C. Schatz and YuHuang Wang, *J. Phys. Chem. Lett.*, 2, 1577-82 (2011) DOI: 10.1021/jz200687u
661. Understanding the electronic structure properties of bare silver clusters as models for plasmonic excitation, Lindsey R. Madison, Mark A. Ratner and George C. Schatz, in *M. A. C. Nascimento et*

- al (eds), *Frontiers in Quantum Methods and Applications in Chemistry and Physics, Progress in Theoretical Chemistry and Physics* (Springer) 29, 37-54 (2015) DOI 10.1007/978-3-319-14397-2_3
662. Time-dependent theory of the rate of photo-induced electron transfer, Hanning Chen, Mark A. Ratner and George C. Schatz, *J. Phys. Chem. C*, 115, 18810-21 (2011) DOI: 10.1021/jp205262u
663. Electromagnetic field enhancement for wedge-shaped metal nanostructures, Ali M. Angulo, Cecilia Noguez and George C. Schatz, *J. Phys. Chem. Lett.*, 2, 1978-83 (2011). DOI: 10.1021/jz200825a
664. Tunneling currents that increase with molecular elongation, Ignacio Franco, Gemma C. Solomon, George C. Schatz, Mark A. Ratner, *J. Amer. Chem. Soc.* 133, 15714-20 (2011) DOI: 10.1021/ja205908q
665. Nanoparticle superlattices engineering with DNA, Robert J. Macfarlane, Byeongdu Lee, Matthew R. Jones, Nadine Harris, George C. Schatz, Chad A. Mirkin, *Science* 334, 204-208 (2011) DOI: 10.1126/science.1210493
666. Dynamic QM/MM: a hybrid approach to simulating gas-liquid interactions, Scott Yockel and George C. Schatz, *Top. Curr. Chem.*, 307, 43-68 (2012) DOI: 10.1007/128_2011_130
667. Computational studies of the properties of DNA-linked nanomaterials, One-Sun Lee and George C. Schatz, *Advances in Chemical Physics* (ed. A. R. Dinner, Wiley, 2012) Vol 149, pp197-249.
668. O(³P) + CO₂ collisions at hyperthermal energies: dynamics of nonreactive scattering, oxygen isotope exchange, and oxygen-atom abstraction, L. Y. Yeung, M. Okumura, J. Zhang, T. K. Minton, J. T. Paci, A. Karton, J. M. L. Martin, J. P. Camden, and G. C. Schatz, *J. Phys. Chem. A* 116, 64-84 (2011), doi: 10.1021/jp2080379.
669. Kinetics of the reaction of the heaviest hydrogen atom with H₂, the ⁴Heμ + H₂ → ⁴HeμH + H reaction: Experiments, accurate quantal calculations, and variational transition state theory, including kinetic isotope effects for a factor of 36.1 in isotopic mass, D. G. Fleming, D. J. Arseneau, O. Sukhorukov, J. H. Brewer, S. L. Mielke, D. G. Truhlar, G. C. Schatz, B. C. Garrett and K. A. Peterson, *J. Chem. Phys.* 136, 184310 (2011) DOI: 10.1063/1.3657440
670. Observation of size-dependent thermalization in CdSe nanocrystals using time-resolved photoluminescence, Daniel C. Hannah, Nicholas J. Dunn, Sandrine Ithurria, Dmitri V. Talapin, Lin X. Chen, Matthew Pelton, George C. Schatz, Richard D. Schaller, *Phys. Rev. Lett.* 107, 177403/1-5 (2011) DOI: 10.1103/PhysRevLett.107.177403 107, 259901/1 (2011).
671. Electron donor-acceptor interactions with flanking purines influence the efficiency of thymine photodimerization, Zhengzheng Pan, Mahesh Hariharan, Joshua D. Arkin, Almaz S. Jalilov, Martin McCullagh, George C. Schatz, Frederick D. Lewis, *J. Am. Chem. Soc.* 133, 20793-98 (2011). DOI: 10.1021/ja205460f E: 134, 3611-11 (2012)
672. Observation of Multiple Vibrational Modes in Ultrahigh Vacuum Tip-Enhanced Raman Spectroscopy Combined with Molecular-Resolution Scanning Tunneling Microscopy N. Jiang, E. T. Foley, J. M. Klingsporn, M. D. Sonntag, N. A. Valley, J. A. Dieringer, T. Seideman, G. C. Schatz, M. C. Hersam and R. P. Van Duyne *Nano Lett.*, 12, 5061-67 (2012) DOI: 10.1021/nl2039925 E6506.

673. Modeling the effect of small gaps in surface-enhanced Raman spectroscopy, J. M. McMahon, S. Li, L. K. Ausman, G. C. Schatz, *J. Phys. Chem. C*, 116, 1627-37 (2012). DOI: 10.1021/jp207661y
674. Spatial nonlocality in the calculation of Hamaker coefficients, R. Esquivel-Sirvent and G. C. Schatz, *J. Phys. Chem. C*, 420-424 (2012) DOI: 10.1021/jp209577v
675. LSPR imaging of silver triangular nanoprisms: correlating scattering with structure using electrostatics for plasmon lifetime analysis, M. G. Blaber, A.-I. Henry, J. M. Bingham, G. C. Schatz, R. P. Van Duyne, *J. Phys. Chem. C*, 116, 393-403 (2012) DOI: 10.1021/jp209466k.
676. Single-molecule tip-enhanced Raman spectroscopy, M. D. Sonntag, J. M. Klingsporn, L. K. Garibay, J. M. Roberts, J. M. Dieringer, T. Seideman, K. Scheidt, L. Jensen, G. C. Schatz, R. P. Van Duyne, *J. Phys. Chem. C*, 116, 478-483 (2012). DOI: 10.1021/jp209982h
677. Computational modeling of plasmon-enhanced light absorption in a multicomponent dye sensitized solar cell, H. Chen, M. G. Blaber, S. D. Standridge, E. J. DeMarco, J. T. Hupp, M. A. Ratner, G. C. Schatz, *J. Phys. Chem. C* 116, 10215-10221 (2012). DOI:10.1021/jp301950q
678. CO₂ hydrogenation to formic acid on Ni (111), G. Peng, S. J. Sibener, G. C. Schatz, S. T. Ceyer and M. Mavrikakis, *J. Phys. Chem. C*, 116, 3001-3006 (2012) DOI: 10.1021/jp210408x
679. An experimental-computational study of shear interactions within double-walled carbon nanotube bundles, T. Filleter, S. Yockel, M. Naraghi, J. T. Paci, O. Compton, M. Lodriguito, S. T. Nguyen, G. C. Schatz, H. Espinosa, *Nano Lett.*, 12, 732-42 (2012) DOI: 10.1021/nl203686d
680. Editorial for January 2012 for JPC A/B/C, A. B. McCoy, S. Hammes-Schiffer, C. J. Murphy, G. C. Schatz, *J. Phys. Chem. B*, 116, 1 (2012).
681. Anion effects in the scattering of CO₂ from the room-temperature ionic liquids [bmin][BF₄] and [bmin][Tf₂N]: insights from trajectories, X. Li, G.C. Schatz and D. J. Nesbitt, *J. Phys. Chem. B*, 116, 3587-3602 (2012). DOI: 10.1021/jp2123357
682. Time-dependent density functional methods for surface enhance Raman scattering (SERS) studies, Jonathan M. Mullin, Jochen Autschbach, George C. Schatz, *Comp. Theor. Chem.*, 987, 32-41 (2012). DOI:10.1016/j.comptc.2011.08.027
683. A combined linear response quantum mechanics and classical electrodynamics (QM/ED) method for the calculation of surface enhanced Raman spectra, Jonathan Mullin, George C. Schatz, *J. Phys. Chem. A* 116, 1931-38 (2012). DOI: 10.1021/jp2087829
684. Spatial confinement of electromagnetic hot and cold spots in gold nanocubes, J. Haggui, M. Dridi, J. Plain, S. Marguet, H. Perez, G. C. Schatz, G. P. Wiederrecht, S. K. Gray, R. Bachelot, *ACS Nano*, 6, 1299-1307 (2012). DOI: 10.1021/nn2040389
685. Dipole Re-Radiation effects in surface enhanced Raman scattering, Logan K. Ausman and George C. Schatz, in *The Mie Theory*, W. Hergert and T. Wriedt, eds, Springer Series in Optical Sciences 169, Springer-Verlag, Berlin, 2012, Chapt. 5, 135-155.
686. Assembly of reconfigurable one-dimensional colloidal superlattices due to a synergy of fundamental nanoscale forces, Kaylie L. Young, Matthew R. Jones, Jian Zhang, Robert J. MacFarlane, Raul Esquivel-Sirvent, Rikkert J. Nap, Jinsong S. Wu, George C. Schatz, Byeongdu

- Lee and Chad A. Mirkin, PNAS 109, 2240-2245 (2012). DOI: 10.1073/pnas.1119301109
687. Near-field optical properties of Au-nanocubes: confinement of hot and cold spots, M. Haggui, M. Dridi, J. Plain, S. Marguet, H. Perez, G. C. Schatz, G. P. Wiederrecht, S. K. Gray, R. Bachelot, SPIE Proceedings, 8424, Nanophotonics IV, 842415 (2012). DOI:10.1117/12.922414
688. Emerging themes in biophysical chemistry, G. C. Schatz, J. Phys. Chem. Lett., 3, 1072-73 (2012).
689. New subsections for JPC A/B/C and JPC Letters, A. B. McCoy, S. Hammes-Schiffer, C. J. Murphy, P. Kamat, G. C. Schatz, J. Phys. Chem. A/B/C, 116, 3507/4117, 7611 (2012).
690. Electronic interactions in helical stacked arrays of the modified DNA base pyrrolocytosine, Prakash P. Neelakandan, Martin McCullagh, George C. Schatz, Frederick D. Lewis, J. Phys. Chem. B 116, 5199-5204 (2012). DOI:10.1021/jp302385c
691. Enhancing the melting properties of small molecule-DNA hybrids through designed hydrophobic interactions: an experimental-computational study, Ibrahim Eryazici, Ilyas Yildirim, George C. Schatz, SonBinh T. Nguyen, J. Am. Chem. Soc. 134, 7450-7458 (2012) DOI:10.1021/ja300322a
692. A- to B- form transition in DNA between gold surfaces, One-Sun Lee, Vince Y. Cho and George C. Schatz, J. Phys. Chem. B, 116, 7000-7005 (2012). DOI:10.1021/jp300877e
693. Carbonization in polyacrylonitrile (PAN) based carbon fibers studied by ReaxFF molecular dynamics simulations, Biswajit Saha and George C. Schatz, J. Phys. Chem. B, 116, 4684-92 (2012). DOI:10.1021/jp300581b
694. CO₂ hydrogenation to formic acid on Ni (110), Guowen Peng, S. J. Sibener, G. C. Schatz and M. Mavrikakis, Surf. Sci. 606, 1050-1055 (2012). DOI:10.1016/j.susc.2012.02.027
695. Surface plasmon coupling of compositionally heterogeneous core-satellite nanoassemblies, Jun Hee Yoon, Yong Zhou, Martin G. Blaber, George C. Schatz, Sangwoon Yoon, J. Phys. Chem. Lett, 4, 1371-1378 (2013) DOI: 10.1021/jz400602f
696. On the origin of photoluminescence in silicon nanocrystals: pressure-dependent structural and optical studies, Danniell C. Hannah, Jihua Yang, Paul Podsiadlo, Maria K. Y. Chan, Arnaud Demortiere, David J. Gosztola, Vitali, B. Prakapenka, George C. Schatz, Uwe Kortshagen Richard J. Schaller, Nano Lett. 12, 4200-4205 (2012) DOI:10.1021/nl301787g
697. Dispersible gold nanorod dimers with sub-5 nm gaps as local amplifiers for surface-enhanced Raman scattering, K. D. Osberg, M. Rycenga, N. Harris, A. L. Schmucker, M. R. Langille, G. C. Schatz, C. A. Mirkin, Nano Lett., 12, 3828-32 (2012). DOI:10.1021/nl301793k
698. Hyperthermal oxidation of graphite and diamond, J. T. Paci, T. K. Minton, G. C. Schatz, Accts. Chem. Res. 45, 1973-81 (2012). DOI:10.1021/ar200317y
699. QM/MM studies of gas-liquid collisional energy transfer, Xiaohu Li and George C. Schatz, in Theory and applications in computational chemistry: the first decade of the second millennium: International Congress TACC-2012, AIP Conf. Proc. 1456, 131-138 (2012). doi:<http://dx.doi.org/10.1063/1.4730652>
700. Structural effects in the electromagnetic enhancement mechanism of surface-enhanced Raman scattering: dipole reradiation and rectangular symmetry effects in nanoparticle arrays. Logan K. Ausman, Shuzhou Li and George C. Schatz, J. Phys. Chem. C, 116, 17318-27 (2012). DOI:

10.1021/jp2122938

701. Modeling the electron-impact dissociation of methane, Marcin Ziolkowski, Anna Vikar, Maricris Lodriguito Mayes, Akos Bencsura, G. Lendvay, George C. Schatz, *J. Chem. Phys.* 137, 22A510 (2012). DOI:10.1063/1.4733706
702. Liquid plasmonics: manipulating surface plasmon polaritons via phase transitions, S. R. C. Vivekchand, Clifford J. Engel, Steven M. Lubin, Martin G. Blaber, Wei Zhou, Jae Yong Suh, George C. Schatz, Teri W. Odom, *Nano Lett.* 12, 4324-28 (2012). DOI:10.1021/nl302053g
703. Effect of structural dynamics and base pair sequence on the nature of excited states in DNA hairpins, Sameer Patwardhan, Stefano Tonzoni, Frederick D. Lewis, Laurens D. A. Siebbeles, George C. Schatz, Ferdinand C. Grozema, *J. Phys. Chem. B*, 116, 11447-58 (2012) DOI: 10.1021/jp307146u
704. The optical properties of responsive hybrid Au@polymer nanoparticles, Mario Tagliazucchi, Martin G. Blaber, George C. Schatz, Emily A. Weiss, Igal Szleifer, *ACS Nano* 6, 8397-8406 (2012) DOI: 10.1021/nn303221y
705. Molecular dynamics simulation of β -sheet formation in self-assembled peptide amphiphile fibers, One-Sun Lee, Yamei Liu and George C. Schatz, *J. Nanopart. Res.* 14, 936/1-936/7 (2012) DOI: 10.1007/s11051-012-0936-z
706. Defects in DNA: Lessons from Molecular Motor Design, M. McCullagh, I. Franco, M. A. Ratner and G.C. Schatz, *J. Phys. Chem. Lett.*, 3, 689-93 (2012) DOI: 10.1021/jz201649k
707. Getting your submission right and avoiding reject-without-review, Prashant V. Kamat and George C. Schatz, *J. Phys. Chem. Lett.* 3, 3088-89 (2012). DOI:10.1021/jz3014562
708. Particle-level engineering of thermal conductivity in matrix-embedded semiconductor nanocrystals, Daniel C. Hannah, Sandrine Ithurria, Galyna Krylova, Dmitri V. Talapin, George C. Schatz, Richard D. Schaller, *Nano Lett.*, 12, 5797-5801 (2012). DOI:10.1021/nl303109r
709. A semiconducting organic radical cationic host-guest complex, Albert C. Fahrenbach, Srinivasan Sampath, Dattatray J. Late, Jonathan C. Barnes, Samuel L. Kleinman, Nicholas Valley, Karel J. Hartlieb, Zhichang Liu, Vinayak P. Dravid, George C. Schatz, Richard P. Van Duyne, J. Fraser Stoddart, *ACS Nano*, 6, 9964-71 (2012). DOI:10.1021/nn303553z
710. Molecular dynamics study of the role of the spine of hydration in DNA A-tracts in determining nucleosome occupancy, Xiao Zhu and George C. Schatz, *J. Phys. Chem. B*, 116, 13672-81 (2012). DOI:10.1021/jp3084887 PMID: PMC3508256
711. Near-infrared surface-enhanced Raman spectroscopy (NIR-SERS) for the identification of eosin Y: theoretical calculations and evaluation of two different nanoplasmonic substrates, Nathan G. Greeneltch, Amber S. Davis, Nicholas Valley, Francesca Casadio, George C. Schatz, Richard P. Van Duyne, Nilam C. Shah, *J. Phys. Chem. A*, 116, 11863-69 (2012). DOI:10.1021/jp3081035
Erratum: *J. Phys. Chem. A* 118, 1-3 (2014). DOI:10.1021/jp4123985
712. Eutectic liquid alloys for plasmonics: theory and experiment, Martin G. Blaber, Clifford J. Engel, S. R. C. Vivekchand, Steven M. Lubin, Teri W. Odom, George C. Schatz, *Nano Lett.* 12, 5275-80 (2012). DOI:10.1021/nl3025104

713. State-selected reaction of muonium with vibrationally excited H₂, Pavel Bakule, Donald G. Fleming, Oleksandr Sukhorukov, Katsuhiko Ishida, Francis Pratt, Takamasa Momose, Eiko Torikai, Steven L. Mielke, Bruce C. Garrett, Kirk A. Peterson, *J. Phys. Chem. Lett* 3, 2755-60 (2012). DOI:10.1021/jz3011496
714. Modeling the self-assembly of peptide amphiphiles into fibers using coarse-grained molecular dynamics, One-Sun Lee, Vince Cho, George C. Schatz, *Nano Lett.* 12, 4907-4913 (2012). DOI:10.1021/nl302487m
715. Self-assembly and photopolymerization of sub-2 nm one-dimensional organic nanostructures of graphene, Aparna Deshpande, Chun-Hong Sham, Justice M.P. Alaboson, Jonathan M. Mullin, George C. Schatz, Mark C. Hersam, *J. Am. Chem. Soc.* 134, 16759-64 (2012). DOI:10.1021/ja307061e
716. Combined quantum mechanics (TDDFT) and classical electrodynamics (Mie theory) methods for calculating surface enhanced Raman and hyper-Raman spectra, Jonathan Mullin, Nicholas Valley, Martin G. Blaber, George C. Schatz, *J. Phys. Chem. A*, 116, 9574-81 (2012). DOI:10.1021/jp307003p
717. Experimental and theoretical studies of plasmon-molecule interactions, Hanning Chen, George C. Schatz and Mark A. Ratner, *Reports on Progress in Physics*, 75, 096402/1-35, 2012 DOI:10.1088/0034-4885/75/9/096402
718. New directions in biophysical modeling, G. C. Schatz, *J. Phys. Chem. Lett.* 3, 3663-4 (2012).
719. Theoretical studies of the O + C₂ reaction at hyperthermal energies, Mausumi Ray, Biswajit Saha, George C. Schatz, *J. Phys. Chem. C*, 116, 26577-85 (2012). DOI: 10.1021/jp3066629
720. Structure-enhancement factor relationships in single gold nanoantennas by surface-enhanced Raman excitation spectroscopy, Samuel L. Kleinman, Bhavya, Sharma, Martin G. Blaber, Anne-Isabelle Henry, Nicholas Valley, Richard G. Freeman, Michael J. Natan, George C. Schatz, Richard, P. Van Duyne, *J. Am. Chem. Soc.*, 135, 301-308 (2013). DOI: 10.1021/ja309300d
721. Multiscale simulation as a framework for the enhanced design of nanodiamond-polyethylenimine-based gene delivery, Hansung Kim, Han Bin Man, Biswajit Saha, Adrian M. Kopacz, One-Sun Lee, George C. Schatz, Dean Ho, Wing Kam Liu, *J. Phys. Chem. Lett.*, 3, 3791-97 (2012). DOI: 10.1021/jz301756e PMCID: PMC3538166
722. QM/MM Study of photo-induced reduction of a tetrahedral Ag₂₀⁺ cluster by a Ag atom, Hanning Chen, Mark A. Ratner, George C. Schatz, *J. Phys. Chem. C*, 118, 1755-1762 (2014). DOI: 10.1021/jp310149y
723. Plasmon-sampled surface-enhanced Raman excitation spectroscopy on silver immobilized nanorod assemblies and optimization for near infrared ($\lambda_{ex} = 1064$) studies, Samuel L. Kleinman, Bhavya Sharma, Martin G. Blaber, Anne-Isabelle Henry, Nicholas Valley, R. Griffith Freeman, Michael Natan, George C. Schatz, Richard P. Van Duyne, *J. Am. Chem. Soc.* 135, 301-308 (2013). DOI: 10.1021/jp310846j
724. Controlling orientational order in 1-D assemblies of multivalent triangular prisms, Kevin L. Kohlstedt, Monica Olvera de la Cruz, George C. Schatz, *J. Phys. Chem. Lett.* 4, 203-208 (2013). DOI: 10.1021/jz301953k
725. Extraordinary improvement of the graphitic structure of continuous carbon nanofibers template

- with double wall carbon nanotubes, Dimitry Papkov, Allison, M. Beese, Alexander Goponenko, Yan Zou, Mohammad Naraghi, Horacio D. Espinosa, Biswajit Saha, George C. Schatz, Alexander Moravsky, Raouf Loutfy, Sonbin T. Nguyen, Yuris, Dzenis, *ACS Nano*, 7, 126-42 (2013). DOI:10.1021/nn303423x
726. Light-harvesting and ultrafast energy migration in porphyrin-based metal-organic frameworks, Ho-Jin Son, Shengye Jin, Sameer Patwardhan, Sander J. Wezenberg, Nak Cheon Jeong, Monica So, Christopher E. Wilmer, Amy A. Sarjeant, George C. Schatz, Randall Q. Snurr, Omar K. Farha, Gary P. Wiederrecht, Joseph T. Hupp, *J. Am. Chem. Soc.*, 135, 862-9 (2013). DOI: 10.1021/ja310596a
727. Nanoparticles and Theory, Nadine Harris, Shuzhou Li, George C. Schatz, *AIP Conf. Proc.*, 1504, 31-42 (2012). DOI: 10.1063/1.4771701
728. Editorial for January 2013 for JPC A/B/C, A. B. McCoy, S. Hammes-Schiffer, C. J. Murphy, G. C. Schatz, *J. Phys. Chem. A,B,C* 117, 1-2 (2013). DOI: 10.1021/jp311637k
729. Emerging research frontiers in physical chemistry, Prashant V. Kamat, George C. Schatz, *J. Phys. Chem. Lett.* 4, 233-234 (2013) DOI: 10.1021/jz301955f
730. Immobilized nanorod assemblies: fabrication and understanding of large area SERS substrates, Nathan G. Greeneltch, Martin G. Blaber, Anne-Isabelle Henry, George C. Schatz, Richard P. Van Duyne, *Anal. Chem.* 85(4), 2297-2303 (2013) DOI:10.1021/ac303269w
731. Plasmon-sampled surface-enhanced Raman excitation spectroscopy on silver immobilized nanorod assemblies and optimization for near infrared ($\lambda_{ex}=1064$ nm) studies, Nathan G. Greeneltch, Martin G. Blaber, George C. Schatz, Richard P. Van Duyne, *J. Phys. Chem. C* 117(6), 2554-2558 (2013) DOI:10.1021/jp310846j
732. Single-molecule pulling: phenomenology and interpretation, I. Franco, M. A. Ratner, G. C. Schatz, in *Nano and Cell Mechanics: Fundamentals and Frontiers*, First Edition, Ed. Horacio D. Espinosa and Gang Bao, Wiley, New York, 2013, pp369-388 ISBN: 978-1-1184-6039-9 DOI:10.1002/9781118482568.ch14
733. Tunable and broadband plasmonic absorption via dispersible nanoantennas with sub-10 nm gaps, Bryan F. Mangelson, Daniel J. Park, Kyle D. Osberg, George C. Schatz, Chad A. Mirkin, *Small*, 9, 2250-2254 (2013) DOI:10.1002/smll.201202787
734. Van der Waals torque coupling between slabs composed of planar arrays of nanoparticles, R. Esquivel-Sirvent and George C. Schatz, *J. Phys. Chem. C*, 117, 5492-96 (2013). DOI:10.1021/jp400581j
735. Identification of parameters through which surface chemistry determines the lifetimes of hot electrons in small Au nanoparticles, Kenneth O. Aruda, Mario Tagliacuzzi, Christina M. Sweeney, Daniel C. Hannah, George C. Schatz, Emily A. Weiss, *PNAS*, 110, 4212-17, (2013) S4212 DOI:10.1073/pnas.1222327110
736. A dynamic structural model of expanded RNA CAG repeats: a refined X-ray structure and computational investigations using molecular dynamics and umbrella sampling simulations, Ilyas Yildirim, Ha Jeung Park, Matthew D. Disney, George C. Schatz, *J. Am. Chem. Soc.* 135(9), 3528-38 (2013). DOI:10.1021/ja3108627 PMID: PMC3625063
737. Propagative sidewall alkylcarboxylation that induces red-shifted near-IR photoluminescence in

- single-wall carbon nanotubes, Yin Zhang, Nicholas Valley, Alexandra H. Brozena, Yanmei Piao, Xiaoping Song, George C. Schatz, Yu Huang Wang, *J. Phys. Chem. Lett.*, 4(5), 826-830 (2013). DOI:10.1021/jz400167d
738. Steered molecular dynamics studies of the potential of mean force for peptide amphiphile self-assembly into cylindrical nanofibers, Tao Yu, One-Sun, Lee, George C. Schatz, *J. Phys. Chem. A*, 117, 9004-13 (2013) DOI:10.1021/jp401508w
739. Plasmonics in the ultraviolet with the poor metals Al, Ga, In, Sn, Tl, Pb and Bi, Jeffrey M. McMahon, George C. Schatz, Stephen K. Gray, *PCCP* 15(15), 5415-23 (2013) DOI:10.1039/c3cp43856b Erratum *PCCP* 17, 19670-71 DOI:10.1039/C5CP90112J
740. Long-range plasmophore rules, Gilles R. Bourret, Tuncay Ozel, Martin Blaber, Chad M. Shade, George C. Schatz, Chad A. Mirkin, *Nano. Lett.* 13, 2270-2275 (2013) DOI: 10.1021/nl400884j
741. How to make your next paper scientifically effective, Prashant Kamat, George C. Schatz, *J. Phys. Chem. Lett.* 4, 1578-81 (2013). DOI:10.1021/jz4006916
742. Lasing action in strongly coupled plasmonic nanocavity arrays, Wei Zhou, Montacer Dridi, Jae Yong Suh, Chul Hoon Kim, Dick T. Co, Michael R. Wasielewski, George C. Schatz, Teri W. Odom, *Nature Nano* 8, 506-511 (2013) DOI: 10.1038/NNANO.2013.99
743. The effect of field gradient on SERS, Christine M. Aikens, Lindsey R. Madison and George C. Schatz, *Nature Photonics* 7, 508-10 (2013) DOI:10.1038/nphoton.2013.153
744. Tailorable plasmonic circular dichroism properties of helical nanoparticle superstructures, Chengyi Song, Martin G. Blaber, Gongpu Zhao, Peijun Zhang, H. Christopher Fray, George C. Schatz, Nathaniel L. Rosi, *Nano Lett.* 13, 3256-61 (2013). DOI:10.1021/nl4013776
745. Controlling conformations of conjugated polymers and small molecules: the role of nonbonding interactions, Nicholas E. Jackson, Brett M. Savoie, Kevin L. Kohlstedt, Monica Olvera de la Cruz, George C. Schatz, Lin X. Chen, Mark A. Ratner, *J. Am. Chem. Soc.* 135, 10475-10483 (2013). DOI:10.1021/ja403667s
746. Free energy profile and mechanism of self-assembly of peptide amphiphiles based on a collective assembly coordinate, Tao Yu, George C. Schatz, *J. Phys. Chem. B*, 117, 9004-9013(2013). DOI:10.1021/jp404835q
747. Increasing the impact of published work. Introducing ACS Liveslides, Prashant V. Kamat, George C. Schatz, *J. Phys. Chem. Lett.*, 4, 2377-78 (2013). DOI:10.1021/jz401301z
748. A look at the origin and magnitude of the chemical contribution to the enhancement mechanism of surface-enhanced Raman spectroscopy (SERS): theory and experiment, Nicholas Valley, Nathan Greeneltch, Richard P. Van Duyne and George C. Schatz, *J. Phys. Chem. Lett.* 4, 2599-2604 (2013). DOI: 10.1021/jz4012383
749. Tensile mechanics of α -helical polypeptides, Korosh Torabi and George C. Schatz, *Macromolecules*, 46, 7947-56 (2013). DOI:10.1021/ma4015824
750. High performance SERS substrates: Advances and Challenges, Bhavya Sharma, M. Fernanda Cardinal, Samuel L. Kleinman, Nathan G. Greeneltch, Renee R. Frontiera, Martin G. Blaber, George C. Schatz and Richard P. Van Duyne, *MRS Bulletin*, 38, 615-624 (2013). DOI:

10.1557/mrs.2013.161

751. Ultrafast energy migration in porphyrin-based metal organic frameworks (MOFs), S. Patwardhan, S. Jin, H-J Son, G. C. Schatz, Mater.Res. Soc. Symp. Proc. 1539, 987 (2013) DOI: 10.1557/opl.2013.987
752. Osmolytic co-solute perturbing the surface enhancement of halide ions, Xiaohu Li and George C. Schatz, J. Phys. Chem. Lett. 4, 2885-2889 (2013) DOI:10.1021/jz4014695
753. Brightening of carbon nanotube photoluminescence through the incorporation of sp³ defects, Yanmei Piao, Brendan, Meany, Lyndsey R. Powell, Nicholas Valley, Hyejin Kwon, George C. Schatz, YuHuang Wang, Nature Chemistry, 5, 840-845 (2013). doi:10.1038/nchem.1711
754. Nature of noncovalent interactions in catenane supramolecular complexes: calibrating the MM3 force field with ab initio, DFT and SAPT methods, Tomekia M. Simeon, Mark A. Ratner and George C. Schatz, J. Phys. Chem. A, 117, 7918-27 (2013).DOI: 10.1021/jp400051b PMID: PMC3840798
755. Computational modeling of octahedral iron oxide clusters: hexaaquairon (III) and its dimers, Yang Yang, Mark A. Ratner and George C. Schatz, J. Phys. Chem. C 117, 21706-17 (2013). DOI:10.1021/jp408066h
756. Understanding the surfaces of nanodiamonds, Jeffrey T. Paci, Han B. Man, Biswajit Saha, Dean Ho and George C. Schatz, J. Phys. Chem. C 117, 17256-67 (2013) DOI:10.1021/jp404311a
757. Model for describing plasmon-enhanced lasers that combines rate equations with finite-difference time-domain, Montacer Dridi and George C. Schatz, J. Opt. Soc. Am. B 30, 2791-7 (2013). DOI: 10.1364/JOSAB.30.002791
758. Plasmonically enhanced dye-sensitized solar cells, Michael B. Ross, Martin G. Blaber, George C. Schatz, in Plasmonics: Theory and Applications, T. V. Shahbazyan and M. I. Stockman, eds., Challenges and Advances in Computational Chemistry and Physics 15, Springer Science + Business Media, Dordrecht, 2014, Ch. 3, 1-23 DOI: 10.1007/978-94-007-7805-4_3
759. Direct measurement of lattice dynamics and optical phonon excitation in semiconductor nanocrystals using femtosecond stimulated Raman spectroscopy, Daniel C. Hannah, Kristen E. Brown, Ryan M. Young, Michael R. Wasielewski, George C. Schatz, Dick T. Co, Richard D. Schaller, Phys. Rev. Lett. 111, 107401 (2013) DOI: 10.1103/PhysRevLett.111.107401.
760. Induction and reversal of myotonic dystrophy type 1 pre-mRNA splicing defects by small molecules, Jessica L. Childs-Disney, Ewa Stepniak-Konieczna, Tuan Tran, Ilyas Yildirim, Hajeung Park, Catherine Z. Chen, Jason Hoskins, Noel Southall, Juan J. Marugan, Samarjit Patnaik, Wei Zheng, Chris P. Austin, George C. Schatz, Krzysztof Sobczak, Charels A. Thornton, Matthew D. Disney, Nature Comm. 4, 3044 (2013) DOI: 10.1038/ncomms3044 PMID: PMC3710115
761. Free-energy landscape for peptide amphiphile self-assembly: stepwise versus continuous assembly mechanisms, Tao Yu, George C. Schatz, J. Phys. Chem. B, 117, 14059-14064 (2013). DOI: 10.1021/jp409305e
762. Using DNA to design plasmonic metamaterials with tunable optical properties, Kaylie L. Young, Michael B. Ross, Martin G. Blaber, Matthew Rycenga, Matthew R. Jones, Chuan Zhang, Adv. Mater., 26, 653-659 (2013). DOI:10.1002/adma.201302938

763. Plasmon-enhanced solar chemistry: electrostatics and quantum mechanics, Hanning Chen, George C. Schatz and Mark A. Ratner, in *Solar Energy Conversion: Dynamics of Interfacial Electron and Excitation Transfer*, Ed. Piotr Piotrowiak, RSC Energy and Environment Series No. 8, The Royal Society of Chemistry, 2013, pp. 111-134 DOI:10.1039/9781849735445-00111.
764. Thymine photodimer formation in DNA hairpins. Unusual conformations favor (6-4) vs. (2+2) adducts, Mahesh Hariharan, Karsten Siegmund, Clifton Saurel, Martin McCullagh, George C. Schatz, Frederick D. Lewis, *Photochem. Photobiol. Sci.*, 13, 266-271 (2014) DOI: 10.1039/C3PP50283J PMID: PMC3902035
765. Metal oxide nanoparticle growth on graphene via chemical activation with atomic oxygen, James E. Johns, Justice M.P. Alaboson, Sameer Patwardhan, Christopher R. Ryder, George C. Schatz, Mark C. Hersam, *J. Am. Chem. Soc.* 135, 18121-18125 (2013). DOI:10.1021/ja408248z
766. Growth dynamics for DNA-guided nanoparticle crystallization, Subas Dhakal, Kevin L. Kohlstedt, George C. Schatz, Chad A. Mirkin, Monica Olvera de la Cruz, *ACS Nano*, 7, 10948-10959 (2013) DOI:10.1021/nn404476f E:8, 2098 (2014) DOI:10.1021/nn5008447
767. Structure of the myotonic dystrophy type 2 RNA and designed small molecules that reduce toxicity, Jessica L. Childs-Disney, Ilyas Yildirim, HaJeung, Park, Jeremy R. Lohman, Lirui Guan, Tuan Tran Partha Sarkar, George C. Schatz, Mathew D. Disney, *ACS Chem. Biol.* 9, 538-550 (2014) DOI:10.1021/cb4007387 PMID: PMC3944380
768. Structure and electronic spectra of purine-methyl viologen charge transfer complexes, Almaz S. Jalilov, Sameer Patwardhan, Arunoday Singh, Tomekia Simeon, Amy A. Sarjeant, George C. Schatz, Frederick D. Lewis, *J. Phys. Chem. B* 118, 125-133 (2014). DOI:10.1021/jp410348b PMID: PMC3930082
769. In situ scanning electron microscope peeling to quantify surface energy between multiwall carbon nanotubes and graphene, Michael R. Roenbeck, Xiaoding Wei, Allison M. Beese, Mohammad Naraghi, Al'one Furmanchuk, Jeffre T. Paci, George C. Schatz, Horacio D. Espinosa, *ACS Nano* 8, 124-138 (2013). DOI:10.1021/nn402485n
770. Collisions of sodium atoms with liquid glycerol: insights into solvation and ionization, Justin P. Wiens, Gilbert M. Nathanson, William A. Alexander, Timothy K. Minton, Lakshmi Sankaran, George C. Schatz, *J. Am. Chem. Soc.* 136, 3065-74 (2014). DOI:10.1021/ja4106144
771. The increasing impact of multimedia and social media in scientific publications, Prashant V. Kamat and George C. Schatz, *J. Phys. Chem. Lett.*, 5, 233-234 (2014). DOI:10.1021/jz402623m
772. Editorial for January 2014 for JPC A/B/C, George C. Schatz, Anne B. McCoy, Sharon Hammes-Schiffer, Catherine J. Murphy, *J. Phys. Chem. A*, 118, 1-3 (2014). DOI:10.1021/jp411739e
773. Time-dependent density functional methods for Raman spectra in open-shell systems, Fredy W. Aquino, George C. Schatz, *J. Phys. Chem. A*, 118, 517-525 (2014) DOI:10.1021/jp411039m
774. Surface nanophotonics theory. J. M. McMahon, S. K. Gray and G. C. Schatz, In: Andrews D. L., Scholes, G. D. and Wiederrecht, G. P. (eds), *Comprehensive Nanoscience and Technology*, Vol. 3, (Oxford, 2011), pp. 187-208 ISBN: 978-0-12-374396-1

775. Ground and excited state electronic spectra of perylene diimide dimers with flexible and rigid geometries in DNA conjugates, Prakash P. Neelakandan, Tarek A. Zeidan, Marting McCullagh, George C. Schatz, Josh Vura-Weiss, Chul Hoon Kim, Michael R. Wasielewski and Frederick D. Lewis, *Chem. Sci.* 5, 973-981 (2014).
776. Cell death versus cell survival instructed by supramolecular cohesion of nanostructures, Christina J. Newcomb, Shantanu Sur, Julia H. Ortony, One-Sun Lee, John B. Matson, Job Boekhoven, Jeong Min Yu, George C. Schatz, Samuel I. Stupp, *Nature Comm.* 5, 4321/1-10 (2014) DOI: 10.1038/ncomms4321
777. Overcoming the myths of the review process and getting your paper ready for publication, Prashant V. Kamat, Gregaory Scholes, Oleg Prezhdo, Francisco Zaera, Timothy Zwier and George C. Schatz, *J. Phys. Chem. Lett.* 5, 896-899 (2014). DOI:10.1021/jz500162r
778. Two-photon and time-resolved fluorescence spectroscopy as probes for structural determination in Amyloid- β peptides and aggregates, Travis B. Clark, Marcin Ziolkowski, George C. Schatz and Theodore Goodson, *J. Phys. Chem. B*, 118, 2351-59 (2014). DOI: 10.1021/jp500883s
779. Hydrophobic Organic Linkers in the Self-Assembly of Small Molecule-DNA Hybrid Dimers: A Computational/Experimental Study of the Role of Linkage Direction in Product Distributions and Stabilities, Illyas Yildirim, Ibrahim Eryazici, S. T. Nguyen, and G. C. Schatz, *J. Phys. Chem. B* 118, 2366-76 (2014) DOI: 10.1021/jp501041 PMCID PMC3954456
780. Shape-selective deposition and assembly of anisotropic nanoparticles, Yu Zhou, Xiaozhu Zhou, Daniel J. Park, Korosh Torabi, Keith A. Brown, Matthew R. Jones, Chuan Zhang, George C. Schatz, Chad A. Mirkin, *Nano Lett.* 14, 2157-61 (2014). DOI:10.1021/nl500471g
781. Cite with a Sight, Prashant Kamat and George C. Schatz, *J. Phys. Chem. Lett.* 5, 1241-2 (2014) DOI:10.1021/jz500430j
782. Molecular dynamics simulations and electronic excited state properties of a self-assembled peptide amphiphile nanofiber with metalloporphyrin arrays, Tao Yu, One-Sun Lee and George C. Schatz, *J. Phys Chem. A*, 118, 8553-62 (2014). DOI:10.1021/jp502459r
783. $O_2(X^3\Sigma_g^-)$ and $O_2(a^1\Delta_g)$ charge exchange with simple ions, Marcin Ziolkowski, George C. Schatz, A. A. Viggiano, Anthony Midey and Itzhak Dotan, *J. Chem. Phys.* 140, 214307/1-12 (2014).
784. Aluminum and indium plasmonic nanoantennas in the ultraviolet, Michael B. Ross and George C. Schatz, *J. Phys. Chem. C* 118, 12506-12514 (2014) DOI:10.1021/jp503323u
785. Synthesis and characterization of a plasmonic-semiconductor composite containing rationally designed, optically tunable gold nanorod dimers and anatase TiO_2 , Bryan F. Mangelson, Matthew R. Jones, Daniel J. Park, Chad M. Shade, George C. Schatz, Chad A. Mirkin, *Chem. Mat.* 26, 3818-24 (2014) DOI: 10.1021/cm5014625
786. EFRC Feature Articles, Anne B. McCoy, Sharon Hammes-Schiffer, Catherine J. Murphy, George C. Schatz, *J. Phys. Chem. C*, 118, 13329 (2014). DOI: 10.1021/jp503709n
787. Mesoscale molecular network formation in amorphous organic materials, Brett M. Savoie, Kevin L. Kohlstedt, Nicholas E. Jackson, Lin X. Chen, Monica Olvera de la Cruz, George C. Schatz, Tobin J. Marks, Mark A. Ratner, *PNAS*, 111(28), 10055-10060 (2014) DOI: 10.1073/pnas.1409514111

788. Why did you accept my paper?, Prashant V. Kamat, Oleg Prezhdo, Joan-Emma Shea, Gregory Scholes, Francisco Zaera, Timothy Zwier, George C. Schatz, *J. Phys. Chem. Lett.* 5, 2443 (2014) DOI: 10.1021/jz501139d
789. A square-planar tetracoordinate oxygen-containing Ti_4O_{17} clusters stabilized by two 1,1'-Ferrocenedicarboxylato ligands, Zhichang Liu, Marco Frascioni, Xiaohu Li, Dennis Cao, Zhixue Zhu, Severin T. Schneebeli, George C. Schatz, J. Fraser Stoddart, *Angew. Chemie*, 53, 9193-9197 (2014), DOI: 10.1002/anie.201402603
790. Using nanoscale and mesoscale anisotropy to engineer the optical response of three-dimensional plasmonic metamaterials, Michael B. Ross, Martin G. Blaber, George C. Schatz, *Nature Communications*, 5, 4090 (2014) DOI: 10.1038/ncomms5090.
791. Multireference ab initio study of ligand field d-d transitions in octahedral transition-metal oxide clusters, Yang Yang, Mark A. Ratner and George C. Schatz, *J. Phys. Chem. C* 118, 29196-29208 (2014) DOI: 10.1021/jp5052672.
792. Inhomogeneous surface plasmon polaritonics, Jonathan J. Foley, Jeffrey M. McMahon, George C. Schatz, Hayk Harutyunyan, Gary P. Wiederrecht, Stephen K. Gray, *ACS Photonics*, 1, 2014, 739-745 (2014) DOI: 10.1021/ph500172f
793. Inherent carbonaceous impurities on arc-discharge multiwalled carbon nanotubes and their implications for nanoscale interfaces, Zhi An, Al'ona Furmanchuk, Rajaprakash Ramachandramoorthy, Tobin Filleter, Michael R. Roenbeck, Horacio D. Espinosa, George C. Schatz, SonBinh T. Nguyen, *CARBON*, 80, 1-11 (2014) DOI:10.1016/j.carbon.2014.07.069
794. What's in a Name?, Prashant V. Kamat, George C. Schatz, *J. Phys. Chem. Lett.* 5, 2879 (2014). DOI:10.1021/jz5014888
795. Hollow spherical gold nanoparticle superstructures with tunable diameters and visible to near-infrared extinction, Chen Zhang, Yong Zhou, Andrea Merg, Chengyi Song, George C. Schatz, Nathaniel L. Rosi, *Nanoscale*, 6, 12328-12332 (2014). DOI:10.1039/C4NR04289A
796. Ultrafast photoluminescence in quantum-confined silicon nanocrystals arises from an amorphous surface layer, Daniel C. Hannah, Jihua Yang, Nicolas J. Kramer, George C. Schatz, Uwe R. Kortshagen, Richard D. Schaller, *ACS Photonics*, 1, 960-967 (2014). DOI:10.1021/ph500145p
797. Interplay of LNA and 2'-o-methyl RNA in the structure and thermodynamics of RNA hybrid systems: a molecular dynamics study using the revised AMBER force field and comparison with experimental results, Ilyas Yildirim, Elzbieta Kierzek, Ryszard Kierzek, George C. Schatz, *J. Phys. Chem. B*, 118, 14177-87 (2014). DOI:10.1021/jp506703g
798. Introducing article transfer from letters to regular articles, Prashant V. Kamat, George C. Schatz, *J. Phys. Chem. Lett.* 5, 3391 (2014). DOI:10.1021/jz501963f
799. Mastering the art of scientific publication, Prashant V. Kamat, Jillian M. Buriak, George C. Schatz and Paul S. Weiss, *J. Phys. Chem. Lett.* 5, 3519-21 (2014). DOI:10.1021/jz502010v
800. Shear and friction between carbon nanotubes in bundles and yarns, Jeffrey T. Paci, Al'ona Furmanchuk, Horacio D. Espinosa, George C. Schatz, *Nano Lett.* 14, 6138-47 (2014). DOI:10.1021/nl502210r

801. Building physical chemistry with BRICKs, Prashant V. Kamat, George C. Schatz, *J. Phys. Chem. Lett.*, 5, 4000-4001 (2014). DOI:10.1021/jz502174p
802. Systematic Study of Antibonding Modes in Gold Nanorod Dimers and Trimers, Kyle Osberg, Nadine Harris, Tuncay Ozel, Jessie C. Ku, George C. Schatz, Chad A. Mirkin, *Nano Lett.* 14, 6949-54(2014) DOI:10.1021/nl503207j
803. Radiative effects in plasmonic aluminum and silver nanospheres and nanorods, Michael B. Ross and George C. Schatz, *J. Phys. D: Appl. Phys.* 48, 184004 (2015), DOI: 10.1088/0022-3727/48/18/184004.
804. Introducing perovskite solar cells to undergraduates, Sameer Patwardhan, Duyen H. Cao, Shelby Hatch, Omar K. Farha, Joseph T. Hupp, Mercouri G. Kanatzidis, and George C. Schatz, *J. Phys. Chem. Lett.* 6, 251-55 (2015) DOI: 10.1021/jz502648y
805. A prolific first five years, P. V. Kamat, B. Mennucci, O. Prezhdo, G. Scholes, F. Zaera, T. Zwieter, G. C. Schatz, *J. Phys. Chem. Lett.* 6, 180-182 (2015). DOI:10.1021/jz502524s
806. Plasmonic photonic crystals realized through DNA-programmable assembly, D. J. Park, C. Zhang, J. C. Ku, Y. Zhou, G. C. Schatz and C. A. Mirkin, *PNAS*, 112, 977-81 (2015). DOI:10.1073/pnas.1422649112
807. Editorial for January 2015, A. B. McCoy, J. -E. Shea, C. J. Murphy, G. C. Schatz, *J. Phys. Chem. A/B/C*, 119, 1-4 (2015). DOI:10.1021/jp511796t
808. Uniform circular disks with synthetically tailorable diameters: two-dimensional nanoparticles for plasmonics, M. N. O'Brien, M. R. Jones, K. L. Kohlstedt, G. C. Schatz and C. A. Mirkin, *Nano Lett.* 15, 1012-1017 (2015). DOI:10.1021/nl5038566
809. Reply to "Comment on 'Ultrafast Photoluminescence in Quantum-Confined Silicon Nanocrystals Arises from an Amorphous Surface Layer'", D. C. Hannah, J. Yang, N. J. Nicolaas, G. C. Schatz, U. R. Kortshagen, R. D. Schaller, *ACS Photonics*, 2, 456-58(2015) DOI:10.1021/ph500490a
810. X-ray radiation induces deprotonation of the bilin chromophore in crystalline d. radiodurans phytochrome, F. Le, E. S. Burgie, T. Yu, A. Heroux, G. C. Schatz, R. D. Vierstra, A. M. Orville, *J. Am. Chem. Soc.* 137. 2792-95 (2015). DOI:10.1021/ja510923m
811. Apertureless cantilever-free pen arrays for scanning photochemical printing, Y. Zhou, Z. Xie, K. A. Brown, D. J. Park, X. Zhou, P.-C. Chen, M. Hirtz, Q. -Y. Lin, V. P. Dravid, G. C. Schatz, Z. Zheng, C. A. Mirkin, *Small*, 8, 913-918 (2015). DOI:10.1002/smll.201402195
812. Local electric field factors by a combined charge-transfer and point-dipole interaction model, Nazanin Davari, Shokouh Haghani, Per-Olof Astrand and George C. Schatz, *RSC Advances*, 5, 31594-31605 (2015) DOI: 10.1039/c5ra04183j
813. DNA demonstrates unprecedented control over photonic crystal fabrication, Daniel J. Park, Jessie C. Ku, George C. Schatz, Chad A. Mirkin, *SPIE Newsroom* April 6, 2015. <http://spie.org/x112978.xml> DOI: 10.1117/2.1201501.005823

814. Know the difference: scientific publications versus scientific reports, P. V. Kamat and G. C. Schatz, *J. Phys. Chem. Lett.* 6, 858-9 (2015) DOI:10.1021/acs.jpcclett.5b00286
815. Calculations of surface-enhanced Raman spectra including orientational and Stokes effects using TDDFT/Mie theory QM/ED method, George C. Schatz and Nicholas A. Valley, in *Frontiers of surface-enhanced Raman scattering*, Ed. Yukihiro Ozaki, Katrin Kneipp, Ricardo Aroca, Wiley, p. 1-17, 2014. DOI:10.1002/9781118703601.ch1
816. What controls the hybridization thermodynamics of spherical nucleic acids?, P. S. Randeria, M. R. Jones, K. L. Kohlstedt, R. J. Banga, M. Olvera de la Cruz, G. C. Schatz, C. A. Mirkin, *J. Am. Chem. Soc.* 137, 3486-89 (2015) DOI:10.1021/jacs.5b00670
817. Local electric field factors by a combined charge-transfer and point-dipole interaction model, Nazanin Davari, Shokouh Haghdani, Per-Olof Aastrand, G. C. Schatz, *RSC Adv.* 5, 31594-605 (2015) DOI:10.1039/C5RA04183J
818. Understanding Open Access, G. C. Schatz, *J. Phys. Chem. Lett.* 6, 1285 (2015). DOI:10.1021/acs.jpcclett.5b00385
819. Charge transport across DNA-based three-way junctions, R. M. Young, P. N. Arunoday, A. Thazhathveetil, V. Y. Cho, Y. Zhang, N. Renaud, F. C. Grozema, D. N. Beratan, M. A. Ratner, G. C. Schatz, Y. A. Berlin, F. D. Lewis, M. R. Wasielewski, *J. Am. Chem. Soc.* 137, 5113-22 (2015). DOI:10.1021/jacs.5b00931
820. Nanoscale form dictates mesoscale function in plasmonic DNA-nanoparticle superlattices, M. B. Ross, J. C. Ku, V. M. Vaccarezza, G. C. Schatz, C. A. Mirkin, *Nature Nano* 10 453-8 (2015) DOI:10.1038/nnano.2015.68
821. Conformal, macroscopic crystalline nanoparticle sheets assembled with DNA, J. C. Ku, M. B. Ross, G. C. Schatz, C. A. Mirkin, *Adv. Materials*, 27, 3159-3163 (2015) DOI:10.1002/adma.201500858
822. Conformational order in aggregates of conjugated polymers, N. E. Jackson, K. L. Kohlstedt, B. M. Savoie, M. Olvera de la Cruz, G. C. Schatz, L. X. Chen, M. A. Ratner, *J. Am. Chem. Soc.* 137, 6254-62 (2015) DOI:10.1021/jacs.5b00493
823. Real-time tunable lasing from plasmonic nanocavity arrays, Ankun Yang, Thang B. Hoang, Montacer Dridi, Claire Deeb, Maiken H. Mikkelsen, George C. Schatz, Teri W. Odom, *Nature Communications* 6, 6939 (2015) DOI: 10.1038/ncomms7939
824. Lasing action in periodic arrays of nanoparticles, Montacer Dridi, George C. Schatz, *J. Opt. Soc. Am. B* 32, 818-23 (2015) DOI: 10.1364/JOSAB.32.000818
825. Reverse non-equilibrium molecular dynamics demonstrate that surface passivation controls thermal transport at semiconductor-solid interfaces, Daniel C. Hannah, J. Daniel Gezelter, Richard D. Schaller, George C. Schatz, *ACS Nano*, 9, 6278-87 (2015). DOI:10.1021/acsnano.5b01724
826. Molecular-level engineer of adhesion in carbon nanomaterial interfaces, M. R. Roenbeck, A. Furmanchuk, Z. An, J. T. Paci, X. Wei, S. T. Nguyen, G. C. Schatz, H. Espinosa, *Nano Lett.* 15,

- 4504-16 (2015). DOI:10.1021/acs.nanolett.5b01011
827. Strong coupling between plasmonic gap modes and photonic lattice modes in DNA-assembled gold nanocube arrays, Q. -Y. Lin, Z. Li, K. A. Brown, M. N. O'Brien, M. B. Ross, Y. Zhou, S. Butun, P. -C. Chen, G. C. Schatz, V. P. Dravid, K. Aydin, C. A. Mirkin, *Nano Lett* 15, 4699-4703 (2015) DOI:10.1021/acs.nanolett.5b01548
828. Ten reasons why peer review makes sense, P. V. Kamat, G. C. Schatz, *J. Phys. Chem. Lett.* 6, 2588-89 (2015) DOI:10.1021/acs.jpcllett.5b01280
829. Solution-dispersible metal nanorings with deliberately controllable compositions and architectural parameters for tunable plasmonic response, T. Ozel, M. J. Ashley, G. R. Bourret, M. B. Ross, G. C. Schatz, C. A. Mirkin, *Nano Lett.* 15, 5273-78 (2015) DOI:10.1021/acs.nanolett.5b01594
830. Allosteric transcriptional regulation via changes in the overall topology of the core promoter, Steven J. Philips, Monica Canalizo-Hernandez, Ilyas Yildirim, George C. Schatz, Alfonso Mondragon, Thomas V. O'Halloran, *Science* 349, 877-881 (2015). DOI:10.1126/science.aaa9809 PMID:[PMC4617686](https://pubmed.ncbi.nlm.nih.gov/2617686/)
831. Journal impact factor and the real impact of your paper, Prashant V. Kamat, George. C. Schatz, *J. Phys. Chem. Lett.* 6, 3074-75 (2015) DOI:10.1021/acs.jpcllett.5b01527
832. Defect tolerance and the effect of structural inhomogeneity in plasmonic DNA-nanoparticle superlattices, M. B. Ross, J. C. Ku, M. G. Blaber, C. A. Mirkin, G. C. Schatz, *PNAS* 112, 10292-7 (2015). DOI:10.1073/pnas.1513058112
833. Adjusting the metrics of 1-D helical gold nanoparticle superstructures using multivalent peptide conjugates, A. D. Merg, J. Slocik, M. G. Blaber, G. C. Schatz, R. Naik, N. L. Rosi, *Langmuir*, 31, 9492-501 (2015) DOI:10.1021/acs.langmuir.5b02208
834. Evaluating single-molecule Stokes and anti-Stokes SERS for Nanoscale Thermometry, E. A. Pozzi, A. B. Zrimsek, C. M. Lethiec, G. C. Schatz, M. C. Hersam, R. P. Van Duyne, *J. Phys. Chem. C* 119, 21116-24 (2015). DOI:10.1021/acs.jpcc.5b08054
835. Computational investigation of RNA CUG repeats responsible for myotonic dystrophy 1. I. Yildirim, D. Chakraborty, M. D. Disney, D. J. Wales, G. C. Schatz, *J. Chem. Theory Comp*, 11, 4943-58 (2015). DOI:10.1021/acs.jctc.5b00728 PMID: [PMC4606397](https://pubmed.ncbi.nlm.nih.gov/2616397/)
836. Multi-step mechanism of carbonization in templated polyacrylonitrile derived fibers: ReaxFF model uncovers origins of graphite alignment, B. Saha, A. Furmanchuk, Y. Dzenis, G. C. Schatz, *Carbon* 94, 694-704 (2015). DOI:10.1016/j.carbon.2015.07.048
837. Introducing Viewpoints in the Journal of Physical Chemistry A/B/C, *J. Phys. Chem. B*, 119, 12155 (2015). DOI:10.1021/acs.jpccb.5b08412
838. Enhancing DNA-mediated assemblies of supramolecular cage dimers through tuning core flexibility and DNA length – A combined experimental-modeling study, Bong Jin Hong, Vincent Y. Cho, Reiner Bleher, George C. Schatz, SonBinh T. Nguyen, *J. Amer. Chem.*

- Soc. 137, 13381-13388 (2015). DOI:10.1021/jacs.5b08678
839. Theoretical Investigation of charge transfer in Metal organic frameworks for electrochemical device applications, Sameer Patwardhan and George C. Schatz, *J. Phys. Chem. C* 119, 24238-47 (2015). DOI:10.1021/acs.jpcc.5b06065
840. Modular and chemically responsive oligonucleotide “bonds” in nanoparticle superlattices, Stacey N. Barnaby, Ryan V. Thaner, Michael B. Ross, Keith A. Brown, George C. Schatz, Chad A. Mirkin, *J. Amer. Chem. Soc.* 137, 13566-13571 (2015). DOI:10.1021/jacs.5b07908
841. Influence of surfactant bilayers on the refractive index sensitivity and catalytic properties of anisotropic gold nanoparticles, Martinsson, Erik; Shahjamali, Mohammad M.; Large, Nicolas; Zaraee, Negin; Zhou, Yu; Schatz, George C.; Mirkin, Chad A.; Aili, Daniel, *Small*, 12, 330-342 (2015) DOI: 10.1002/sml.201502449
842. Light driven Ca²⁺ ion pump: how does it work? Cheng-Tsung Lai, Yu Zhang, George C. Schatz, *J. Phys. Chem. B* 119, 15110-15117 (2015) DOI:10.1021/acs.jpcc.5b07578
843. Superlattice plasmons in hierarchical Au nanoparticle arrays, Danqing Wang, Ankun Yang, Alexander J. Hryn, George C. Schatz and Teri W. Odom, *ACS Photonics* 2, 1789-94 (2015) DOI:10.1021/acsp Photonics.5b00546
844. Optical properties of One-, Two-, and Three-Dimensional Arrays of Plasmonic Nanostructures, M. B. Ross, J. C. Ku, B. Lee, C. A. Mirkin and G. C. Schatz, *J. Phys. Chem. C* 120, 816-830 (2016) DOI:10.1021/acs.jpcc.5b10800
845. Reaching out within physical chemistry, Kamat, Prashant V.; Mennucci, Benedetta; Prezhdo, Oleg; Scholes, Gregory; Zaera, Francisco; Zwier, Timothy; Schatz, George C. *J. Phys. Chem. Lett* 7, 103-4 (2016). DOI:10.1021/acs.jpcclett.5b02734
846. Editorial for January 2016 for JPC A/B/C, A. B. McCoy, J-E. Shea, C. J. Murphy, G. C. Schatz, *J. Phys. Chem. A* 120, 1-4 (2016) DOI:10.1021/acs.jpca.5b10811
847. Liquid-phase Beam Pen Lithography, Shu He, Zhuang Xie, Daniel J. Park, Xing Liao, Keith A. Brown, Peng-Cheng Chen, Yu Zhou, George C. Schatz, Chad A. Mirkin, *Small*, 12, 988-993 (2016) DOI:10.1002/sml.201502666
848. Tunable Excited-State Properties and Dynamics as a Function of Pt-Pt Distance in Pyrazolate-Bridged Pt(II) Dimers, Samantha Brown-Xu, Matthew S. Kelley, Kelly A. Fransted, Arnab Chakraborty, George C. Schatz, Felix N. Castellano, Lin X. Chen, *J. Phys. Chem. A*, 120, 543-550 (2016) DOI:10.1021/acs.jpca.5b11233
849. Energy landscapes and functions of supramolecular systems, Faifan Tantakitti, Job Boekhoven, Xin Wang, Roman V. Kazantsev, Tao Yu, Jiahe Li, Ellen Zhuang, Roya Zandi, Julia H. Ortony, Christina J. Newcomb, Liam C. Palmer, Gajendra S. Shekhawat, Monic Olvera de la Cruz, George C. Schatz, Samuel I. Stupp, *Nature Materials*, 15, 469-477 (2016) DOI:10.1038/nmat4538

850. Simultaneous covalent and noncovalent hybrid polymerizations, Zhilin Yu, Faifan Tantakitti, Liam C. Palmer, George C. Schatz, Samuel I. Stupp, *Science* 351, 497-502 (2016) DOI:10.1126/science.aad4091
851. Probing the chemistry of alumina atomic layer deposition using operando surface-enhanced Raman spectroscopy, Sichel S. Masango, Ryan A. Hackler, Anne-Isabelle Henry, Michael O. McAnally, George C. Schatz, Peter C. Stair, Richard P. Van Duyne, *J. Phys. Chem. C* 120, 3822-33 (2016). DOI:10.1021/acs.jpcc.5b11487
852. Unraveling near-field and far-field relationships for 3D SERS substrates-a combined experimental and theoretical analysis, D. Kuroski, N. Large, N. Chiang, N. Greeneltch, K. T. Carron, T. Seideman, G. C. Schatz, R. P. Van Duyne, *Analyst*, 141, 1779-88 (2016) DOI:10.1039/C5AN01921D
853. Reactive force field modeling of zinc oxide nanoparticle formation, Craig J. Tainter and George C. Schatz, *J. Phys. Chem. C*, 120, 2950-61 (2016) DOI:10.1021/acs.jpcc.5b09511
854. Ultrafast and nonlinear surface-enhanced Raman spectroscopy, N. L. Gruenke, F. M. Cardinal, M. O. McAnally, R. R. Frontiera, G. C. Schatz, R. P. Van Duyne, *Chem. Soc. Rev.* 45, 2263 - 2290 (2016) DOI:10.1039/c5cs00763a
855. Plasmonic metallurgy enabled by DNA, M. B. Ross, J. C. Ku, B. Lee, C. A. Mirkin, G. C. Schatz, *Adv. Mat.* 28, 2790-2794 (2016) DOI:10.1002/adma.201505806
856. Connection between Hybrid Functionals and Importance of the Local Density Approximation, M. A. Mosquera, C. H. Borca, M. A. Ratner and G. C. Schatz, *J. Phys. Chem. A*, 120, 1605-1612 (2016) DOI: 10.1021/acs.jpca.5b10864
857. Supramolecular gelation of rigid triangular macrocycles through rings of multiple C-H...O interactions acting cooperatively, Zhichang Liu, Junling Sun, Yu Zhou, Yu Zhang, Yilei Wu, Siva Krishna Mohan Nalluri, Yuping Wang, Avik Samanta, Chad A. Mirkin, George C. Schatz, J. Fraser Stoddart, *J. Org. Chem.* 81, 2581-2588 (2016). DOI:10.1021/acs.joc.6b00281
858. Greg Scholes takes over at Deputy Editor of JPC Letters, George C. Schatz and Gregory Scholes, *JPC Letters*, 7, 1154 (2016). DOI:10.1021/acs.jpcllett.6b00457
859. Dependence of plasmon energies on acoustic normal modes of Ag_n (n=20,84,120) clusters. Clotilde M. Lethiec, Lindsey R. Madison, George C. Schatz, *JPC C*, 120, 20572-78 (2016). DOI:10.1021/acs.jpcc.5b12497
860. Fundamental limitations to plasmonic hot-carrier solar cells, Yu Zhang, ChiYung Yam, George C. Schatz, *J. Phys. Chem. Lett.* 7, 1852-58 (2016) DOI: 10.1021/acs/jpclett.6b00879
861. Nitrogenase-mimic iron-containing chalcogels for photochemical reduction of dinitrogen

- to ammonia, Jian Liu, Matthew S. Kelley, Weiqiang Wu, Abhishek Banerjee, Alexios P. Douvalis, Jinson Wu, Yongbo Zhang, George C. Schatz, Mercouri G. Kanatzidis, PNAS, 113, 5530-5535 (2016). DOI: 10.1073/pnas.1605512113
862. Size-dependent coherent-phonon plasmon modulation and deformation characterization in gold bipyramids and nanojavelins, Matthew S. Kirschner, Clotilde M. Lethiec, Xiao-Min Lin, George C. Schatz, Lin X. Chen, Richard D. Schaller, ACS Photonics, 3, 758-763 (2016). DOI:10.1021/acsp Photonics.6b00136.
863. Covalent functionalization and passivation of exfoliated black phosphorus via aryl diazonium chemistry, Christopher R. Ryder, Joshua D. Wood, Spencer A. Wells, Yang Yang, Deep Jariwala, Tobin J. Marks, George C. Schatz, Mark C. Hersam, Nature Chemistry, 597-602 (2016) DOI:10.1038/nchem.2505
864. Structure-function relationships for surface-enhanced Raman spectroscopy-active plasmonic paper, M. B. Ross, M. J. Ashley, A. L. Schmucker, S. Singamaneni, R. R. Naik, G. C. Schatz, C. A. Mirkin, J. Phys. Chem. C 120, 20789-97 (2016) DOI:10.1021/acs.jpcc.6b02019
865. Ag-Ag₂S Hybrid Nanoprisms: structural versus plasmonic evolution, M. M. Shahjamali, Y. Zhou, N. Zeraee, C. Xue, J. Wu, N. Large, C. M. McGuirk, F. Boey, V. Dravid, Z. Cui, G. C. Schatz, C. A. Mirkin, ACS Nano 10, 5362-5373 (2016). DOI:10.1021/acsnano.6b01532
866. Molecularly tunable fluorescent quantum defects, H. Kwon, A. Furmanchuk, M. Kim, B. Meany, Y. Guo, G. C. Schatz, Y. H. Wang, JACS 138, 6878-6885 (2016) DOI:10.1021/jacs.6b03618
867. Nanoscale chemical imaging of a dynamics molecular phase boundary with ultrahigh vacuum tip-enhanced Raman spectroscopy, N. Jiang, N. Chiang, L. R. Madison, E. A. Pozzi, M. R. Wasielewski, T. Seideman, M. A. Ratner, M. C. Hersam, G. C. Schatz, R. P. Van Duyne, Nano Lett. 16, 3898-3904 (2016). DOI:10.1021/acs.nanolett.6b01405
868. SERS Detection of Ricin B-Chain via N-Acetyl-Galactosamine Glycopolymers, Victoria M. Szlag, Matthew J. Styles, Lindsey R. Madison, Antonio R. Campos, Bharat S. Wagh, Dustin Sprouse, George C. Schatz, Theresa M. Reineke, Christy L. Hayes, ACS Sensors, 1, 842-46 (2016) DOI:10.1021/acssensors.6b00209
869. Sequential double excitations from linear-response time-dependent density functional theory, Martin A. Mosquera, Lin X. Chen, Mark A. Ratner, George C. Schatz, J. Chem. Phys. 144, 204105/1-11, (2016). DOI:10.1063/1.4950876
870. High-resolution distance dependence study of surface-enhanced Raman scattering enabled by atomic layer deposition, Sicelo S. Masango, Ryan A. Hackler, Nicolas Large, Anne-Isabelle Henry, Michael O. McAnally, George C. Schatz, Peter C. Stair, Richard P. Van Duyne, Nano Lett. 16, 4251-59 (2016). DOI:10.1021/acs.nanolett.6b01276
871. Semiempirical Modeling of Ag Nanoclusters: New Parameters for Optical Property Studies Enable

- Determination of Double Excitation Contributions to Plasmonic Excitation, Rebecca L. Giesecking, Mark A. Ratner, George C. Schatz, *J. Phys. Chem. A* 120, 4542-49 (2016). DOI:10.1021/acs.jpca.6b04520
872. Surface-Enhanced Raman Spectroscopy Detection of Ricin B Chain in Human Blood, Antonio R. Campos, Zhe Gao, Martin G. Blaber, Rong Huang, George C. Schatz, Richard P. Van Duyne, Christy L. Haynes, *J. Phys. Chem. C* 120, 20961-69 (2016) DOI:10.1021/acs.jpcc.6b03027
873. Kinetic Master Equation Modeling of an Artificial Protein Pump, Yu Zhang, Cheng-Tsung Lai, Bruce J. Hinds, George C. Schatz, *J. Phys. Chem. C* 120, 11495-14501 (2016), 120(27). DOI:10.1021/acs.jpcc.6b03076
874. Molecular Transport Junctions Created By Self-Contacting Gapped Nanowires, Jong Kuk Lim One-Sun, Lee, Jae-Won Jang, Sarah Hurst, George C. Schatz, Chad A. Mirkin, *Small* 12, 4349-56 (2016) DOI:10.1002/sml.201601214
875. In solution SERS sensing using mesoporous silica-coated gold nanorods, Zhe Gao, Nathan D. Burrows, Nicholas A. Valley, George C. Schatz, Catherine J. Murphy, Christy L. Haynes, *Analyst* 141, 5088-95 (2016) DOI:10.1039/C6AN01159D; *E* 141, 5088–5095 (2016). DOI:10.1039/c6an90098d *E*:141, 6604.
876. Contraction and Expansion of Stimuli-Responsive DNA Bonds in Flexible Colloidal Crystals, Jarad A. Mason, Christine R. Laramy, Cheng-Tsung Lai, Matthew N. O'Brien, Qing-Yuan Lin, Vinayak P. Dravid, George C. Schatz, Chad A. Mirkin, *J. Am. Chem. Soc.* 138 (28), pp 8722–8725 (2016) DOI:10.1021/jacs.6b05430
877. Effect of cation rotation on charge dynamics in hybrid lead halide perovskites, Maria C. Gelvez-Rueda, Duyen H. Cao, Sameer Patwardhan, Nicolas Renaud, Constantinos C. Stoumpos, George C. Schatz, Joseph T. Hupp, Omar K. Farha, Tom J. Savenije, Mercuri G. Kanatzidis, Ferdinand C. Grozema, *J. Phys. Chem. C*, 120, 16577-85 (2016) DOI:10.1021/acs.jpcc.6b06722
878. Enzymatically controlled vacancies in nanoparticle crystals, Stacey N. Barnaby, Michael B. Ross, Ryan V. Thaner, Byeongdu Lee, George C. Schatz, Chad A. Mirkin, *Nano Lett.* 16, 5114-5119 (2016) DOI:10.1021/acs.nanolett.6b02042
879. Operational regimes in picosecond and femtosecond pulse-excited ultrahigh vacuum SERS, Eric A. Pozzi, Natalie L. Gruenke, Naihao Chiang, Dmitry V. Zhdanov, Nan Jiang, Tamar Seideman, George C. Schatz, Mark C. Hersam, Richard P. Van Duyne, *J. Phys. Chem. Lett.* 7, 2971–2976 (2016). DOI:10.1021/acs.jpcl.6b01151
880. Design considerations for RNA spherical nucleic acids (NSAs), Stacey N. Barnaby, Grant A. Perelman, Kevin L. Kohlstedt, Alyssa B. Chinen, George C. Schatz, Chad A. Mirkin, *Bioconjugate Chem.* 27, 2123-31 (2016). DOI:10.1021/acs.bioconjchem.6b00350
881. Enabling singlet fission by controlling intramolecular charge transfer in n-stacked covalent terylenediimide dimers, Eric A. Margulies, Claire E. Miller, Yilei Wu, Lin Ma, George C. Schatz, Ryan M. Young, Michael R. Wasielewski, *Nature Chem.* 8, 1120-25 (2016) DOI:10.1038/nchem.2589
882. Singlet fission via an excimer-like intermediate in 3,6-bis(thiophen-2-yl) diketopyrrolopyrrole derivatives, Catherine M. Mauck, Patrick E. Hartnett, Eric A. Margulies, Line Ma, Claire E. Miller, George C. Schatz, Tobin J. Marks, Michael R. Wasielewski, *J. Am. Chem. Soc.* 138, 11749-61

- (2016). DOI:10.1021/jacs.6b05627
883. Interfacial effects on nanoscale wrinkling in gold-covered polystyrene, Craig T. Chapman, Jeffrey T. Paci, Won-Kyu Lee, Clifford J. Engel, Teri Odom, George C. Schatz, *ACS Applied Materials & Interfaces* 8, 24339-44 (2016) DOI:10.1021/acsami.6b08554
884. Coupled wave equations theory of surface-enhanced femtosecond stimulated Raman scattering, Michael O. McAnally, Jeffrey M. McMahon, Richard P. Van Duyne, George C. Schatz, 145, 094106/1-/10 (2016) DOI:10.1063/1.4961749
885. Near-quantitative yield for transfer of near-infrared excitons within solution-phase assemblies, Ki-Ryong Lee, Stephanie Homan Bettis, Mohamad S. Kodaimati, George C. Schatz, Emily A. Weiss, *J. Phys. Chem. C* 120, 22186-22194 (2016) DOI:10.1021/acs.jpcc.6b06880
886. Reducing CO₂ to CO and H₂O on Ni(110): the influence of subsurface hydrogen, Wei Lin, Kelsey M. Stocker, George C. Schatz, *J. Phys. Chem. C* 120, 23061-23068 (2016) DOI: 10.1021/acs.jpcc.6b07849
887. Virtual issue in memory of Ahmed Zewail, Mostafa A. El-Sayed and George C. Schatz, *J. Phys. Chem. A*, 120, 7405-7, *J. Phys. Chem. B*, 120 10043-45, *J. Phys. Chem. C*, 120, 21145-21147 (2016) DOI:10.1021/acs.jpca.6b08645
888. Bisboronic acids for selective, physiologically relevant direct glucose sensing with surface-enhanced Raman spectroscopy, Bhavya Sharma, Pradeep Bugga, Lindsey R. Madison, Anne-Isabelle Henry, Martin G. Blaber, Nathan G. Greeneltch, Naihao Chiang, Milan Mrksich, George C. Schatz, Richard P. Van Duyne, *J. Am. Chem. Soc.* 138, 13952-13959 (2016) DOI:10.1021/jacs.6b07331
889. Reversible shape and plasmon tuning in hollow AgAu nanorods, Sadegh Yazdi, Josee R. Daniel, Nicolas Large, George C. Schatz, Denis Broudreau, Emilie Ringe, *Nano Lett.* 16, 6939-45 (2016) DOI:10.1021/acs.nanolett.6b02946
890. Supramolecular double-helix formation by diastereoisomeric conformations of configurationally enantiomeric macrocycles, Avik Samanta, Zhichang Liu, Krishna Mohan Siva, Yu Zhang, George C. Schatz, J. Fraser Stoddart, *J. Amer. Chem. Soc.* 138, 14469-80 (2016). DOI:10.1021/jacs.6b09258
891. Quantum mechanical identification of quadrupolar plasmonic excited states in silver nanorods, Rebecca L. Gieseck, Mark A. Ratner, George C. Schatz, *J. Phys. Chem. A*, 120, 9324-29 (2016). DOI:10.1021/acs.jpca.6b09649
892. Surface-enhanced femtosecond stimulated Raman spectroscopy at 1MHz repetition rates, Lauren E. Buchanan, Natalie L. Gruenke, Michael O. McAnally, Bodgan Negru, Hannah E. Mayhew, Vartkess A. Apkarian, George C. Schatz, Richard P. Van Duyne, *J. Phys. Chem. Lett.* 7, 4629-34 (2016). DOI:10.1021/acs.jpcllett.6b02175
893. Electronic structure and potential reactivity of sila-aromatic molecules, Yang Yang, Martin A. Mosquera, Kwan Skinner, Andres E. Becerra, Vasgen Shamamian, George C. Schatz, Mark A. Ratner, Tobin J. Marks, *J. Phys. Chem. A*, 120, 9476-88 (2016). DOI:10.1021/acs.jpca.6b09526
894. Energetic and dynamics analysis of transport of Na⁺ and K⁺ through a cyclic peptide nanotube in water and in lipid bilayers, Yeonho Song, Ji Hye Lee, Hoon Hwang, George C. Schatz, Hyonseok

- Hwang, *J. Phys. Chem. B*, 120, 11912-11922 (2016). DOI:10.1021/acs.jpccb.6b09638
895. Magneto-optical response of cobalt interacting with plasmonic nanoparticle superlattices, Michael B. Ross, Marc R. Bourgeois, Chad A. Mirkin and George C. Schatz, *J. Phys. Chem. Lett.* 7, 4732-38 (2016). DOI:10.1021/acs.jpcclett.6b02259
896. Aluminum film-over-nanosphere substrates for deep-UV surface-enhanced resonances Raman spectroscopy, Bhavya Sharma, M. Fernanda Cardinal, Michael B. Ross, Alyssa B. Zrimsek, Sergei V. Bykov, David Punihaoale, Sanford A. Asher, George C. Schatz, Richard P. Van Duyne, *Nano Lett.* 16, 7968-73 (2016). DOI:10.1021/acs.nanolett.6b04296
897. Celebrating our 120th Anniversary, George C. Schatz, *J. Phys. Chem. Lett.* 7, 4977-79 (2016) DOI:10.1021/acs.jpcclett.6b02537, *JPCA*, 120, 9679-81, *JPC B*,120, 12417-19, *JPCC* 120, 27731-33.
898. Programmable and reversible plasmon mode engineering, Ankun Yang, Alexander J. Hryn, Marc R. Bourgeois, Won-Kyu Lee, Jintian Hu, George C. Schatz, Teri W. Odom, *PNAS* 113, 14201-6 (2016) DOI:10.1073/pnas.1615281113
899. Implementation of INDO/SCI with COSMO implicit solvation and benchmarking for solvatochromic shifts, Rebecca L. Gieseking, Mark A. Ratner, George C. Schatz, *J. Phys. Chem. A*, 120, 9878-85 (2016) DOI:10.1021/acs.jpca.6b10487
900. Single-molecule chemistry with surface- and tip-enhanced Raman spectroscopy, Alyssa B. Zrimsek, Naihao Chiang, Michael Mattei, Stephanie Zaleski, Michael O. McAnally, Craig T. Chapman, Anne-Isabelle Henry, George C. Schatz, Richard P. Van Duyne, *Chem. Rev.* 117(11), 7583-7613 (2017) DOI:10.1021/acs.chemrev.6b00552
901. Balancing the effects of extinction and enhancement for optimal signal in surface-enhanced femtosecond stimulated Raman spectroscopy, Natalie L. Gruenke, Michael O. McAnally, George C. Schatz, Richard P. Van Duyne, *J. Phys. Chem. C* 120(51), 29449-29454 (2016) DOI:10.1021/acs.jpcc.6b10727
902. JPCL New Year's Editorial, G. D. Scholes, J. Bisquert, B. Mennucci, O. Prezhdo, F. Zaera, T. Zwieter, G. C. Schatz, *J. Phys. Chem. Lett* 8, 41 (2017) DOI:10.1021/acs.jpcclett.6b02781
903. Optical properties and structural relationships of the silver nanoclusters Ag₃₂(SG)₁₉ and Ag₁₅(SG)₁₁, S. -H. Yau, B. A. Ashenfelter, A. Desireddy, A. P. Ashwell, O. P. Varnavski, G. C. Schatz, T. P. Bigioni, T. Goodson III, *J. Phys. Chem. C*, 121, 1349-61 (2017). DOI:10.1021/acs.jpcc.6b10434
904. Tip-enhanced Raman Voltammetry: coverage dependence and quantitative modeling, Michael Mattei, Gyeongwon Kang, Guillaume Goubert, Dhabih V. Chulhai, George C. Schatz, Lasse Jensen, Richard P. Van Duyne, *Nano Lett.* 17(1), 590-596 (2017) DOI: 10.1021/acs.nanolett.6b04868
905. Advantages of conical pores for ion pumps, Yu Zhang, George C. Schatz, *J. Phys. Chem. C*, 121(1), 161-168(2017). DOI:10.1021/acs.jpcc.6b10713
906. Direct observation of a charge transfer state preceding high yield singlet fission in terylenediimide thin films, E. A. Margulies, J. L. Logsdon, C. E. Miller, L. Ma, E. Simonoff, R. M. Young, G. C. Schatz, M. R. Wasielewski, *J. Am. Chem. Soc.* 139, 663-71 (2017). DOI:10.1021/jacs.6b07721

907. Molecular dynamics simulations and experimental studies of gold nanoparticle template HDL-like nanoparticles for cholesterol metabolism therapeutics, Cheng-Tsung Lai, Wangqiang Sun, Rohun U. Palekar, Shad, C. Thaxton, George C. Schatz, ACS AMI, 9, 1247–1254 (2017). DOI:10.1021/acsami.6b12249
908. Ultrahigh-vacuum tip-enhanced Raman spectroscopy, E. A. Pozzi, G. Goubert, N. Chiang, N. Jiang, C. T. Chapman, M. O. McAnally, A. –I. Henry, T. Seideman, G. C. Schatz, M. C. Hersam, R. P. Van Duyne, Chem. Rev. 117(7), 4961-4982 (2017), DOI: 10.1021/acs.chemrev.6b00343
909. Energetic and frictional effects in the transport of ions in a cyclic peptide nanotube, Yongil Seo, Yeonho Song, George C. Schatz, Hyonseok Hwang, Bull. Korean Chem. Soc. 38, 19-26 (2017) DOI:10.1002/bkcs.11035
910. Improved scaling of molecular network calculations: the emergence of molecular domains, A. g. Gagorik, B. Savoie, N. Jackson, A. Agrawal, A. Choudhary, M. A. Ratner, G. C. Schatz, K. L. Kohlstedt, J. Phys. Chem. Lett. 8, 415-421 (2017). DOI:10.1021/acs.jpcclett.6b02921
911. Directional emission from dye-functionalized plasmonic DNA superlattice microcavities, D. J. Park, J. C. Ku, L. Sun, C. M. Lethiec, N. P. Stern, G. C. Schatz, C. A. Mirkin, PNAS, 114, 457-461 (2017). DOI:10.1073/pnas.1619802114
912. Editorial for January 2017 for JPC A/B/C, A. B. McCoy, J. E. Shea, C. J. Murphy, G. C. Schatz, J. Phys. Chem. A/B/C, 121, 1-3 (2017) DOI:10.1021/acs.jpca.6b11794
913. Review of plasmon-induced hot-electron dynamics and related SERS-chemical effects, Rebecca L. Giesecking, Mark A. Ratner, George C. Schatz, in **Frontiers of Plasmon Enhanced Spectroscopy**, Volume 1, Ed. Y. Ozaki, G. C. Schatz, D. Graham and T. Itoh, ACS Symposium Series Vols. 1245, American Chemical Society, Washington, D. C., 2016, pp 1-22. DOI: 10.1021/bk-2016-1245.ch001
914. The photoluminescence spectral profiles of water-soluble aggregates of PbS quantum dots assembled through reversible metal coordination, Chen Wang, Mohammad S. Kodaimati, George C. Schatz, Emily A. Weiss, Chem. Comm. 53, 1981-84 (2017) DOI:10.1039/c6cc07950d
915. A time-dependent density functional theory study of the impact of ligand passivation on the plasmonic behavior of Ag nanoclusters, Adam P. Ashwell, Mark A. Ratner and George C. Schatz, Adv. Quantum. Chem. 75, 117-145 (2017) Ed. J. R. Savin and E.J. Brandas, Burlington: Academic Press. DOI: 10.1016/bs.aiq.2017.01.011
916. Identification of Dimeric Methylalumina Surface Species during Atomic Layer Deposition using Operando Surface-Enhanced Raman Spectroscopy, R. A. Hackler, M. O. McAnally, G. C. Schatz, P. C. Stair, and R. P. Van Duyne, J. Am. Chem. Soc., 139, 2456-2463 (2017), DOI: 10.1021/jacs.6b12709
917. Plasmon-coupled resonance energy transfer: a real-time electrodynamic approach, Wendu Ding, Liang-Yan Hsu and George C. Schatz, J. Chem. Phys. 146, 064109/1-064109/11 (2017) DOI: 10.1063/1.4975815

918. Understanding nanoparticle-mediated nucleation pathways of anisotropic nanoparticles, Christine R. Laramy, Lam-Kiu Fong, Matthew R. Jones, Matthew N. O'Brien, George C. Schatz, Chad A. Mirkin, *Chem. Phys. Lett.* 389-392 (2017) DOI: 10.1016/j.cplett.2017.01.050.
919. Exciton absorption spectra by linear response methods: application to conjugated polymers, Martin A. Mosquera, Nicholas E. Jackson, Thomas J. Fauvell, Matthew S. Kelley, Lin X. Chen, George C. Schatz, Mark A. Ratner, *J. Am. Chem. Soc.* 139, 3728–3735 (2017) DOI:10.1021/jacs.6b12405
920. Wrinkles in polytetrafluoroethylene on polystyrene: persistence lengths and the effect of nano-inclusions, Jeffrey T. Paci, Craig T. Chapman, Won-Kyu Lee, Teri W. Odom and George C. Schatz, *ACS Appl. Mat. Interfaces*, 9(10), 9079-9088 (2017) DOI:10.1021/acsami.6b14789
921. Mechanisms of hydrogen-assisted CO₂ reduction on Nickel, Wei Lin, Kelsey M. Stocker, George C. Schatz, *J. Am. Chem. Soc.* 139, 4663-6 (2017). DOI:10.1021/jacs.7b01538
922. Polarization-dependent optical response in anisotropic nanoparticle-DNA superlattices, Lin Sun, Haixin Lin, Daniel J. Park, Marc. R. Bourgeois, Michael B. Ross, Jessie C. Ku, George C. Schatz, Chad A. Mirkin, *Nano Lett.* 17, 2313-2318 (2017). DOI:10.1021/acs.nanolett.6b05101
923. Distance-dependence of inter-particle energy transfer in the near-infrared within electrostatic assemblies of PbS quantum dots, M. S. Kodaimati, C. Wang, C. Chapman, G. C. Schatz and E. A. Weiss, *ACS Nano*, 11(5), 5041-5050 (2017). DOI:10.1021/acs.nano.7b017
924. Modeling singlet fission in rylene and diketopyrrolopyrrole derivatives: the role of the charge transfer state in superexchanges and excimer formation, Claire E. Miller, Michael R. Wasielewski and George C. Schatz, *J. Phys. Chem. C*, 121(19), 10345-10350 (2017). DOI:10.1021/acs.jpcc.7b02697
925. Theoretical modeling of voltage effects and the chemical mechanism in surface-enhanced Raman scattering, Rebecca Giesecking, Mark A. Ratner and George C. Schatz, *Far. Disc.* 205, 149 - 171 (2017) DOI:10.1039/c7fd00122c
926. All-atom molecular dynamics simulations of peptide amphiphile assemblies that spontaneously form twisted and helical ribbon structures, Cheng-Tsung Lai, Nathaniel L. Rosi, George C. Schatz, *J. Phys. Chem. Lett.* 8, 2170-74 (2017). DOI:10.1021/acs.jpcclett.7b00745
927. Plasmon-coupled resonance energy transfer, Liang-Yuan Hsu, Wendu Ding, George C. Schatz, *J. Phys. Chem. Lett.* 8, 2357-67. DOI:10.1021/acs.jpcclett.7b00526
928. Preface, Yukihiro Ozaki, George C. Schatz, Duncan Graham, Tamitake Itoh, *ACS Symp. Series*, 1246 (vol 2), 2016. DOI:10.1021/bk-2016-1246.pr001
929. Virtual issue on best practices for reporting the properties of materials and devices, Jillian M. Buriak, Christopher W. Jones, Prashant V. Kamat, Kirk S. Schanze, George C. Schatz, Gregory D. Scholes, Paul S. Weiss, *Chem. Mat.* 28, 3525-26 (2016) DOI:10.1021/acs.chemmater.6b01854
930. What does “Important New Physical Insights” Mean? Tips for writing better papers, George C. Schatz, *J. Phys. Chem. A* 121, 3627-8 (2017) DOI:10.1021/acs.jpca.7b04302
931. Conical nanopores for efficient ion pumping and desalination, Yu Zhang and George C. Schatz, *J. Phys. Chem. Lett.* 8, 2842-8 (2017). DOI:10.1021/acs.jpcclett.7b01137

932. Understanding the vibrational mode-specific polarization effects in femtosecond Raman-induced Kerr-effect spectroscopy, M. O. McAnally, Y-S. Guo, G. Balakrishnan, G. C. Schatz and R. P. Van Duyne, *Opt. Lett.* 41, 5357-60 (2016). DOI:10.1364/OL.41.005357
933. Quantitative Determination of the Differential Raman Scattering Cross-Sections of Glucose by Femtosecond Stimulated Raman Scattering, M. O. McAnally, B. T. Phelan, R. M. Young, M. R. Wasielewski, G. C. Schatz, and R. P. Van Duyne, *Anal. Chem.*, 89, 6931-6935 (2017), DOI: 10.1021/acs.analchem.7b01335
934. Studying Stimulated Raman activity in Surface-Enhanced Femtosecond Stimulated Raman Spectroscopy by Varying the Excitation Wavelength, L. E. Buchanan, M. O. McAnally, N. L. Bruenke, G. C. Schatz, R. P. Van Duyne, *J. Phys. Chem. Lett.* 8, 3328-33 (2017), DOI: 10.1021/acs.jpcllett.7b01342
935. Semiempirical modeling of electrochemical charge transfer, R. L. Giesecking, M. A. Ratner and G. C. Schatz, *Far. Disc.* 99, 547-563 (2017) DOI:10.1039/c6fd00234j
936. Modeling super-resolution SERS using a T-matrix method to elucidate molecule-nanoparticle coupling and the origins of localization errors, C. W. Heaps and G. C. Schatz, *J. Chem. Phys.* 146, 224201/1-11 (2017) DOI: 10.1063/1.4984120
937. The competing effects of core rigidity and linker flexibility in the nanoassembly of trivalent small molecule-DNA hybrids (SMDH3s)—a synergistic experimental-modeling study, V. Y. Cho, B. J. Hong, K. L. Kohlstedt, G. C. Schatz, S. T. Nguyen, *Nanoscale*, 9, 12652-12663 (2017) DOI: 10.1039/c7nr01931a
938. Virtual issue celebrating the life and career of Millie Dresselhaus G. C. Schatz, G. D. Scholes, P. J. Stang, C. J. Burrows, F. M. Winnick, A. P. Alivisatos, C. M. Lieber, P. S. Weiss, J. M. Buriak, *Chem. Mat.* 29, 5017-18 (2017) DOI:10.1021/acs.chemmater.7b02398
939. Expanding applications of SERS through versatile nanomaterials engineering, M. F. Cardinal, E. Vander Ende, R. A. Hackler, M. O. McAnally, P. C. Stair, G. C. Schatz, R. P. Van Duyne, *Chem. Soc. Rev.* 46, 3886-3903 (2017). DOI:10.1039/C7CS00207F
940. Unraveling the near- and far-field relationship of 2D surface-enhanced Raman spectroscopy substrates using wavelength-scan surface-enhanced Raman excitation spectroscopy, D. Kurouski, N. Large, N. Chiang, A.-I. Henry, T. Seideman, G. C. Schatz, R. P. Van Duyne, *J. Phys. Chem. C* 121, 14737-44 (2017). DOI:10.1021/acs.jpcc.7b04787
941. Physical chemistry in India, G. C. Schatz, S. S. M. Konda, *J. Phys. Chem. B* 121, 6287-93 (2017). A, 4843-49; C 13977-83. DOI:10.1021/acs.jpcc.7b05682
942. Understanding the electronic structure properties of bare silver clusters as models for plasmonic excitation, L. R. Madison, M. A. Ratner, G. C. Schatz, in *Progress in Theoretical Chemistry and Physics*, 29, 37-52, (2015) DOI:10.1007/978-3-319-14397-2_3
943. ACS virtual issue on deep eutectic solvents, M. C. Kroon, D. T. Allen, J. F. Brennecke, P. E. Savage, G. C. Schatz, *J. Chem. Eng. Data*, 62, 1927-28 (2017). DOI:10.1021/acs.jced.7b00545
944. Band-edge engineering for controlled multi-modal nanolasing in plasmonic superlattices, Danqing Wang, Ankun Yang, Weijia Wang, Yi Hua, Richard D. Schaller, G. C. Schatz, Teri W. Odom, *Nature Nanotechnology* 12, 889-894 (2017). DOI:10.1038/nnano.2017.126

945. Self-assembled plasmonic metamolecules exhibiting tunable magnetic response at optical frequencies, M. R. Bourgeois, A. T. Liu, M. B. Ross, J. M. Berlin, G. C. Schatz, *J. Phys. Chem. C*, 121, 15915-21 (2017). DOI:10.1021/acs.jpcc.7b03817
946. Structures and dynamics of electron injection and charge recombination in i-motif DNA conjugates, T. Fujii, A. K. Thazhathveetil, I. Yildirim, R. M. Rount, M. R. Wasielewski, G. C. Schatz, F. D. Lewis, *J. Phys. Chem. B*, 121, 8058-8068 (2017). DOI:10.1021/acs.jpcc.7b04996
947. Perspective Collections in the limelight, G. D. Scholes, J. Bisquert, M. Forsyth, B. Mennucci, O. Prezhd, F. Zaera, T. Zwier, G. C. Schatz, *J. Phys. Chem. Lett.* 8, 3718-9 (2017). DOI:10.1021/acs.jpcclett.7b01914
948. Transient melting and recrystallization of semiconductor nanocrystals under multiple electron-hole pair excitation, M. S. Kirschner, D. C. Hannah, B. T. Diroll, Xiaoyi Zhang, Michael Wagner, Dugan Hayes, Angela Chang, Clare Rowland, Clotilde LeThiec, G. C. Schatz, L. X. Chen, R. D. Schaller, *Nano Lett.* 5314-5320 (2017). DOI:10.1021/acs.nanolett.7b01705
949. Deterministic symmetry breaking of plasmonic nanostructures enabled by DNA-programmable assembly, M. R. Jones, K. L. Kohlstedt, M. N. O'Brien, J. Wu, G. C. Schatz, C. A. Mirkin, *Nano Lett.* 5830-5835 (2017) DOI: 10.1021/acs.nanolett.7b03067
950. Nanostructured organic semiconductor films for molecular detection with surface-enhanced Raman spectroscopy, M. Yilmaz, E. Babur, M. Ozdemir, R. L. Gieseck, Y. Dede, U. Tamer, G. C. Schatz, A. Facchetti, H. Usta, G. Demirel, *Nature Materials*, 16, 918-925 (2017). DOI: 10.1038/NMAT4957
951. Peptide amphiphile self-assembly, Aysenur Iscen and George C. Schatz, *European Physics Letters*, 119, 38002 (2017). DOI: 10.1209/0295-5075/119/38002
952. Native electron capture dissociation maps to iron-binding channels in horse spleen ferritin, O. S. Skinner, M. O. McAnally, R. P. Van Duyne, G. C. Schatz, K. Breuker, P. D. Compton, N. L. Kelleher, *Anal. Chem.* 89, 1071-16 (2017). DOI:10.1021/acs.analchem.7b01581
953. Observation of single molecule plasmon-driven electron transfer in isotopically edited 4,4'-bipyridine gold nanosphere oligomers, E. A. Sprague-Klein, M. O. McAnally, D. V. Zhdanov, A. B. Zrimsek, V. A. Apkarian, T. Seideman, G. C. Schatz, R. P. Van Duyne, *J. Am. Chem. Soc.* 15212-15221 (2017). DOI:10.1021/jacs.7b08868
954. Structural engineering in plasmon nanolasers, Danqing Wang, Weijia Wang, Michael P. Knudson, George C. Schatz, Teri W. Odom, *Chem. Rev.* 118, 2865-2881 (2018) DOI:10.1021/acs.chemrev.7b00424
955. Virtual issue on metal-halide perovskite nanocrystals-A bright future for optoelectronics, J. M. Buriak, P. V. Kamat, K. S. Schanze, A. P. Alivisatos, C. J. Murphy, G. C. Schatz, G. D. Scholes, P. J. Stang, P. S. Weiss, *Chem. Mat.*, 29(21), 8915-8917 (2017) DOI:10.1021/acs.chemmater.7b04336
956. Virtual issue in honor of the 150th birthday of Marie Curie: Highlighting female physical chemists, G. C. Schatz, A. B. McCoy, J. -E. Shea, C. J. Murphy, G. D. Scholes, *J. Phys. Chem. B*, 9983-85 (2017). DOI:10.1021/acs.jpcc.7b09653

957. Fabrication of gold nanosphere oligomers for surface-enhanced femtosecond stimulated Raman spectroscopy, Bogdan Negru, Michael O. McAnally, Hannah E. Mayhew, Tyler, W. Ueltschi, Lingxuan Peng, Emily A. Sprague-Klein, George C. Schatz, Richard P. Van Duyne, *J. Phys. Chem. C* 121, 27004-27008 (2017). DOI: 10.1021/acs.jpcc.7b09664
958. In the limelight: Perspective collections on perovskites, Gregory D. Scholes, Juan Bisquert, Maria Forsyth, Benedetta Mennucci, Oleg Prezhdo, Francisco Zaera, Timothy Zwier, George C. Schatz, *J. Phys. Chem. Lett.* 8, 5688 (2017) DOI:10.1021/acs.jpcclett.7b02970
959. Hydrogenation of CO to methanol on Ni(110) through subsurface hydrogen, Adam P. Ashwell, Wei Lin, Michelle S. Hofman, Yuxin Yang, Mark A. Ratner, Bruce E. Koel, George C. Schatz, *J. Am. Chem. Soc.* 139, 17582-17589 (2017). DOI:10.1021/jacs.7b09914
960. Phonon-driven oscillatory plasmonic excitonic nanomaterials, Matthew S. Kirschner, Wendu Ding, Yuxiu Li, Craig T. Chapman, Aiwen Lei, Xiao-Mi9n Lin, Lin X. Chen, George C. Schatz, Richard D. Schaller, *Nano Lett.* 18, 442-448 (2017). DOI:10.1021/acs.nanolett.7b04354
961. Probing intermolecular vibrational symmetry breaking in self-assembled monolayers with ultrahigh vacuum tip-enhanced Raman spectroscopy, Naihao Chiang, Nan Jiang, Lindsey R. Madison, Eric A. Pozzi, Michael R. Wasielewski, Mark A. Ratner, Mark C. Hersam, Tamar Seideman, George C. Schatz, Richard P. Van Duyne, *J. Am. Chem. Soc.* 139, 18664-18669 (2017). DOI:10.1021/jacs.7b10645
962. Wavefunctions, density functionals, and artificial intelligence for materials and energy research: future prospects and challenges, Martin A. Mosquera, Bo Fu, Kevin L. Kohlstedt, George C. Schatz, Mark A. Ratner, *ACS Energy Lett.* 3, 155-162 (2017). DOI:10.1021/acsenerylett.7b01058
963. Deducing the adsorption geometry of rhodamine 6G from the surface-induced mode renormalization in surface-enhanced Raman spectroscopy, Colin Van Dyck, Bo Fu, Richard P. Van Duyne, George C. Schatz, Mark A. Ratner, *J. Phys. Chem. C*, 122, 465-473 (2018). DOI:10.1021/acs.jpcc.7b09441
964. Ultrafast dynamics of two copper bis-phenanthroline complexes measured by transient x-ray absorption spectroscopy, Matthew S. Kelley, Megan L. Shelby, Michael W. Mara, Kristoffer Haldrup, Dugan Hayes, Ryan G. Hadt, Xiaoyi Zhang, Andrew B. Sticrath, Romain Ruppert, Jean-Pierre Sauvage, Diling Zhu, Henrik T. Lemke, Matthieu Chollet, George C. Schatz, Lin X. Chen, *J. Phys. B* 50, 154006 (2017). DOI:10.1088/1361-6455/aa7b97
965. Model for describing plasmonic nanolasers using Maxwell-Liouville equations with finite-difference time-domain calculations, Dhara J. Trivedi, Danqing Wang, Teri W. Odom, George C. Schatz, *Phys. Rev. A* 96, 053825 (2017) DOI: 10.1103/PhysRevA.96.053825
966. Editorial: 2017 in Perspective, Gregory D. Scholes, Juan Bisquert, Maria Forsyth, Benedetta Mennucci, Oleg Prezhdo, Francisco Zaera, Timothy Zwier, George C. Schatz, *J. Phys. Chem. Lett.* 9, 138-140 (2018) DOI:10.1021/acs.jpcclett.7b03309
967. Editorial for January 2018 for JPC A/B/C, Anne B. McCoy, Joan-Emma Shea, Catherine J. Murphy, George C. Schatz, *J. Phys. Chem. C* 122, 107 (2018). DOI:10.1021/acs.jpcc.7b11431
968. Ultra-high vacuum tip-enhanced Raman spectroscopy, Naihao Chiang, Guillaume Goubert, Eric A. Pozzi, Michael O. McAnally, Craig Chapman, Nan Jiang, George C. Schatz, Richard P. Van Duyne, in "Recent Developments in Plasmon-supported Raman spectroscopy: 45 years of

- enhanced Raman signals”, ISBN 9781786344236 ed. Katrin Kneipp, Yukihiro Ozaki, Zhong-Qun Tian, World Scientific, Singapore, 2018, 231-254.
969. SERS theory: the chemical effect of Rhodamine 6G Adsorption on Silver Surfaces on its Raman spectrum, Lindsey R. Madison, Mark A. Ratner, George C. Schatz, in “Recent Developments in Plasmon-supported Raman spectroscopy: 45 years of enhanced Raman signals”, ISBN 9781786344236 ed. Katrin Kneipp, Yukihiro Ozaki, Zhong-Qun Tian, World Scientific, Singapore, 2018, 401-414.
970. Shape and size control of substrate-grown gold nanoparticles for surface-enhanced Raman spectroscopy detection of chemical analytes, M. J. Ashley, M. R. Bourgeois, R. R. Murthy, C. R. Laramy, M. B. Ross, R. R. Naik, G. C. Schatz, C. A. Mirkin, *J. Phys. Chem. C* 122, 2307-2314 (2018). DOI:10.1021/acs.jpcc.7b11440
971. Highly stable, ultrasmall polymer-grafted nanobins (usPGNSs) with stimuli-responsive capability, B. J. Hong, A. Iscen, A. J. Chipre, M. M. Li, One-Sun Lee, J. N. Leonard, G. C. Schatz, S. B. T. Nguyen, *J. Phys. Chem. Lett.* 9, 1133-1139 (2018). doi: 10.1021/acs.jpcclett.7b03312
972. Mechanisms of formaldehyde and C₂ formation from methylene reacting with CO₂ adsorbed on Ni(110), Wei Lin and George C. Schatz, *J. Phys. Chem. C*, 122, 13827-13833 (2018). DOI:10.1021/acs.jpcc.8b00945
973. New sections for JPC A/B/C, Anne B. McCoy, Joan-Emma Shea, Catherine J. Murphy, George C. Schatz, *J. Phys. Chem. A*, 122, 2611 (2018). DOI:10.1021/acs.jpca.8b01720
974. Understanding the vibrational mode-specific polarization effects in femtosecond Raman-induced Kerr-effect spectroscopy, Michael O. McAnally, Yinsheng Guo, Gurusamy Balakhishnan, George C. Schatz, Richard P. Van Duyne, *Opt. Lett.* 41, 5357-60 (2016). DOI:10.1364/OL.41.005357
975. Peptide amphiphile self-assembly, Aysenur Iscen, George C. Schatz, *EPL* 119, 38002/1-/6 (2017). DOI:10.1209/0295-5075/119/38002
976. Virtual Issue on New Physical Insights, George C. Schatz, *J. Phys. Chem. A* 122, 3959-61 (2018). DOI:10.1021/acs.jpca.8b01561
977. Probing molecular-scale catalytic interactions between oxygen and cobalt phthalocyanine using tip-enhanced Raman spectroscopy, Duc Nguyen, G. Kan, N. Chiang, Xu, Chen, T. Seideman, M. C. Hersam, G. C. Schatz, R. P. Van Duyne, *J. Am. Chem. Soc.* 140, 5948-54 (2018). DOI: 10.1021/jacs.8b01154
978. Coherent vibrational wavepacketdynamics in platinum (II) dimers and their implications, Pyosang Kim, M. S. Kelley, Arnab Chakraborty, Nolan L. Wong, Richard P. Van Duyne, George C. Schatz, Felix N. Castellano, Lin X. Chen, *J. Phys. Chem. C* 122, 14195-14204 (2018) DOI:10.1021/acs.jpcc.8b01636
979. The role of structural enthalphy in spherical nucleic acid hybridization, Lam-Kiu Fong, Ziwei Wang, G. C. Schatz, E. Luijten, C. A. Mirkin, *J. Am. Chem. Soc.* 140, 6226-6230 (2018) DOI:10.1021/jacs.8b03459
980. Bias-dependent chemical enhancement and Nonclassical Stark Effect in Tip-Enhanced Raman Spectromicroscopy of CO-Terminated Ag Tips, Rebecca L. M. Giesecking, Joonhee Lee, Nicholas Tallarida, Vartkess Ara Apkarian, George C. Schatz, *J. Phys. Chem. Lett* 9, 3074-3080 (2018)

DOI:10.1021/acs.jpcclett.8b01343

981. Stretchable nanolasing from hybrid quadrupole plasmons, Danqing Wang, Marc R. Bourgeois, Won-Kyu Lee, Ran Li, Dhara Trivedi, Michael P. Knudson, Weijia Wang, George C. Schatz, Teri W. Odom, *Nano Lett.* 18, 4549-4555 (2018) DOI:10.1021/acs.nanolett.8b01774
982. Hydrogenation of CO on Ni(110) by energetic deuterium, Michelle S. Hofman, Yuxin Yang, Wei Lin, Xiaofang Yang, George C. Schatz, Bruce E. Koel, *J. Phys. Chem. C*, 122, 14671-14677 (2018). DOI:10.1021/acs.jpcc.8b03820