

Publications of Robert Benny Gerber

1. R.B. Gerber; Variational Properties of Adiabatic Molecular Wave Functions for Collisional States Intern. *J. Quant. Chem.* **1**, 781–798 (1967).
2. C.A. Coulson and R.B. Gerber; A Lower Bound Property of Adiabatic phase Shifts *Mol. Phys.* **14**, 117–131 (1968).
3. C.A. Coulson and R.B. Gerber; Effects of Complex-Values Electronic Wave Functions on Nuclear Motions Intern. *J. Quant. Chem.* **2**, 607–640 (1968).
4. R.B. Gerber; On the Order of Accuracy of the Born–Oppenheimer Approximation for Molecular Collision States *Proc. Roy. Soc. A309*, 221–244 (1969).
5. R.B. Gerber and M. Karplus; Upper Bounds on Many-Channel Scattering phase Shifts by an Adiabatic-Type Approximation *J. Chem. Phys.* **51**, 2726–2734 (1969).
6. R.B. Gerber and M. Karplus; On the Determination of the phase of the Scattering Amplitude from the Differential Cross Section *Phys. Rev. D1*, 998–1012 (1970).
7. R.B. Gerber and M. Karplus; On the Determination of the phases of Electromagnetic Scattering Amplitudes from Experimental Data *J. Chem. Phys.* **56**, 1921–1936 (1972).
8. R.B. Gerber; Determination of the Scattering Amplitude from the Cross Section for Scattering by an Arbitrary Noncentral Potential *Phys. Rev. A5*, 2151–2162 (1972).
9. R.B. Gerber; Solution of the Inversion Problem for Nonspherically Symmetric Separable Potentials *J. Phys.* **5**, L242–L245 (1972).
10. R.B. Gerber; Semiclassical Approximations for Scattering by Nonlocal Potentials: I. The Effective Mass Method *J. Chem. Phys.* **58**, 4936–4948 (1973).
11. R.B. Gerber; Semiclassical Approximations for Scattering by Nonlocal Potentials: II. Simple Applications to Atomic Collisions *J. Chem. Phys.* **58**, 4949–4961 (1973).
12. R.B. Gerber; Construction of a Nonlocal Potential from the Scattering Amplitude in the Born Approximation *Chem. Phys. Lett.*, **18**, 436–440 (1973).
13. R.B. Gerber; Inversion Procedure for a Certain Class of Nonspherically Symmetric Potentials *J. Phys.* **A6**, 770–777 (1973).
14. R.B. Gerber and N.C. Rosenbach; Properties of an Analytically Solvable Model of Multi-Channel Scattering *Phys. Rev. A9*, 301–315 (1974).
15. V. Yakhot and R.B. Gerber; Excimer Emission Spectrum in Noble Gas Systems *Chem. Phys.* **8**, 366–370 (1975).
16. V. Yakhot, M. Berkowitz and R.B. Gerber; Theory of Excimer Vibrational Relaxation and U.V. Emission in Solid Neon *Chem. Phys.* **10**, 61–66 (1975).
17. R.B. Gerber and M. Shapiro; A Numerical Method for the Determination of Atom–Atom Scattering Amplitudes from the Measured Differential Cross Sections *Chem. Phys.* **13**, 227–233 (1976).
18. M. Shapiro and R.B. Gerber; Extraction of Interaction Potentials from the Elastic Scattering Amplitudes: An Accurate Quantum-Mechanical Procedure *Chem. Phys.* **13**, 235–242 (1976).
19. R.B. Gerber; Analytical Approximation for Vib-Rotational Cross Sections in Molecular Collisions *Chem. Phys.* **16**, 19–27 (1976).
20. E. Keren, R.B. Gerber and A. Ben-Shaul; Computer Simulation of the Cl + HBr Chemical Laser: Effects of Rotational Nonequilibrium *Chem. Phys.* **21**, 1–19 (1977).
21. M. Shapiro, R.B. Gerber, U. Buck and J. Schleusener; A Method for the Deconvolution of Differential Cross Sections Measured in Molecular Beam Experiments *J. Chem. Phys.* **67**, 3570–3576 (1977).
22. M. Berkowitz and R.B. Gerber; Vibrational Relaxation of Molecules in Solids: The Role of Rotational and of Translational Modes *Chem. Phys. Lett.* **49**, 260–264 (1977).
23. R.B. Gerber and M. Berkowitz; Role of Rotational and Translational Local Modes in Vibrational Relaxation in Solids: A Study of NH and ND in Ar *Phys. Rev. Lett.* **39**, 1000–1004 (1977).
24. N.C. Pyper, I.P. Grant and R.B. Gerber; Relativistic Effects on Interactions Between Heavy Atoms: The Hg–Hg Potential *Chem. Phys. Lett.* **49**, 479–483 (1977).
25. R.B. Gerber, N.C. Zaritsky and U. Minglegrin; An Optical Potential Approach to the Calculation of Vibrational Relaxation Rates *Mol. Phys.* **35**, 1247–1269 (1978).
26. N.C. Zaritsky, U. Minglegrin and R.B. Gerber; Vib-Rotational Relaxation in Li + N₂ Collisions: Calculations with the Optical Potential Method *Mol. Phys.* **35**, 1269–1281 (1978).
27. R.B. Gerber, M. Berkowitz and V. Yakhot; Librational Relaxation of Impurity Molecules in Host Crystals *Mol. Phys.* **36**, 355–363 (1978).
28. R.B. Gerber and M. Berkowitz; Rotational Mode Participation in Long-Distance Vibrational Energy Transfer in Solids *Chem. Phys. Lett.* **56**, 105–108 (1978).
29. R.B. Gerber, A.T. Yinnon and J.N. Murrell; Sudden Decoupling Approximations for Atom–Surface Scattering *Chem. Phys.* **31**, 1–9 (1978).
30. J.N. Murrell, A.T. Yinnon and R.B. Gerber; Applications of Symmetry in Coupled-Channel Atom–Surface Scattering Calculations *Chem. Phys.* **33**, 131–135 (1978).
31. A.T. Yinnon, S. Bosanac, R.B. Gerber and J.N. Murrell; Coupled-Channel Calculations and the Accuracy of Sudden Approximation for Atom–Surface Scattering *Chem. Phys. Lett.* **58**, 364–367 (1978).
32. S. Bosanac, R.B. Gerber and U. Buck; Regge Pole Analysis of Differential Cross Sections for Elastic Molecular Scattering *Chem. Phys. Lett.* **58**, 359–363 (1978).
33. R.B. Gerber, M. Shapiro, U. Buck and J. Schleusener; Quantum-Mechanical Inversion of the Differential Cross Section: Determination of the He–Ne Potential *Phys. Rev. Lett.* **41**, 236–239 (1978).
34. M.S. Child and R.B. Gerber; Inversion of Inelastic Atom–Atom Scattering Data: Recovery of the Potential *Mol. Phys.* **38**, 421–432 (1979).
35. M. Berkowitz and R.B. Gerber; Theory of Vibrational Relaxation in Solids: The Competition Between Local Phonon and Roton Receiving Modes *Chem. Phys.* **37**, 369–388 (1979).
36. R.B. Gerber and M.A. Ratner; A Semiclassical Self-Consistent Field (SC-SCF) Approximation for Eigenvalues of Coupled-Vibration Systems *Chem. Phys. Lett.* **68**, 195–198 (1979).
37. R.B. Gerber; Direct Inversion Methods for Obtaining Intermolecular Potentials from Elastic and Inelastic Scattering Data, in: *Lectures in Biological and Chemical Physics* (A

volume in honor of S. Lifson's 65th Birthday), edited by M. Balaban (Balaban Science Services, New York, 1979).

38. R.B. Gerber and A.T. Yinnon; Approximate Solution of the Inversion Problem for Atom-Surface Scattering *J. Chem. Phys.* **73**, 3232–3238 (1980).

39. A.T. Yinnon, U. Minglegrin and R.B. Gerber; Dynamics of Molecular Scattering from Stepped Surfaces *J. Chem. Phys.* **73**, 5363–5370 (1980).

40. R.B. Gerber, V. Buch and U. Buck; Direct Inversion Method for Obtaining Anisotropic Potentials from Rotationally Inelastic and Elastic Cross Sections *J. Chem. Phys.* **72**, 3596–3603 (1980).

41. R.B. Gerber, A.T. Yinnon, Y. Shimoni and D.J. Kouri; Rotationally Inelastic Molecule-Surface Scattering in the Sudden Approximation *J. Chem. Phys.* **73**, 4397–4412 (1980).

42. R.B. Gerber, V. Buch, U. Buck, G. Maneke and J. Schleusener; Direct Inversion of Rotationally Inelastic Cross Sections: Determination of the Anisotropic Ne-D₂ Potential *Phys. Rev. Lett.* **44**, 1397–1400 (1980).

43. M.A. Ratner, V. Buch and R.B. Gerber; The Semiclassical Self-Consistent-Field Approach to Energy Levels of Coupled Vibrational Modes. II. The Semiclassical State-Interaction Procedure *Chem. Phys.* **53**, 345–356 (1980).

44. R.B. Gerber, L.H. Beard and D.J. Kouri; Vibrational Deactivation of Diatomic Molecules by Collisions with Solid Surfaces *J. Chem. Phys.* **74**, 4709–4725 (1981).

45. V. Buch, M.A. Ratner and R.B. Gerber; A Semiclassical Approximation for Matrix Elements Involving Nonorthogonal Bound States *Mol. Phys.* **42**, 497–500 (1981).

46. R.B. Gerber; Semiclassical Approximation for Off-Shell T-Matrix Elements for Collisions of Composite Particles *Mol. Phys.* **42**, 693–702 (1981).

47. D.E. Fitz, A.O. Bawagan, L.H. Beard, D.J. Kouri and R.B. Gerber; Rotational-Translational Energy Exchange in Molecule-Surface Collisions *Chem. Phys. Lett.* **80**, 537–541 (1981).

48. R.B. Gerber; The Extraction of Intermolecular Potentials from Molecular Scattering Data - Direct Inversion Methods, in: *Intermolecular Forces* (Proceedings of the 14th Jerusalem Symposium on Quantum Chemistry and Biochemistry), edited by B. Pullman (Reidel Publishing Co., Dordrecht, Holland, (1981).

49. R.B. Gerber, R. Roth and M.A. Ratner; Approximate Inversion Method for Obtaining Polyatomic Potential Energy Surfaces from Ro-Vibrational Spectra *Mol. Phys.* **44**, 1335–1353 (1981).

50. A.O. Bawagan, L.H. Beard, R.B. Gerber and D.J. Kouri; Vibrational-Rotational Translational Energy Exchange in Molecule - Surface Collisions *Chem. Phys. Lett.* **84**, 339–443 (1981).

51. V. Buch, R.B. Gerber and M.A. Ratner; Distributions of Energy Spacings and Wave Function Properties in Rotationally Excited States of Polyatomic Molecules: I. Numerical Experiments on Coupled Morse Oscillators *J. Chem. Phys.* **76**, 5397–5405 (1982).

52. V. Buch, M.A. Ratner and R.B. Gerber; Properties of Rotationally Excited Polyatomic Molecules and Their Energy Variation: Transition Moment and Energy Spacing Distributions *Mol. Phys.* **46**, 1129–1140 (1982).

53. R.B. Gerber, V. Buch and M.A. Ratner; Statistical Wave Function Method for Highly Excited Vibrational States of Polyatomics *Chem. Phys. Lett.* **89**, 171–174 (1982).

54. R.B. Gerber, V. Buch and M.A. Ratner; Self-Consistent Field and Statistical Wave Function Methods for Excited

Vibrational States of Polyatomic Molecules, in: *Intramolecular Dynamics* (Proceedings of the 14th Jerusalem Symposium on Quantum Chemistry and Biochemistry), edited by J. Jortner and B. Pullman (Reidel Publishing Co., Dordrecht, Holland 1982), pp. 171–190.

55. R.B. Gerber, V. Buch and M.A. Ratner; Time-Dependent Self-Consistent Field Approximation for Intramolecular Energy Transfer. I. Formulation and Application to Dissociation of van der Waals Molecules *J. Chem. Phys.* **77**, 3022–3030 (1982).

56. R.B. Gerber, M.A. Ratner and V. Buch; Simplified Time-Dependent Self-Consistent Field Approximation for Intramolecular Dynamics *Chem. Phys. Lett.* **91**, 173–177 (1982).

57. D.J. Kouri and R.B. Gerber; Quantum Mechanical Treatments of Rotationally Inelastic Molecule-Surface Scattering *Isr. J. Chem.* **22**, 321–328 (1982).

58. Z. Kirson, R.B. Gerber and A. Nitzan; Excitation and Emission of Metal Electrons in Atom-Surface Collisions *Surface Science* **124**, 279–296 (1983).

59. J.I. Gersten, R.B. Gerber, D.K. Dacol and H.A. Rabitz; Molecular Scattering from Disordered Surfaces in the Sudden Approximation *J. Chem. Phys.* **78**, 4277–4287 (1983).

60. R. Elber and R.B. Gerber; Dissociation Dynamics in High Energy Molecule-Surface Collisions: The Dissociation Rainbow Effect *Chem. Phys. Lett.* **97**, 4–8 (1983).

61. R.M. Roth, R.B. Gerber and M.A. Ratner; Vibrational Levels in the Self-Consistent Field Approximation with Local and with Normal Modes: Results for H₂O and CO₂ *J. Phys. Chem.* **87**, 2376–2382 (1983).

62. G.C. Schatz, V. Buch, M.A. Ratner and R.B. Gerber; Dissociation Dynamics of Rotationally Excited van der Waals Clusters: I₂XY → I₂ + X + Y (X, Y = He, Ne) *J. Chem. Phys.* **79**, 1808–1822 (1983).

63. B. Barbov, G.C. Schatz, M.A. Ratner and R.B. Gerber; Dynamical Instabilities and Structural Changes in Molecules *Mol. Phys.* **50**, 353–368 (1983).

64. R. Elber and R.B. Gerber; Multiple Collision Rotational Rainbow Effect in Molecule-Surface Scattering *J. Chem. Phys.* **79**, 4087–4088 (1983).

65. V. Buch, M.A. Ratner and R.B. Gerber; Dissociation Dynamics of Ar₃ in the Time Dependent Self-Consistent Field (TDSCF) Approximation *Chem. Phys. Lett.* **101**, 44–48 (1983).

66. R.B. Gerber and R. Elber; Vibrational and Rotational Excitation in High-Energy Molecule-Surface Collisions: Dominance of the Rotational Mode *Chem. Phys. Lett.* **102**, 466–469 (1983).

67. R. Elber and R.B. Gerber; Formation of Metastables and Dissociative Trapping in High Energy Molecule-Surface Collisions *J. Phys. Chem.* **88**, 1571–1575 (1984).

68. Z. Kirson, R.B. Gerber, A. Nitzan and M.A. Ratner; Dynamics of Metal Electron Excitation in Atom-Surface Collisions: A Quantum Wave Packet Approach *Surface Science* **137**, 527–550 (1984).

69. T.R. Proctor, D.J. Kouri and R.B. Gerber; ΔM_J-Transitions in Homonuclear Molecule Surface Scattering off Corrugated Surfaces: Square and Rectangular Lattice Symmetry and Purely Repulsive Interaction *J. Chem. Phys.* **80**, 3845–3858 (1984).

70. R.B. Gerber, A.T. Yinnon and R. Kosloff; Effects of Isolated Impurities on Atom Scattering from Crystalline Surfaces. Exact Quantum-Mechanical Calculations *Chem. Phys. Lett.* **105**, 523–526 (1984).

71. A.T. Yinnon, R. Kosloff and R.B. Gerber; Time-Dependent Wavepacket Calculations of Atom Scattering from Surfaces with Impurities *Chem. Phys.* **87**, 441–449 (1984).

72. I. Benjamin, V. Buch, R.B. Gerber and R.D. Levine; Spacings Distribution for Highly Excited Vibrational States: The Role of Dynamical Symmetry *Chem. Phys. Lett.* **107**, 515–521 (1984).
73. R.M. Roth, M.A. Ratner and R.B. Gerber; Inversion of Polyatomic Ro-Vibrational Spectra into a Molecular Potential Energy Surface: Application to CO₂ *Phys. Rev. Lett.* **52**, 1288–1291 (1984).
74. R.B. Gerber and R. Elber; Centrifugal Mechanism for Molecular Dissociation in High-Energy Collisions with Solid Surfaces *Chem. Phys. Lett.* **107**, 141–144 (1984).
75. A.T. Yinnon, R. Kosloff and R.B. Gerber; Atom Scattering from Disordered Surfaces: Calculations for a Model of Xe + Ar Mixed Overlayer *Surf. Sci.* **148**, 148–152 (1984).
76. V. Buch, R.B. Gerber and M.A. Ratner; A Statistical Wave function Model for C–H, C–D Overtone Linewidths: Application to C₆H₆, C₆D₆, C₆HD₅, C₆HF₅ *J. Chem. Phys.* **81**, 3393–3399 (1984).
77. R.B. Gerber and A. Nitzan; Dynamics on Surfaces - Concluding Remarks on the Jerusalem Symposium. *Proceedings of 17th Jerusalem Symposium on Theoretical Chemistry and Biochemistry: Dynamics on Surfaces*, edited by B. Pullman, J. Jortner, R.B. Gerber and A. Nitzan (Reidel, Dordrecht, Holland, pp. 461–466, 1984).
78. E. Kolodney, A. Amirav, R. Elber and R.B. Gerber; Energy Transfer and Dissociation in Collisions of I₂ with MgO(100) *Chem. Phys. Lett.* **111**, 366–371 (1984).
79. E. Kolodney, A. Amirav, R. Elber and R.B. Gerber; Dissociation and Energy Transfer in Molecular Impact on Surfaces: Experimental and Theoretical Studies of I₂/MgO(100) and I₂/Sapphire *Surf. Sci.* **148**, 153–154 (1984).
80. E. Kolodney, A. Amirav, R. Elber and R.B. Gerber; Large Energy Transfer in Hyperthermal Heavy Atom-Surface Scattering: Hg on MgO(100) *Chem. Phys. Lett.* **113**, 303–307 (1984).
81. R. Schinke and R.B. Gerber; Phonon Sudden Theory of Debye–Waller Attenuation: Temperature Dependence of Rotational Energy Transfer in Molecule-Surface Scattering *J. Chem. Phys.* **82**, 1567–1576 (1985).
82. Z. Kirson, R.B. Gerber, A. Nitzan and M.A. Ratner; Dynamics of Metal Electron Excitation in Molecular Dipole–Surface Collisions *Surf. Sci.* **151**, 531–542 (1985).
83. R. Elber and R.B. Gerber; Multiple-Collision Model for Molecular Dissociation in Impact on Solid Surfaces *Chem. Phys.* **92**, 363–379 (1985).
84. R. Elber, R.B. Gerber and D.J. Kouri; Multiple Collision Model for High Energy Molecular Dissociation on Surfaces: Effects of Corrugation and of Phonon Participation *Chem. Phys.* **97**, 345–356 (1985).
85. N. Moiseyev, T. Maniv, R. Elber and R.B. Gerber; Lifetimes of Rotational Resonances in Molecule-Surface Scattering: Quantum vs. Classical Results *Mol. Phys.* **55**, 1369–1381 (1985).
86. L.A. Eslava, R.B. Gerber and M.A. Ratner; Relaxation of Vibrationally Highly Excited Diatomics in van der Waals Clusters. A Study of I₂ (Ne) N; N = 4,8,16 *Mol. Phys.* **56**, 47–64 (1985).
87. R. Elber and R.B. Gerber; Excitation of Molecular Rotation and of Solid Vibrations in High-Energy Collisions of I₂ with MgO(100) *Chem. Phys. Lett.* **119**, 269–274 (1985).
88. R.B. Gerber; Potentials for Polyatomic Systems from Spectroscopic and Scattering Data: Multidimensional Inversion Methods Comments At. *Mol. Phys.* **17**, 65–89 (1985).
89. A.T. Yinnon, E. Kolodney, A. Amirav and R.B. Gerber; Atom–Surface Potentials by Inversion of Diffraction Data: Application to He/MgO(100) *Chem. Phys. Lett.* **123**, 268–272 (1986).
90. M.A. Ratner and R.B. Gerber; Excited Vibrational States of Polyatomic Molecules: The Semiclassical Self-Consistent Field Approach *J. Phys. Chem.* **90**, 20–29 (1986) (Feature Article).
91. K.B. Whaley, A. Nitzan and R.B. Gerber; Quantum Diffusion of Hydrogen on Metal Surfaces *J. Chem. Phys.* **84**, 5181–5195 (1986).
92. Z. Bacic and R.B. Gerber; Dissociation Dynamics of Mass-Asymmetric Molecules in Impact on Solid Surfaces *J. Phys. Chem.* **90**, 2912–2922 (1986).
93. A.T. Yinnon, R.B. Gerber, D.K. Dacol and H. Rabitz; The Sudden Approximation for Scattering from Noncrystalline Surfaces: Applications to Models of Adsorbed Impurities and to Mixed Overlayers *J. Chem. Phys.* **84**, 5955–5960 (1986).
94. Z. Bacic, R.B. Gerber and M.A. Ratner; Vibrational Levels and Tunneling Dynamics by the Optimal Coordinates, Self-Consistent Field (OC-SCF) Method: A Study of HCN ↔ HNC *J. Phys. Chem.* (Issue in honor of R.A. Marcus) **90**, 3606–3612 (1986).
95. R.B. Gerber and A. Amirav; Dynamics of Dissociation and Energy Transfer in Molecular Collisions with Surfaces *J. Phys. Chem.* **90**, 4483–4491 (1986) (Feature Article).
96. K.B. Whaley, A. Nitzan and R.B. Gerber; Low-Temperature Atom Diffusion on Surfaces: Tunneling and Energy Band Structure in: *Tunneling - Proceedings of the 18th Jerusalem Symposium on Quantum Chemistry*, edited by J. Jortner and B. Pullman (Reidel, Dordrecht, The Netherlands, 1986), p. 60.
97. R.B. Gerber, M.A. Ratner and Z. Bacic; Mean-Field Approach to Vibrational Energy Levels and Tunneling Dynamics in Polyatomic Systems, in: *Tunneling - Proceedings of the 18th Jerusalem Symposium*, edited by J. Jortner and B. Pullman (Reidel, Dordrecht, The Netherlands, 1986), p. 25.
98. L.L. Gibson, R.M. Roth, M.A. Ratner and R.B. Gerber; The Semiclassical Self-Consistent-Field Method for Polyatomic Vibrations: Use of Hyperspherical Coordinates for H₂O and CO₂ *J. Chem. Phys.* **85**, 3425–3431 (1986).
99. R.B. Gerber; Molecular Scattering from Surfaces: Theoretical Methods and Results *Chem. Rev.* **87**, 29–79 (1987) (Topical issue on Chemical Dynamics).
100. R.B. Gerber, R. Kosloff and M. Berman; Time-Dependent Wavepacket Calculations of Molecular Scattering from Surfaces *Comput. Phys. Rep.* **5**, 59–114 (1986).
101. R. Alimi, A. Brokman and R.B. Gerber; Theoretical Studies of Photodissociation Dynamics in Large Clusters and Solids, in: *Stochasticity and Intramolecular Redistribution of Energy*, edited by R. Lefebvre and S. Mukamel (Reidel, Dordrecht, The Netherlands, 1987), p. 233–244.
102. M.A. Ratner, R.B. Gerber and V. Buch; Excited Vibrational States: Semiclassical Self-Consistent Field and Statistical Considerations, in: *Stochasticity and Intramolecular Redistribution of Energy*, edited by R. Lefebvre and S. Mukamel (Reidel, Dordrecht, The Netherlands, 1987), p. 57–80.
103. R.B. Gerber and M.A. Ratner; Self-Consistent Field Methods for Vibrational Excitation in Polyatomic Systems *Adv. Chem. Phys.* **70**, 97–132 (1988).
104. D.K. Dacol, H. Rabitz and R.B. Gerber; Atom Scattering from Disordered Surfaces: Randomly Corrugated Hard Walls and the Sudden Approximation *J. Chem. Phys.* **86**, 1616–1623 (1987).

105. R.B. Gerber and M.A. Ratner; Mean Field Methods for Vibrational States and Dynamics: New Developments *J. Phys. Chem.* **92**, 3252–3260 (1988) (issue of invited lectures at the American Conference on Theoretical Chemistry).
106. R.H. Bisseling, R. Kosloff, R.B. Gerber, M.A. Ratner, L. Gibson and C. Cerjan; Exact Time-Dependent Quantum Mechanical Dissociation Dynamics of I₂He: Comparison of Exact Time-Dependent Quantum Calculation with the Quantum Time-Dependent Self-Consistent Field (TDSCF) Approximation *J. Chem. Phys.* **87**, 2760–2765 (1987).
107. A.T. Yinnon, R. Kosloff, R.B. Gerber, B. Poelsema and G. Comsa; Cross Sections for the Scattering from Surface Imperfections: Vacancies and CO-Absorbates on Pt(111) *J. Chem. Phys.* **88**, 3722–3731 (1988).
108. G.C. Schatz, R.B. Gerber and M.A. Ratner; Energies and Lifetimes of Predissociative States of van der Waals Molecules: Self-Consistent Field Calculations for I₂ (v)He, I₂ (v) Ne *J. Chem. Phys.* **88**, 3709–3714 (1988).
109. H. Romanowski, R.B. Gerber and M.A. Ratner; The Anharmonic Stretching–Bending Potential of CO₂ from Inversion of Spectroscopic Data *J. Chem. Phys.* **88**, 6757–6767 (1988).
110. H. Romanowski, M.A. Ratner and R.B. Gerber; Determination of Polyatomic Potential Energy Surfaces from Vibration–Rotation Spectra: An Inversion Method Applied to CO₂ *Comput. Phys. Comm.* (Special Issue on Vibrational Dynamics) **51**, 161–171 (1988).
111. P. Hofmann, R.B. Gerber, M.A. Ratner, L.C. Baylor and E. Weitz; Dynamics of Energy Flow from CH Overtone Excitations: Theoretical and Experimental Studies of CH₃C≡CH, *J. Chem. Phys.* **88**, 7434 (1988).
112. R. Alimi, R.B. Gerber and V.A. Apkarian; Dynamics of Molecular Reactions in Solids: Photodissociation of HI in Crystalline Xe *J. Chem. Phys.* **89**, 174–183 (1988).
113. R.B. Gerber, T.R. Horn and M.A. Ratner; Approximate Separability and Choice of Coordinates for Excited Vibrations of Polyatomic Molecules and Clusters, in: *The Structure of Small Molecules and Ions*, R. Naaman, ed. (Plenum, NY, 1989), pp. 9–27.
114. R.C. Mowery, H.F. Bowen, D.J. Kouri, A.T. Yinnon and R.B. Gerber; Quantum Oscillations in Molecule–Surface Scattering: Energy Dependence of Transition Probabilities *J. Chem. Phys.* **89**, 3925–3926 (1988). (Communication).
115. A.T. Yinnon, R. Kosloff and R.B. Gerber; Atom Scattering from Isolated Adsorbates on Surfaces: Rainbows, Diffraction Interferences and Trapping Resonances *J. Chem. Phys.* **88**, 7209–720 (1988).
116. R.B. Gerber and G. Petrella; M J Transitions in Molecular Scattering from Isolated Adsorbates on Surfaces *Chem. Phys. Lett.* **147**, 126–132 (1988).
117. L. Shen, R.B. Gerber and M.A. Ratner; Static Mean Field Theory for Molecular Vibrations: Self Consistent Correlation Corrections *Chem. Phys. Lett.* **155**, 119–126 (1989).
118. G. Petrella, A.T. Yinnon and R.B. Gerber; Atom Scattering from Isolated Molecular Adsorbates on Surfaces: Effects of Adsorbate Orientation *Chem. Phys. Lett.* **158**, 250–256 (1989).
119. R.B. Gerber, R. Alimi and V.A. Apkarian; Ion Migration Following Charge Transfer Reactions in Rare Gas Solids: The Role of Hole Hopping *Chem. Phys. Lett.* **158**, 257–262 (1989).
120. T.R. Horn, R.B. Gerber and M.A. Ratner; Vibrational States of Very Floppy Clusters: Approximate Separability and the Choice of Good Curvilinear Coordinates for XeHe₂, I₂ He *J. Chem. Phys.* **91**, 1813–1823 (1989).
121. R. Alimi, A. Brokman and R.B. Gerber; Molecular Dynamics Simulations of Reactions in Solids: Photodissociation of Cl₂ in Solid Xe *J. Chem. Phys.* **91**, 1611–1617 (1989).
122. R.B. Gerber, T.R. Horn, C.J. Williams and M.A. Ratner; Vibrational States of van der Waals and Hydrogen Bonded Clusters: A Self-Consistent Field Approach, in: *Dynamics of Polyatomic van der Waals Complexes*, edited by N. Halberstadt and K.C. Janda (Plenum Press, N.Y. 1990) pp. 343–345.
123. R. Alimi, R.B. Gerber and V.A. Apkarian; Dynamics of Molecular Reactions in Solids: Photodissociation of F₂ in Solid Ar *J. Chem. Phys.* **92**, 3551–3558 (1990).
124. M.A. Ratner, R.B. Gerber, T.R. Horn and C.J. Williams; Static Self Consistent Field Methods for Anharmonic Problems: An update in: *Advances in Molecular Vibrations*, edited by J.M. Bowman (JAI Press, Ct.) Vol. 1A (1991), pp. 215–253.
125. R. Alimi and R.B. Gerber; Solvation Effects on Chemical Reaction Dynamics in Clusters: Photodissociation of HI in Xe_nHI *Phys. Rev. Lett.* **64**, 1453–1456 (1990).
126. M.I. McCarthy, R.B. Gerber and M. Shapiro; Quantum Theory of the Photodissociation of IBr Adsorbed on an MgO(001) Surface *J. Chem. Phys.* **92**, 7708–7715 (1990).
127. M.I. McCarthy and R.B. Gerber; Molecular Dynamics Simulations of the Photodissociation of ICl Adsorbed on an MgO(001) Surface *J. Chem. Phys.* **93**, 887–896 (1990).
128. R. Alimi, R.B. Gerber, A.D. Hammerich, R. Kosloff and M.A. Ratner; Validity of Time-Dependent Self-Consistent Field (TDSCF) Approximation for Unimolecular Dynamics: A Test for Photodissociation of the Xe•••HI Cluster *J. Chem. Phys.* **93**, 6484–6490 (1990).
129. R.B. Gerber and R. Alimi; Quantum Effects in Molecular Reaction Dynamics in Solids: Photodissociation of HI in Solid Xe *Chem. Phys. Lett.* **173**, 393–396 (1990).
130. T.R. Horn, R.B. Gerber, J.J. Valentini and M.A. Ratner; Vibrational States and Structure of Ar₃: The Role of 3-Body Forces *J. Chem. Phys.* **94**, 6728–6736 (1991).
131. R. Alimi, R.B. Gerber and V.A. Apkarian; Photodissociation Dynamics of F₂ in Solid Kr: Theory versus Experiment *Phys. Rev. Lett.* **66**, 1295–1297 (1991).
132. R.B. Gerber and A.T. Yinnon; Properties of Atom Scattering from Percolation Lattices: He Scattering from Substitutionally Disordered Xe + Kr Monolayers *Chem. Phys. Lett.* **181**, 553–557 (1991).
133. R.B. Gerber and R. Alimi; Mixed Quantum/Classical Molecular Dynamics Simulations of Chemical Reactions in Clusters and in Solids *Isr. J. Chem.* **81**, 383–393 (1991) (Special issue in honor of R. Pauncz).
134. R.B. Gerber and R. Alimi; Quantum Molecular Dynamics by a Perturbation-Corrected Time Dependent Self Consistent Field Method *Chem. Phys. Lett.* **184**, 69–75 (1991).
135. R.B. Gerber, R. Alimi, A. Garcia-Vela and Y. Hurwitz; Dynamics of Photoinduced Reactions in Clusters in: *Mode Selective Chemistry* (Proc. of the 28th Jerusalem Symposium on Quantum Chemistry and Biochemistry), edited by B. Pullman, J. Jortner and R.D. Levine (Kluwer Academic Publishers, Dordrecht, Holland), pp. 201–215 (1991).
136. A. Garcia-Vela, R.B. Gerber and J.J. Valentini; Dynamics of Molecular Photodissociation in Clusters: A Study of Ar•••HCl *Chem. Phys. Lett.* **186**, 223–228 (1991).
137. R. Alimi, A. Garcia-Vela and R.B. Gerber; A Remedy for Zero-Point Energy Problems in Classical Trajectories: A Combined Semiclassical/Classical Molecular Dynamics Algorithm *J. Chem. Phys.* **96**, 2034–2038 (1992).
138. R.B. Gerber; Theory of Atom Scattering from Ordered and from Disordered Surfaces. in: *Theory of Molecular Pro-*

cesses, edited by G. Delgado-Barrio (IOP, Bristol, U.K., 1993), pp. 299–316.

139. R.B. Gerber, A.T. Yinnon, M. Yanuka and D. Chase; Atom Scattering Studies of Structurally Desordered Surfaces *Surf. Sci.* (Special issue of lectures given at the Conference on Molecule-Surface Interactions, Julich, 1991) 272, 81–93 (1992).

140. M.I. McCarthy, R.B. Gerber, K.A. Trentelman, P. Strupp, D.H. Fairbrother, P.C. Stair and E. Weitz; Photodissociation Dynamics of CH₃I Adsorbed on MgO(100): Theory and Experiment *J. Chem. Phys.* 97, 5168–5176 (1992).

141. A. Garcia-Vela, R.B. Gerber and J.J. Valentini; Effects of Solvation by a Single Atom on Photodissociation: Classical and Quantum/Classical Studies of HCl Photolysis in Ar^{•••}HCl *J. Chem. Phys.* 97, 3297–3306 (1992).

142. R. Alimi, R.B. Gerber, J.G. McCaffrey, H. Kunz and N. Schwentner; Delayed and Direct Cage Exit in Photodissociation of Cl₂ in Solid Ar *Phys. Rev. Lett.* 69, 856–859 (1992).

143. A. Garcia-Vela, R.B. Gerber and D.G. Imre; Mixed Quantum Wavepacket/Classical Trajectory Treatment of the Photodissociation Process Ar^{•••}HCl → Ar + H + Cl *J. Chem. Phys.* 97, 7242–7250 (1992).

144. A. Garcia-Vela and R.B. Gerber; Hybrid Quantum/Semiclassical Wavepacket Method for Molecular Dynamics: Applications to Photolysis of Ar^{•••}HCl *J. Chem. Phys.* 98, 427–436 (1993).

145. A. Garcia-Vela, R.B. Gerber, D.G. Imre and J.J. Valentini; Quantum Resonances and Interference Effects in the UV Photodissociation of Ar–HCl *Chem. Phys. Lett.* 202, 473–478 (1993).

146. Y. Hurwitz, Y. Rudich, R. Naaman and R.B. Gerber; Solvent Atom on Bimolecular Reactions: Collision of O(³P) with Hydrocarbon–Argon Clusters *J. Chem. Phys.* 98, 2941–2946 (1993).

147. T.R. Horn, R.B. Gerber and M.A. Ratner; Vibrational States of ArCO₂: Analysis of an Internal Dynamical Transition Using Self-Consistent Field Techniques *J. Phys. Chem.* 97, 3151–3158 (1993).

148. R. Alimi, V.A. Apkarian and R.B. Gerber; Effect of Pressure on Molecular Photodissociation in Matrices: Molecular Dynamics Simulations of Cl₂ in Xe *J. Chem. Phys.* 98, 331–335 (1993).

149. H.F. Brown, D.J. Kouri, R.C. Mowrey, A.T. Yinnon and R.B. Gerber; Molecular-Corrugated Surface Collisions: Close-Coupling Wavepacket and Quasi-Classical Trajectory Calculations for N₂–Scattering from Corrugated Lattices *J. Chem. Phys.* 99, 704–720 (1993).

150. J. Segall, Y. Wen, R. Singer, C. Wittig, A. Garcia-Vela and R.B. Gerber; Evidence for Cage Effect in UV Photolysis of HBr in Ar^{•••}HBr: Experimental and Theoretical Results *Chem. Phys. Lett.* 207, 504–509 (1993).

151. A.B. McCoy, Y. Hurwitz and R.B. Gerber; Dynamics of Photo-Induced Reactions in Hydrogen-Bonded Clusters: Classical Studies of the Photodissociation of (HCl)₂ *J. Phys. Chem.* (Special issue on Femtosecond Chemistry) 97, 12516–12522 (1993).

152. A.B. McCoy, A. Garcia-Vela and R.B. Gerber; Solvation Effects on Photochemical Reactions in Weakly Bound Clusters, in: *Ultrafast Reaction Dynamics and Solvent Effects*, edited by Y. Gaudiel and P.J. Rossky (American Institute of Physics, 1994), pp. 516–527.

153. R.B. Gerber and A. Krylov; Dynamics of the Cage Effect for Molecular Photodissociation in Solids, in: *Reaction Dynamics in Condensed Phases and Clusters*. (Proceedings of the 26th

Jerusalem Symposium), edited by B. Pullman, J. Jortner and R.D. Levine, pp. 509–520 (1994). (Kluwer Publishers, Dordrecht).

154. A. Garcia-Vela, R.B. Gerber, D.G. Imre and J.J. Valentini; Resonances in the Photolysis of HCl in Ar–HCl: Imaging of a Resonance Wave function in the Photofragment Angular Distribution *Phys. Rev. Lett.* 71, 931–934 (1993).

155. Z. Li and R.B. Gerber; Treatment of Zero-Point Motions in Cluster Dynamics: Semiclassical Time-Dependent Self-Consistent Field Simulation of (Ne)_N *J. Chem. Phys.* 99, 8637–8643 (1993).

156. M. Yanuka, A.T. Yinnon, R.B. Gerber, P. Zeppenfeld, K. Kern, U. Becher and G. Comsa; He Scattering from Substitutionally Disordered Mixed Monolayers: Experimental and Theoretical Studies of Xe + Kr on Pt(111) *J. Chem. Phys.* 99, 8280–8289 (1993).

157. B. Vekhter, M.A. Ratner and R.B. Gerber; Dynamic Mean-Field Models with Correlated Modes *J. Chem. Phys.* 99, 7916–7924 (1993).

158. A. Garcia-Vela, R.B. Gerber and U. Buck; Photolysis of HCl in the Ar₂–HCl and Ar–HCl Clusters: The Cluster Size Effect *J. Phys. Chem.* 98, 3518–3526 (1994). (Special Issue in honor of J. Jortner).

159. A.E. Roitberg, R.B. Gerber and M.A. Ratner; A Perturbed Mean Field Approach to the Decay Rates of Excited Vibrational States in Extended Systems: An Application to I₂ (Ne)_n *J. Chem. Phys.* 100, 4355–4366 (1994).

160. R.B. Gerber, A.B. McCoy and A. Garcia-Vela; Dynamics of Photoinduced Reactions in van der Waals and in Hydrogen-Bonded Clusters, in: “Femtosecond Chemistry”, edited by J. Manz and L. Woste (Verlag Chemie, Berlin) 1995, pp. 499–531.

161. A.I. Krylov and R.B. Gerber; Photodissociation of ICN in Solid and Liquid Ar: Dynamics of the Cage Effect and of Excited-State Isomerization *J. Chem. Phys.* 100, 4242–4252 (1994).

162. R.B. Gerber, A.B. McCoy and A. Garcia-Vela; Photochemical Reactions in Weakly-Bound Clusters *Ann. Rev. Phys. Chem.* 45, 275–314 (1994).

163. A. Vegiri, M.H. Alexander, S. Gregurick, A.B. McCoy and R.B. Gerber; Quantum Monte Carlo Studies of Small B (H₂)_n Clusters *J. Chem. Phys.* 101, 2577–2591 (1994).

164. N. Lipkin, R.B. Gerber, N. Moiseyev and G.M. Nathanson; Atom Scattering Studies of Liquid Structure and Dynamics: Collisions of Xe with a Model of Squalane *J. Chem. Phys.* 100, 8408–8417 (1994).

165. B. Schmidt and R.B. Gerber; Reactive Collisions as A Signature for Melting-Like Transitions in Clusters *Phys. Rev. Lett.* 72, 2490–2493 (1994).

166. B. Schmidt and R.B. Gerber; Solvation Effects on Association Reactions in Microclusters: Classical Trajectory Study of H + Cl (Ar)_n *J. Chem. Phys.* 101, 343–355 (1994).

167. A.B. McCoy, R.B. Gerber and M.A. Ratner; A Quantitative Approximation for the Quantum Dynamics of Hydrogen Transfer: Transition State Dynamics and Decay in ClHCl[–] *J. Chem. Phys.* 101, 1975–1987 (1994).

168. A.I. Krylov, R.B. Gerber and V.A. Apkarian; Adiabatic Approximation and Non-Adiabatic Effects for Open-Shell Atoms in Inert Solvents: F Atoms in Solid Kr *Chem. Phys.* 189, 261–272 (1994). (Special issue on Processes in Solid Matrices).

169. Z. Li and R.B. Gerber; Survival of Weakly Bound Quantum Clusters in Collisions with Atoms *Chem. Phys. Lett.* 229, 650–656 (1994).

170. M. Hintenender, F. Rebentrost, R.B. Gerber and R. Kosloff; Molecular Dynamics Simulations of the Photodissociation of Adsorbed HCl on a MgO(001) Surface *J. Chem. Phys.* **102**, 578–584 (1995).
171. A.I. Krylov and R.B. Gerber; Reorientation Dynamics of Electronic Orbitals in Condensed phases: Simulations of F 2 P Atoms in Solid Kr *Chem. Phys. Lett.* **231**, 395–400 (1994).
172. Z. Li and R.B. Gerber; Electronic Excitation Dynamics of Li(H₂)₂: Dissociation Mechanisms, Lifetimes, and the Validity of a Hybrid Quantum/Classical Approach *J. Chem. Phys.* **102**, 4056–4062 (1995).
173. D.A. Hamburger, A.T. Yinnon, I. Farbman, A. Ben-Shaul and R.B. Gerber; He Scattering from Compact Clusters and from Diffusion-Limited Aggregates on Surfaces: Observable Signatures of Structure *Surf. Sci.* **327**, 165–191 (1995).
174. P. Jungwirth and R.B. Gerber; Quantum Dynamics of Large Polyatomic Systems Using a Classically-Based Separable Potential Method *J. Chem. Phys.* **102**, 6046–6056 (1995).
175. D.A. Hamburger and R.B. Gerber; Optical Theorem and the Inversion of Cross Section Data for Atom Scattering from Defects on Surfaces *J. Chem. Phys.* **102**, 6919–6026 (1995).
176. P. Jungwirth and R.B. Gerber; Quantum Dynamics of Many-Atom Systems by the Classically-Based Separable Potential (CSP) Method: Calculations for I⁻ (Ar)₁₂ in Full Dimensionality *J. Chem. Phys.* **102**, 8855–8864 (1995).
177. A. Roitberg, R.B. Gerber, R. Elber and M.A. Ratner; Anharmonic Wave Functions of Proteins: Quantum Self-Consistent Field Calculations of BPTI *Science* **268**, 1319–1322 (1995).
178. A. Garcia-Vela and R.B. Gerber; Three-Dimensional Quantum Wavepacket Study of the Ar-HCl Photodissociation: A Comparison between Time-Dependent Self-Consistent Field and Exact Treatments *J. Chem. Phys.* **103**, 3463–3473 (1995).
179. Z. Li and R.B. Gerber; Validity of the Time-Dependent Self-Consistent Field (TDSCF) Approximation for Non-Stationary Vibrational State of Quantum Clusters *Chem. Phys. Lett.* **104**, 5803–5814 (1996).
180. A.I. Krylov, R.B. Gerber, M.A. Gaveau, J.M. Mestdagh, B. Schilling and J.P. Visticot; Spectroscopy, Polarization and Non-Adiabatic Dynamics of Electronically Excited Ba(Ar)_n Clusters: Theory and Experiment *J. Chem. Phys.* **104**, 3651–3663 (1996).
181. P. Jungwirth and R.B. Gerber; Quantum Dynamics Simulations of Non-Adiabatic Processes in Many-Atom Systems: Photoexcited Ba(Ar)₁₀ and Ba(Ar)₂₀ Clusters *J. Chem. Phys.* **104**, 5803–5814 (1996).
182. E. Fredj, R.B. Gerber and M.A. Ratner; Semiclassical Molecular Dynamics Simulations of Low-Temperature Clusters: Applications to (Ar)₁₃; (Ne)₁₃; (H₂O)_n, n = 2,3,5 *J. Chem. Phys.* **105**, 1121–1130 (1996).
183. D.A. Hamburger, A.T. Yinnon and R.B. Gerber; Fractal Dimension of Disordered Submonolayers: Determination from He Scattering Data *Chem. Phys. Lett.* **253**, 223–229 (1996).
184. P. Jungwirth, E. Fredj and R.B. Gerber; Ultrafast Quantum Dynamics and Resonance Raman Spectroscopy of Photoexcited I₂ (B) in Large Argon and Xenon Clusters *J. Chem. Phys.* **104**, 9332–9339 (1996).
185. A.I. Krylov, R.B. Gerber and R.D. Coalson; Nonadiabatic Dynamics and Electronic Energy Relaxation of Cl₂ Atoms in Solid Ar *J. Chem. Phys.* **105**, 4626–4635 (1996).
186. S. Broude and R.B. Gerber; Solvation of Metal Atoms in Quantum Clusters: Structural and Vibrational Properties of Hg(H₂)₁₂, Mg(H₂)₁₂ *Chem. Phys. Lett.* **258**, 416–420 (1996).
187. E.S. Altshuler, D.L. Mills and R.B. Gerber; Vibrational Dynamics of H Atoms Chemisorbed on Metal (110) Surfaces *Surf. Sci.* **374**, 229–242 (1997).
188. L.S. Norris, M.A. Ratner, A.E. Roitberg and R.B. Gerber; Moller–Plesset Perturbation Theory Applied to Vibrational Problems *J. Chem. Phys.* **106**, 11261–11267 (1996).
189. J.O. Jung and R.B. Gerber; Vibrational Wave functions and Spectroscopy of (H₂O)_n, n = 2,3,4,5: Vibrational SCF with Correlation Corrections *J. Chem. Phys.* **105**, 10332–10347 (1996).
190. J.O. Jung and R.B. Gerber; Vibrational Wave functions and Energy Levels of Large Anharmonic Clusters: A Vibrational SCF Study of Ar₁₃ *J. Chem. Phys.* **105**, 10682–10690 (1996).
191. M. Hintenender, F. Rebentrost, R. Kosloff and R.B. Gerber; Mixed Quantum/Classical Simulation of the Photolysis of HCl on MgO(001) *J. Chem. Phys.* **105**, 11347–11356 (1996).
192. A.E. Roitberg, R.B. Gerber and M.A. Ratner; A Vibrational Wave function of a Protein: The Anharmonic Coupled Mode Ground and Fundamental Excited States of BPTI *J. Phys. Chem.* **101**, 1700–1706 (1997).
193. A.T. Yinnon, D.A. Lidar-Hamburger, I. Farbman, R.B. Gerber, P. Zeppenfeld, M.A. Krzyrowski and G. Comsa; He Scattering from Random Adsorbates, Disordered Compact Islands and Fractal Submonolayers. Intensity Manifestations of Surface Disorder *J. Chem. Phys.* **106**, 4228–4242 (1997).
194. A.I. Krylov and R.B. Gerber; Photodissociation Dynamics of HCl in Solid Ar: Cage Exit, Nonadiabatic Transitions and Recombination *J. Chem. Phys.* **106**, 6574–6587 (1997).
195. R.B. Gerber, P. Jungwirth, E. Fredj and A.Y. Rom; Quantum Molecular Dynamics Simulations of Processes in Large Clusters: Methods and Applications, in: *Modern Methods for Multidimensional Dynamics Computations in Chemistry*, edited by D.L. Thompson. (World Scientific Publishing, Singapore, 1998), pp. 238–265.
196. P. Jungwirth, E. Fredj, P. Zdanska and R.B. Gerber; Quantum Dynamics of Large Polyatomic Systems Using Classical Separable Potentials: The Computational Implementation *Comput. Chem.* **21**, 419–429 (1997).
197. A.Y. Rom and R.B. Gerber; Quantum Simulations of Energy Transfer and State-to-State Transitions in Collisions of an Atom with a Large Anharmonic Cluster: He + (Ar)₁₃ *J. Chem. Phys.* **107**, 8963–8971 (1997).
198. P. Jungwirth, E. Fredj and R.B. Gerber; Quantum Molecular Dynamics of Large Systems Beyond Separable Approximation: The Configuration Interaction Classical Separable Potential Method *J. Chem. Phys.* **107**, 8963–8974 (1997).
199. S.K. Gregurick, E. Fredj, R. Elber and R.B. Gerber; Vibrational Spectroscopy of Peptides and Peptide-Water Complexes: Anharmonic Coupled-Mode Calculations *J. Phys. Chem. B* **101**, 8595–8606 (1997).
200. M.Y. Niv, A.I. Krylov and R.B. Gerber; Photodissociation, Electronic Relaxation and Recombination of HCl in Ar_n (HCl) Clusters: Nonadiabatic Molecular Dynamics Simulations *Faraday Discuss. Chem. Soc.* **108**, 243–254 (1997).
201. A.Y. Rom, D. Neuhauser and R.B. Gerber; Quantum Mechanical Calculation of Inelastic Scattering of an Atom by a Large Anharmonic Cluster: Application to He + Ar₁₃ *J. Chem. Phys.* **108**, 6084–6092 (1998).
202. A.T. Yinnon, D.A. Lidar (Hamburger), R.B. Gerber, P. Zeppenfeld, M.A. Krzyrowski and G. Comsa; Structure Determination of Disordered Metallic Sub-Monolayers by Helium Scattering: A Theoretical and Experimental Study *Surf. Sci. Lett.* **410**, L721-L726 (1998).

203. E. Fredj, R.B. Gerber and M.A. Ratner; Quantum-Mechanical Simulations of Inelastic Scattering in Collisions of Large Clusters: Ar + (H₂O)₁₁ *J. Chem. Phys.* **109**, 4833–4842 (1998).
204. J. Seong, H. Sun, M.A. Ratner, G.C. Schatz and R.B. Gerber; Vibrational Predissociation Rates and Final State Distributions for He–ICl and He–I₂ Using a Computationally Simple Method *J. Phys. Chem. A* **102**, 9345–9352 (1998). (Special issue in honor of R.D. Levine).
205. E.S. Altshuler, D.L. Mills and R.B. Gerber; Solid and Liquid-like phases of Chemisorbed Hydrogen Monolayers on BCC Metal Surfaces: Structure, Dynamics and Order–Disorder Transitions *Surf. Sci.* **414**, 1–16 (1998).
206. S.K. Gregurick, J.H.-Lin, D.A. Brant and R.B. Gerber; Anharmonic Vibrational Self-Consistent Field Calculations as an Approach to Improving Force Fields for Monosaccharides S.K. Gregurick, J.H.-Y. Lin, D.A. Brant and R.B. Gerber *J. Phys. Chem. B* **103**, 3476–3488 (1999).
207. J.N. Harvey, J.-O. Jung and R.B. Gerber; Ultraviolet Spectroscopy of Water Clusters: Excited Electronic States and Absorption Lineshapes of (H₂O)_n, n = 2–6 *J. Chem. Phys.* (Communication) **109**, 8747–8750 (1998).
208. S. Broude, J.-O. Jung and R.B. Gerber; Combined Diffusion Quantum Monte Carlo - Vibrational Self-Consistent Field (DQMC-VSCF) Method for Excited Vibrational States of Large Polyatomic Systems *Chem. Phys. Lett.* **299**, 437–442 (1999).
209. D.A. Lidar, D. Thirumalai, R. Elber and R.B. Gerber; Fractal Analysis of Protein Potential Energy Landscapes *Phys. Rev. E* **59**, 2231–2243 (1999).
210. P. Jungwirth and R.B. Gerber; Quantum Molecular Dynamics of Ultrafast Processes in Large Polyatomic Systems *Chem. Rev.* **99**, 1583–1606 (1999).
211. P. Jungwirth, M. Roeselova and R.B. Gerber; Optimal Coordinates for Separable Approximations in Quantum Dynamics of Polyatomic Systems: Coordinate Choice Criteria and Error Estimates *J. Chem. Phys.* **110**, 9833–9841 (1999).
212. R.B. Gerber and J.O. Jung; The Vibrational Self-Consistent Field Approach and Extensions: Method and Applications to Spectroscopy of Large Molecules and Clusters, in *Computational Molecular Spectroscopy*, edited by P. Jensen and P.R. Bunker (Wiley, Sussex, U.K.) pp. 365–390.
213. J. Wilkie, M.A. Ratner and R.B. Gerber; A Jastrow Corrected Time Dependent Self-Consistent Field Approximation *J. Chem. Phys.* **110**, 7610–7621 (1999).
214. M.Y. Niv, A.I. Krylov, R.B. Gerber and U. Buck; Photodissociation of HCl Adsorbed on the Surface of a Cluster: Nonadiabatic Molecular Dynamics Simulations *J. Chem. Phys.* **110**, 11047–11053 (1999).
215. G.M. Chaban, J.O. Jung and R.B. Gerber; Ab Initio Calculation of Anharmonic Vibrational States of Polyatomic Systems: Electronic Structure Combined with Vibrational SCF, *J. Chem. Phys.* **111**, 1823–1829 (1999).
216. J. Bruderemann, U. Buck, E. Fredj, R.B. Gerber and M.A. Ratner; Vibrational Excitation in He + (H₂O)₁₁ Collisions: Quantum Calculations and Experiment *J. Chem. Phys.* **111**, 10069–10070 (1999).
217. N.J. Wright and R.B. Gerber; Direct Calculations of Anharmonic Vibrational States of Polyatomic Molecules Using Potential Energy Surfaces Calculated from Density Functional Theory, *J. Chem. Phys.* **112**, 2598–2604 (2000).
218. G.M. Chaban, J.O. Jung and R.B. Gerber; Anharmonic Vibrational Spectroscopy of Hydrogen-Bonded Systems Directly Computed from ab initio Potential Surfaces: (H₂O)_n, n = 2,3; Cl⁻(H₂O)_n, n = 1,2; H⁺(H₂O)_n, n = 1,2; H₂O–CH₃OH *J. Phys. Chem. A* **104**, 2772–2779 (2000).
219. E.M. Knipping, M.J. Lakin, K.L. Foster, P. Jungwirth, D.J. Tobias, R.B. Gerber, D. Dabdub and B.J. Finlayson-Pitts; Experiments and Molecular Dynamics Kinetics Simulations of Ion-Enhanced Interfacial Chemistry on Aqueous NaCl Aerosols *Science* **288**, 301–306 (2000).
220. R. Baumfalk, N.H. Nahler, U. Buck, M.Y. Niv and R.B. Gerber; Photodissociation of HBr adsorbed on the Surface and Embedded in Large Clusters *J. Chem. Phys.* **113**, 329–338 (2000).
221. J. Lundell, M. Pettersson, L. Khriachtchev, M. Rasanen, G.M. Chaban and R.B. Gerber; Infrared Spectrum of HXeI Revisited: Anharmonic Vibrational Calculations and Matrix Isolation Experiments *Chem. Phys. Lett.* **322**, 389–394 (2000).
222. N.J. Wright, R.B. Gerber and D.J. Tozer; Direct Calculation of Anharmonic Vibrational States of Polyatomic Molecules Using Density Functional Theory: Spectroscopic Tests of Recently Developed Functionals *Chem. Phys. Lett.* **324**, 206–212 (2000).
223. D. Chase, M. Manning, J.A. Morgan, G.M. Nathanson and R.B. Gerber; Argon Scattering from Liquid Indium: Simulations with Embedded Atom Potentials and Experiment *J. Chem. Phys.* **113**, 9279–9287 (2000).
224. R.B. Gerber, M. Korolkov, J. Manz, M.Y. Niv and B. Schmidt; A Reflection Principle for the Control of Molecular Photodissociation in Solids: Model Simulations for F₂ in Ar *Chem. Phys. Lett.* **327**, 76–84 (2000).
225. J. Lundell, G.M. Chaban and R.B. Gerber; Anharmonic Vibrational Spectroscopy Calculations for Novel Rare-Gas Containing Compounds: HXeH, HXeCl, HXeBr, and HXeOH, *J. Phys. Chem. A* **104**, 7944–7952 (2000).
226. E.S. Altshuler, D.L. Mills and R.B. Gerber; Simulation of Hydrogen Diffusion on BCC Metal (110) Surfaces: Coverage and Temperature Dependence *Surf. Sci.* **452**, 95–107 (2000).
227. M.Y. Niv, M. Bargheer and R.B. Gerber; Photodissociation and Recombination of F₂ Molecules in Ar₅₄ Clusters: Nonadiabatic Molecular Dynamics Simulations *J. Chem. Phys.* **113**, 6660–6672 (2000).
228. G.M. Chaban, J.O. Jung and R.B. Gerber; The Anharmonic Vibrational Spectroscopy of Glycine: Testing of Ab Initio and Empirical Potentials *J. Phys. Chem. A* **104**, 10035–10044 (2000).
229. J. Lundell, G.M. Chaban and R.B. Gerber; Combined Ab Initio and Anharmonic Vibrational Spectroscopy Calculations for Rare-Gas Containing Fluorohydrides HRgF, *Chem. Phys. Lett.* **331**, 308–316 (2000).
230. A. Cohen, M.Y. Niv and R.B. Gerber; Formation of Novel Rare-Gas Containing Molecules by Molecular Photodissociation in Clusters *Faraday Discuss. Chem. Soc.* **118**, 269–280 (2001).
231. G.M. Chaban, R.B. Gerber, M.V. Korokolov, J. Manz, M.Y. Niv and B. Schmidt; Photodissociation Dynamics of Molecular Fluorine in an argon Matrix Induced by Ultrashort Laser Pulses *J. Phys. Chem. A* (Issue in honor of W.H. Miller) **105**, 2770–2782 (2001).
232. N.J. Wright and R.B. Gerber; Extending the Vibrational Self-Consistent Field Method: Using a Partially Separable Wave Function for Calculating Anharmonic Vibrational States of Polyatomic Molecules *J. Chem. Phys.* **114**, 8763–8768 (2001).
233. G.M. Chaban and R.B. Gerber; Anharmonic Vibrational Spectroscopy of the Glycine-Water Complex: Calculations for Ab Initio, Empirical and Hybrid (QM/HM) Potentials, *J. Chem. Phys.* **115**, 1340–1348 (2001).

234. Z. Bihary, R.B. Gerber and V.A. Apkarian; Vibrational Self-Consistent Field Approach to Anharmonic Spectroscopy of Molecules in Solids: Application to Iodine in Argon Matrix, *J. Chem. Phys.* **115**, 2695–2701 (2001).
235. G.M. Chaban, R.B. Gerber and K.C. Janda; The Transition from Hydrogen Bonding to Ionization in Clusters: Consequences for Anharmonic Vibrational Spectroscopy *J. Phys. Chem. A* **105**, 8223–8332 (2001).
236. Z. Bihary, M. Karavitis, R.B. Gerber and V.A. Apkarian; Spectral Inhomogeneity Induced by Vacancies and Thermal Phonons and Associated Observables in Time- and Frequency Domain Nonlinear Spectroscopy: I₂ Isolated in Argon Matrix *J. Chem. Phys.* **115**, 8006–8013 (2001).
237. G.M. Chaban, J. Lundell and R.B. Gerber; Lifetime and Decomposition Pathways of a Chemically Bound Helium Compound *J. Chem. Phys.* (Communication) **115**, 7343–7344 (2001).
238. G.M. Chaban and R.B. Gerber; Ab Initio Calculations of Anharmonic Vibrational Spectroscopy for Hydrogen Fluoride (HF)_n ($n = 3,4$), and Mixed Hydrogen-Fluoride/Water (HF)_n(H₂O)_n ($n = 1,2,4$) Clusters *Spectrochim. Acta* (Special Issue on Vibrational Spectroscopy) **58**, 887–898 (2002).
239. M. Pettersson, L. Khriachtchev, A. Lignell, M. Rasanen, Z. Bihary and R.B. Gerber; HKrF in Solid Krypton *J. Chem. Phys.* **116**, 2508–2515 (2002).
240. Z. Bihary, G.M. Chaban and R.B. Gerber; Vibrational Spectroscopy and Matrix-Site Geometries of HArF, HKrF, HXeCl and HXeI in Rare-Gas Solids *J. Chem. Phys.* **116**, 5521–5529 (2002).
241. H. Yang, N.J. Wright, A.M. Gagnon, R.B. Gerber and B.J. Finlayson-Pitts; An Upper Limit to the Concentration of An Complex at the Air–Water Interface at 298K: Infrared Experiments and Ab Initio Calculations *Phys. Chem. Chem. Phys.* **4**, 1832–1838 (2002).
242. N. Matsunaga, G.M. Chaban and R.B. Gerber; Degenerate Perturbation Theory Corrections for the Vibrational Self-Consistent Field Approximations: Method and Applications *J. Chem. Phys.* **117**, 3541–3547 (2002).
243. S.K. Gregurick, G.M. Chaban and R.B. Gerber; An Initio and Improved Empirical Potentials for the Calculation of the Anharmonic Vibrational States and Intramolecular Couplings of N-Methylacetamide *J. Phys. Chem. A* **106**, 8696–8707 (2002).
244. Z. Bihary, G.M. Chaban and R.B. Gerber; Stability of a Chemically Bound Helium Compound in High-Pressure Solid Helium *J. Chem. Phys.* (Communication) **117**, 5105–5108 (2002).
245. M. Bargheer, M.Y. Niv, R.B. Gerber and N. Schwentner; Ultrafast Solvent-Induced Spin-Flip and Non-Adiabatic Coupling: ClF in Argon Solids *Phys. Rev. Lett.* **89**, 108301/1–4 (2002).
246. G.M. Chaban, J. Lundell and R.B. Gerber; Theoretical Study of Decomposition Pathways for HArF and HKrF *Chem. Phys. Lett.* **364**, 628–633 (2002).
247. M. Bargheer, R.B. Gerber, M.V. Korolkov, O. Kuhn, J. Manz, M. Schroder and N. Schwentner; Subpicosecond Spin-Flip Induced by the Photodissociation Dynamics of ClF in an Ar Matrix *Phys. Chem. Chem. Phys.* **4**, 5554–5562 (2002).
248. R.B. Gerber, B. Brauer, S.K. Gregurick and G.M. Chaban; Calculation of Anharmonic Vibrational Spectroscopy of Small Biological Molecules *Phys. Chem. Comm.* **5**, 142–150 (2002).
249. R.B. Gerber, G.M. Chaban, S.K. Gregurick and B. Brauer; Vibrational Spectroscopy and the Development of New Force Fields for Biological Molecules, *Biopolymers* **68**, 370–382 (2003). (Special Issue in Memory of S. Lifson).
250. J. Lundell, A. Cohen and R.B. Gerber; Quantum Chemical Calculations on Novel Molecules from Xenon Insertion into Hydrocarbons *J. Phys. Chem. A* **106**, 11950–11955 (2002).
251. P. Jungwirth, R.B. Gerber and M.A. Ratner; Quantum Simulations of Vibrational Dephasing of Molecules in a Cryogenic Environment: HArF in an Ar Cluster, *Isr. J. Chem.* (Topical Issue on Quantum Dynamics) **42**, 157–162 (2002).
252. L. Khriachtchev, H. Tanskanen, A. Cohen, R.B. Gerber, J. Lundell, M. Pettersson, H. Kiljunen and M. Rasanen; A Gate to Organokrypton Chemistry: HKrCCH, *J. Am. Chem. Soc.* (Communication) **125**, 6876–6877 (2003).
253. N.H. Nahler, R. Baumfalk, U. Buck, Z. Bihary, R.B. Gerber and B. Friedrich; Photodissociation of Oriented HXeI Molecules Generated from HI–Xe_n Clusters *J. Chem. Phys.* **119**, 224–231 (2003).
254. G.M. Chaban, S.S. Xantheas and R.B. Gerber; Anharmonic Vibrational Spectroscopy of the F[−](H₂O)_n Complexes, $n = 1,2$ *J. Phys. Chem. A* **107**, 4952 (2003).
255. M. Roeselova, P. Jungwirth, D.J. Tobias and R.B. Gerber; Impact, Trapping and Accommodation of Hydroxyl Radical and Ozone at Aqueous Salt Aerosol Surfaces: A Molecules Dynamics Study *J. Phys. Chem. B* **107**, 12690–12699 (2003).
256. Z. Bihary, G.M. Chaban and R.B. Gerber; Delayed Formation Dynamics of HArF and HKrF in Rare-Gas Matrices *J. Chem. Phys.* **119**, 11278–11284 (2003).
257. A. Cohen, J. Lundell and R.B. Gerber; First Compounds with Argon–Carbon and Argon–Silicon Chemical Bonds *J. Chem. Phys.* (Communication) **119**, 6415–6418 (2003).
258. R.B. Gerber; Formation of Novel Rare-Gas Molecules in Low-Temperature Matrices *Ann. Rev. Phys. Chem.* **55**, 55–78 (2004).
259. Y. Miller, E. Fredj, J.N. Harvey and R.B. Gerber; UV Spectroscopy of Large Water Clusters: Model Calculations for (H₂O)_n, $n = 8,11,20,40,50$ *J. Phys. Chem. A* **108**, 4405–4411 (2004).
260. B. Brauer, G.M. Chaban and R.B. Gerber; Spectroscopically-Tested, Improved Semi-Empirical Potentials for Biological Molecules: Calculations for Glycine, Alanine and Proline *Phys. Chem. Chem. Phys.* **6**, 2543–2556 (2004).
261. N.H. Nahler, M. Farnik, U. Buck, H. Vach and R.B. Gerber; Photodissociation of HCl and Small (HCl)_m Complexes In and On Large Ar Clusters *J. Chem. Phys.* **121**, 1293–1299 (2004).
262. R.B. Gerber, G.M. Chaban, B. Brauer and Y. Miller; First Principles Calculations of Anharmonic Vibrational Spectroscopy of Large Molecules in: *Theory and Applications of Computational Chemistry: The First 40 Years*, edited by C.E. Dykstra, G. Frenking, K.S. Kim and G.E. Scuseria (Elsevier, Holland 2005) Chapter 9 (pp. 165–193).
263. C.A. Brindle, G.M. Chaban, R.B. Gerber and J.C. Janda; Anharmonic Vibrational Spectroscopy Calculations for (NH₃)(HF) and (NH₃)(DF): Fundamental, Overtone and Combination Transitions *Phys. Chem. Chem. Phys.* **7**, 945–754 (2005).
264. D. Shemesh, G.M. Chaban and R.B. Gerber; Photoionization of Glycine: The First Ten Picoseconds *J. Phys. Chem. A* **108**, 11477–11484 (2004).
265. Y. Miller, G.M. Chaban and R.B. Gerber; Theoretical Study of Anharmonic Vibrational Spectra of HNO₃,

HNO₃-H₂O, HNO₄: Fundamental, Overtone and Combination Excitations *Chem. Phys.* **313**, 213–224 (2005).

266. D. Shemesh, R. Baer, T. Seideman and R.B. Gerber; Photoionization Dynamics of Glycine Adsorbed on a Silicon Cluster: “On-the-Fly” Simulations *J. Chem. Phys.* **122**, 184704 (2005).

267. E.C. Brown, A. Cohen and R.B. Gerber; Prediction of a Linear Polymer Made of Xenon and Carbon *J. Chem. Phys.* (Communication) **122**, 171101/1–4 (2005).

268. A. Adesokan, E. Fredj, E.C. Brown and R.B. Gerber; Anharmonic Vibrational Spectroscopy Calculations of 5,6 Dihydrouracil and its Complex with Water *Mol. Phys.* (Special Issue in honor of J.P. Simons) **103**, 1505–1520 (2005).

269. R.B. Gerber; New Chemistry of the Noble Gas Elements: Novel Molecules, Polymers and Crystals *Bull. Isr. Chem. Soc.* **18**, 7–14 (2005).

270. D. Shemesh and R.B. Gerber; Different Chemical Dynamics for Different Conformers of Biological Molecules: Photoionization of Glycine *J. Chem. Phys.* (Communication) **122**, 241104/1–4 (2005).

271. Y. Miller, G.M. Chaban and R.B. Gerber; Ab Initio Vibrational Calculations for H₂SO₄ and H₂SO₄-H₂O: Spectroscopy and the Nature of the Anharmonic Couplings *J. Phys. Chem. A* **109**, 6565–6574 (2005).

272. B. Brauer, R.B. Gerber, M. Kabelac, P. Hobza, J.M. Bakker, A.G. Abo Rizik and M.S. de Vries; Vibrational Spectroscopy of the G•••C Base Pair: Experiment, Harmonic and Anharmonic Calculations and the Nature of the Anharmonic Couplings *J. Phys. Chem. A* **109**, 6974–6984 (2005).

273. Y. Miller, G.M. Chaban, B.J. Finlayson-Pitts and R.B. Gerber; Photochemical Processes Induced by Vibrational Overtone Excitations: Dynamics Simulations for cis-HONO, trans-HONO, HNO₃ and HNO₃-H₂O *J. Phys. Chem. A* **110**, 5342–5354 (2006). (Special issue in the honor of J.C. Light).

274. K.A. Ramazan, L.M. Wingen, Y. Miller, G.M. Chaban, R.B. Gerber, S.S. Xantheas and B.J. Finlayson-Pitts; A New Experimental and Theoretical Approach to the Heterogeneous Hydrolysis of NO₂: The Key Role of Molecular Nitric Acid and Its Complexes with Water *J. Phys. Chem. A* **110**, 6886–6897 (2006). (Special issue in honor of D. Golden).

275. D. Shemesh and R.B. Gerber; Classical Trajectory Simulations of Photoionization Dynamics of Tryptophan: Intramolecular Energy Flow, Hydrogen-Transfer Processes and Conformational Transitions *J. Phys. Chem. A* **110**, 8401–8408 (2006) (Special issue in memory of C. Lifshitz).

276. D. Shemesh and R.B. Gerber; Dynamical Simulations of Photoionization of Small Biological Molecules In: *Principles of Mass Spectrometry Applied to Biomolecules*, Edited by C. Lifshitz and J. Laskin (Wiley Interscience, New York 2006). Chapter 6, pp. 213–237.

277. R.B. Gerber; La Surprenante Chimie des Gaz Inertes (in French) *Pour la Science*, March 2006 issue, pp. 68–74.

278. L. Pele, B. Brauer and R.B. Gerber; Acceleration of Correlation-Corrected Vibrational Self-Consistent Field (CC-VSCF) Calculation Times for Large Polyatomic Molecules *Theor. Chem. Acc.* **117**, 69–72 (2007).

279. L. Sheng, A. Cohen and R.B. Gerber; Theoretical Prediction of Chemically-Bound Compounds Made of Argon and Hydrocarbons *J. Am. Chem. Soc.* (Communication) **128**, 7156–7157 (2006).

280. L. Sheng and R.B. Gerber; High Coordination Chemically Bound Compounds of Noble Gases with Hydrocarbons: Ng(CCH)₄ and Ng(CCH)₆, (Ng = Xe or Kr) *J. Chem. Phys.* (Communication) **124**, 231103/1–3 (2006).

281. Y. Miller and R.B. Gerber; Dynamics of Vibrational Overtone Excitations of H₂SO₄, H₂SO₄-H₂O: Hydrogen-Hopping and Photodissociation Processes *J. Am. Chem. Soc.* (Communication) **128**, 9594–9595 (2006).

282. T. Ansbacher and R.B. Gerber; New Organic Noble Molecules: Energetics, Stability and Potential Energy Surfaces of HCCXeCCH and HCCKrCCH *Phys. Chem. Chem. Phys.* **8**, 4175–4181 (2006).

283. H. Eshet, M.A. Ratner and R.B. Gerber; Selective Energy and phase Transfer in the Photodissociation of I₂ in Argon Clusters: Quantum Dynamics Simulations *Chem. Phys. Lett.* **431**, 199–203 (2006).

284. E. Segev, M. Grumbach and R.B. Gerber; Evolution of Conformational Changes in the Dynamics of Small Biological Molecules: A Hybrid MD/RRK Approach *Phys. Chem. Chem. Phys.* **8**, 4915–4923 (cover article) (2006).

285. L. Sheng and R.B. Gerber; Stability and Structure of Oligomers and Polymers Made of Xenon and Hydrocarbons: Theoretical Predictions *J. Chem. Phys.* (Communication) **125**, 201101/1–3 (2006).

286. L. Sheng and R.B. Gerber; Predicted Stability and Structure of (HXeCCH)_n (n = 2 or 4) Clusters and of Crystalline HXeCCH *J. Chem. Phys.* (Communication) **126**, 021108/1–3 (2007).

287. B. Brauer and R.B. Gerber; Complex Systems in the Gas phase: IR Spectroscopy of Gas-Phase Phenylalanine – Anharmonic Calculations in: *Analysis and Control of Ultrafast Photoinduced Reactions*, edited by O. Kühn and L. Wöste, (Springer, Berlin, 2007) Chapter 3.4.4.3, pp. 185–188.

288. A. Borowski, A. Cohen, R.B. Gerber and O. Kühn; Coherence and Control of Molecular Dynamics and Rare Gas Matrices: Interaction Potentials – The Diatomics-in-Molecules Approach in: *Analysis and Control of Ultrafast Photoinduced Reactions*, edited by O. Kühn and L. Wöste, (Springer, Berlin, 2007) Chapter 4.6, pp. 298–304.

289. A. Cohen and R.B. Gerber; Coherence and Control of Molecular Dynamics and Rare Gas Matrices: Semiclassical Simulations of Nonadiabatic Dynamic in: *Analysis and Control of Ultrafast Photoinduced Reactions*, edited by O. Kühn and L. Wöste, (Springer, Berlin, 2007) Chapter 4.8, pp. 310–317.

290. A.A. Adesokan, D. Pan, E. Fredj, R.A. Mathies and R.B. Gerber; Anharmonic Vibrational Calculations Modeling the Raman Spectra of Intermediates in the Photoactive Yellow Protein (PYP) Photocycle *J. Am. Chem. Soc.* **129**, 4584–4594 (2007).

291. D. Schweke, B. Brauer, R.B. Gerber and Y. Haas; The Vibrational Spectra of N-Phenylpyrrol in the Gas phase, in Argon Matrices and in Single Crystals *Chem. Phys.* **333**, 168–178 (2007).

292. G.M. Chaban and R.B. Gerber; Anharmonic Vibrational Spectroscopy Calculations with Electronic Structure Potentials: Comparison of MP2 and DFT for Organic Molecules *Theoret. Chem. Acc.* (Special Issue in Honor of M.S. Gordon) **120**, 273–279 (2008).

293. A.A. Adesokan, G.M. Chaban, O. Dopfer and R.B. Gerber; Vibrational Spectroscopy of Protonated Imidazole and Complexes with Water Molecules: Ab Initio Anharmonic Calculations and Experiments *J. Phys. Chem. A* (Special Issue in Memory of Roger Miller) **111**, 7374–81 (2007).

294. A. Cohen and R.B. Gerber; Photodissociation of F₂ in Solid Ar: Electronic State Distribution in Cage-Exit *Chem. Phys.* (Special Issue in honor of J. Manz) **338**, 200–206 (2007).

295. A. Cohen and R.B. Gerber; A 1 fs Spin-Flip in a Chemical Reaction: Photodissociation of HF in Solid Ar *Chem. Phys. Lett.* **441**, 48–52 (2007).
296. M. Bargheer, A. Cohen, R.B. Gerber, M. Gühr, M.V. Korolkov, J. Manz, M.Y. Niv, M. Schröder and N. Schwentner; Dynamics of Electronic States and Spin-Flip for Photodissociation of Dihalogens in Matrices: Experiment, Semiclassical Surface-Hopping and Quantum Model Simulations for F₂ and ClF in Solid Ar *J. Phys. Chem. A* (Special Issue in honor of H.S. Lin) **111**, 9573–9585 (2007).
297. M.Z. Steinberg, K. Breuker, R. Elber and R.B. Gerber; The Dynamics of Water Evaporation from Partially Solvated Cytochromic c in the Gas phase *Phys. Chem. Chem. Phys.* **9**, 4690–4697 (2007).
298. Y. Miller, R.B. Gerber and V. Vaida; Photodissociation Yields for Vibrationally Excited States of Sulfuric Acid Under Atmospheric Conditions *Geophys. Res. Lett.* **L16829/1–5** (2007).
299. Y. Miller, G.M. Chaban, J. Zhou, K.R. Asmis, D.M. Neumark and R.B. Gerber; Vibrational Spectroscopy of (SO₄²⁻)·(H₂O)_n Clusters, n = 1–5. Harmonic and Anharmonic Calculations and Experiment *J. Chem. Phys.* **127**, Art. No. 094305/1–11 (2007).
300. D. Shemesh, J. Mullin, M.S. Gordon and R.B. Gerber; Vibrational Spectroscopy of Glycine Adsorbed on Silicon Clusters: Harmonic and Anharmonic Calculations for Models of the Si(100)-2 × 1 Surface *Chem. Phys.* (Special Issue in honor of W. Domcke) **347**, 218–228 (2008).
301. G. von Helden, I. Compagnon, H.N. Blom, M. Frankowski, U. Erlekam, J. Oomens, B. Brauer, R.B. Gerber and G. Meijer; Mid-IR Spectra of Different Conformers of Phenylalanine in the Gas phase *Phys. Chem. Chem. Phys.* **10**, 1248–56 (2008).
302. Y. Miller and R.B. Gerber; Dynamics of Proton Recombination with NO₃⁻ Anion in Water Clusters *Phys. Chem. Chem. Phys.* (Communication) **10**, 1091–93 (2008).
303. H.G. Kjaergaard, A.L. Garden, G.M. Chaban, R.B. Gerber, D.A. Matthews and J.F. Stanton; Calculations of Vibrational Transition Frequencies and Intensities in Water Dimer: Comparison of Different Vibrational Approaches *J. Phys. Chem. A* **112**, 4324–35 (2008).
304. L. Khriachtchev, K. Isokaski, A. Cohen, M. Räsänen and R.B. Gerber; A Small Neutral Molecule with Two Noble Gas Atoms: HXeOXeOH *J. Am. Chem. Soc.* **130**, 6114–6118 (2008).
305. I. Wolf, A. Shapira, R. Giniger, Y. Miller, R.B. Gerber and O. Chesnovsky; Critical Size for Intra-Cluster Proton Transfer to an Anion *Angew. Chem. Int. Ed.* **47**, 6272–4 (2008).
306. A. Cohen and R.B. Gerber; Dynamical u↔g Electronic State Transition in Matrix Photochemistry: Photodissociation of F₂ in Solid Ar *Chem. Phys. Lett.* **453**, 173–77 (2008).
307. L. Pele and R.B. Gerber; On the Number of Significant Mode–Mode Anharmonic Couplings in Vibrational Calculations: CC-VSCF Treatment of Di-, Tri- and Tetra-Peptides *J. Chem. Phys.* Art. No. 165105/1–10 (2008).
308. E. Segev, T. Wyttenbach, M.T. Bowers and R.B. Gerber; Conformational Evolution of Ubiquitin Ions in Electrospray Mass Spectrometry: Molecular Dynamics Simulations at Gradually Increasing Temperatures *Phys. Chem. Chem. Phys.* **10**, 3077–83 (2008).
309. B. Brauer, F. Dubnikova, Y. Zeiri, R. Kosloff and R.B. Gerber; Vibrational Spectroscopy of Triacetone Triperoxide (TATP): Anharmonic Fundamental, Overtones and Combination Bands *Spectrochim. Acta, Part A* **71**, 1438–1445 (2008).
310. E. Tsvivon, S. Zilberg and R.B. Gerber; Predicted Stability of the Organo-Xenon Compound HXeCCH Above the Cryogenic Range *Chem. Phys. Lett.* **460**, 23–26 (2008).
311. M.Z. Steinberg, R. Elber, F.W. McLafferty, R.B. Gerber and K. Breuker; Early Structural Evolution of Native Cytochrome C After Solvent Removal *Chem. Bio. Chem.* **9**, 2417–23 (2008).
312. L. Khriachtchev, M. Räsänen and R.B. Gerber; Noble-Gas Hydrides: New Chemistry at Low Temperatures *Accs. Chem. Res.* **42**, 183–191 (2009).
313. M.A. Kamboures, J.D. Raff, Y. Miller, L.F. Philips, B.J. Finlayson-Pitts and R.B. Gerber; Complexes of HNO₃ and NO₃⁻ with NO₂ and N₂O₄ and Their Potential Role in Atmospheric HONO Formation *Phys. Chem. Chem. Phys.* **10**, 6012–32 (2008).
314. M.A. Kamboures, W. van der Veer, R.B. Gerber and L.F. Philips; Raman Spectra of Complexes of HNO₃ and NO₃⁻ with NO₂ at Surfaces with N₂O₄ in Solution *Phys. Chem. Chem. Phys.* **10**, 4748–53 (2008).
315. A.A. Adesokan and R.B. Gerber; Anharmonic Vibrational Spectroscopy Calculations for Proton-Bound Amino Acid Dimers *J. Phys. Chem. A* (Festschrift for M. Wolfsberg) **113**, 1905–12 (2009).
316. O. Link, E. Vöhringer-Martinez, E. Lungovoj, X. Liu, K. Seifermann, M. Faubel, H. Grubmüller, R.B. Gerber, Y. Miller and B. Abel; Ultrafast phase Transitions in Metastable Water Near Liquid Interfaces *Faraday Discuss.* **141**, (in press).
317. Y. Miller, B.J. Finlayson-Pitts and R.B. Gerber; Ionization of N₂O₄ in Contact with Water: Mechanisms, Timescales and Atmospheric Implications *J. Am. Chem. Soc.* (in press).
318. R.B. Gerber and J. Sebek; Dynamics Simulations of Atmospherically-Relevant Molecular Reactions *Inter. Revs. Phys. Chem.* (in press).