

## 1960 – 1970

1. "Kinetics of the Reaction between Titanium (III) and Mercury (II) in Aqueous Hydrochloric Acid Solutions," S.H. Lin and K. Pan, *J. Chinese Chem. Soc.*, **6**, No. 2, 96 (1960).
2. "Kinetics of the Oxidation of Hypophosphorous Acid by Chromate," K. Pan and S.H. Lin, *J. Chinese Chem. Soc.*, **7**, No. 2, 75 (1960).
3. "Spectrophotometric Study of the Complexes of Ge, Zr and Hf with Gallein," K. Pan, S.H. Lin, Y.L. Wu and Y.M. Chen, *J. Chinese Chem. Soc.*, **10**, 24 (1962).
4. "Improved Calculation of Quasiequilibrium Rate Constants," S.H. Lin and H. Eyring, *J. Chem. Physics*, **39**, No. 6, 1577 (1963).
5. "Thermal Conductivity of Liquids," S.H. Lin, H. Eyring and W.J. Davis, *J. Phys. Chem.*, **68**, 3017 (1964).
6. "The Law of Mass Action and Absolute Reaction Rate Theory," H. Eyring and S.H. Lin, *The Law of Mass Action, Centenary Volume*, Oslo, 117 (1964).
7. "Magnet-optical Rotation of Transition Metal Complexes," S.H. Lin and H. Eyring, *J. Chem. Physics*, **42**, No. 5, 1780 (1965).
8. "Calculation of Statistical Complexions of Harmonic Oscillators," S.H. Lin and H. Eyring, *J. Chem. Physics*, **43**, 2153 (1965).
9. "Crystal and Black-body Radiation," S.H. Lin, In: *Advanced Physical Chemistry*, **Vol. II**, H. Eyring, et al., eds. (New York: Academic Press), Chap. 3 (1966).
10. "Some Properties of Quintet State Carbon Atom," S.H. Lin, *J. Chem. Physics*, **44**, No. 7, 2810 (1966).
11. "Rate of Intercoversion of Electronic and Vibrational Energy," S.H. Lin, *J. Chem. Physics*, **44**, No. 10, 3759 (1966).
12. "Effect of Radiation Damping on Dispersion," S.H. Lin and R. Bersohn, *J. Chem. Physics*, **44**, No. 10, 3768 (1966).
13. "The Dispersion of Electric Birefringence," S.H. Lin, C.Y. Lin and H. Eyring, *J. Phys. Chem.*, **70**, 1756 (1966).
14. "Calculation of the Lifetime of the  $^4\pi$  State of NO," S.H. Lin, *J. Chem. Phys.*, **46**, 279 (1967).
15. "Refined Treatment of Nuclear Magnetic Shielding," S.H. Lin, *Mol. Phys.*, **12**, 91 (1967).

16. "Study of Non-Adiabatic Transitions with Application to NO," S.H. Lin, *Theor. Chim. Acta*, **8**, 1 (1967).
17. "Calculation of Anisotropic Excitation Cross Sections and Polarization of Impact Radiation of He Atoms Induced by Electron and Proton Impacts," S.H. Lin, *J. Chem. Physics*, **48**, No. 7, 3125 (1968).
18. "Spectral Band Shape of Absorption and Emission of Molecules in Dense Media," S.H. Lin, *Theor. Chim. Acta, (Berl.)*, **10**, 310 (1968).
19. "Effect of Partial Deuteration and Temperature on Triplet-State Lifetimes," S.H. Lin and R. Bersohn, *J. Chem. Physics*, **48**, 6, 2732 (1968).
20. "Computation of Statistical Complexions by the Method of Steepest Descent," J.C. Tou and S.H. Lin, *J. Chem. Physics*, **49**, 9, 4187 (1968).
21. "Calculations of Anisotropic Photoionization Cross Sections. I. Hydrogen Atom," S.H. Lin, *Can. J. Phys.*, **46**, 24, 2719 (1968).
22. "Significant Structure Theory of Liquids Applied to the Shock Compression of Argon," S.H. Lin, D. Tweed and H. Eyring, *Proc. Natl. Acad. Sci. U.S.*, **61**, 1171 (1968).
23. "Exact Solution of an Electron Trapped in a Spherical Cavity and Applications to the F Center in Alkali Halides," J. D. Zahrt and S.H. Lin, *Theoret. Chim. Acta*, **12**, 256 (1968).
24. "Orientation of Target Molecules by Beam Excitation," R. Bersohn and S.H. Lin, *Adv. Chem. Phys.*, **16**, 67 (1969).
25. "Optical Absorption Spectra of the Ordered Phases in the Praseodymium Oxide-Oxygen System," J.M. Warmkessel, S.H. Lin and L. Eyring, *Inorg. Chem.*, **8**, 875 (1969).
26. "The Heavy Atom Effect on the Phosphorescence of Aromatic Hydrocarbons. I," S.H. Lin and D. Tweed, *Intern. J. Quantum Chem.*, **3S**, 315 (1969).
27. "Quenching of Phosphorescence by Paramagnetic Molecules in Rigid Media I," C.O. Hill and S.H. Lin, *Intern. J. Quantum Chem.*, **3S**, 307 (1969).
28. "Hydrogen Bonding," S.H. Lin, In: *Advanced Physical Chemistry*, **Vol. V**, H. Eyring, et al., eds. (New York: Academic Press), p 439 (1970).
29. "Kinetics of Heterogeneous Chemical Reactions. II," S.H. Lin and H. Eyring, *Proc. Natl. Acad. Sci. U.S.A.*, **62**, 156 (1970).

30. "Effect of Partial Deuteration of Triplet-state Lifetimes," S.H. Lin, *Trans. Faraday Soc.*, **66**, 1879 (1970).
31. "Quenching of Phosphorescence of Paramagnetic Molecules in Rigid Media. II. Quenching of Perdeuterated Naphthalene by  $\text{CO}^{++}$ ,  $\text{Cr}^{+3}$ ,  $\text{Cu}^{++}$ , and  $\text{Ni}^{++}$ ," C.O. Hill and S.H. Lin, *J. Chem. Phys.*, **53**, 608 (1970).
32. "Detonation," S.H. Lin and H. Eyring, *Ann. Rev. Phys. Chem.*, **21**, 225 (1970).
33. "The Energy Gap Law and Franck-Condon Factor in Radiationless Transitions," S.H. Lin, *J. Chem. Phys.*, **53**, 3766 (1970).
34. "The Heavy Atom Effect on the Phosphorescence of Aromatic Hydrocarbons. II. Quenching of Perdeuterated Naphthalene by Alkali Halides," R.H. Hofeldt, R. Sahai and S.H. Lin, *J. Chem. Phys.*, **53**, 4512 (1970).
35. "The Activated Complex in Some High Temperature Heterogeneous Reactions," H. Eyring and S.H. Lin, In: *International Conference on Heterogeneous Kinetics of Elevated Temperature (New York: Plenum Press)*, p1 (1970).
36. "The Study of Hysteresis in the High Order Phase Transitions," S.H. Lin, In: *The Chemistry of Extended Defects in Non-metallic Solids*, L. Eyring and M. O'Keefe, eds. (Amsterdam: North-Holland), p 444 (1970).

## 1970 – 1980

37. "Calculation of the Energy Density Function by the Method of Steepest-Descent," S.H. Lin, *Mol. Phys.*, **20**, 953 (1971).
38. "Calculation of Statistical Complexions of Polyatomic Molecules and Ions," S.H. Lin and C.Y. Lin Ma, *Adv. Chem. Phys.*, **21**, 143 (1971).
39. "Calculation of the Reaction Cross Section from a Rate Constant by the Method of Steepest-Descent," S.H. Lin and H. Eyring, *Proc. Natl. Acad. Sci. U.S.A.*, **68**, 402 (1971).
40. "Scattering and Capturing by Inverse Fourth Power Potential in Low Energy Range," J.A. Coombs and S. H. Lin, *J. Chem. Phys.*, **54**, 2285 (1971).
41. "Kinetics of Heterogeneous Chemical Reactions III. A Theoretical Model of Pesticide Accumulation in Soil," S. H. Lin, R. Sahai and H. Eyring, *Proc. Natl. Acad. Sci. U.S.A.*, **68**, 777 (1971).

42. "Band Shape of Optical Rotatory Dispersion," S.H. Lin, *J. Chem. Phys.*, **54**, 1177 (1971).
43. "Computation of the Statistical Complexions of Molecules and Ions," K.H. Lau and S.H. Lin, *J. Chem. Phys.*, **75**, 981 (1971).
44. "The Heavy Atom Effect on the Phosphorescence of Aromatic Hydrocarbons. III. Quenching of C<sub>6</sub>D<sub>6</sub> by Alkali Halides," R. Sahai, R.H. Hofeldt and S.H. Lin, *Trans. Faraday Soc.*, **67**, 1 (1971).
45. "Solution of the Time-dependent Schrödinger Equation by the Laplace Transform Method," S.H. Lin and H. Eyring, *Proc. Natl. Acad. Sci. U.S.A.*, **68**, 76 (1971).
46. "Application of the Method of Steepest-Descent to the Calculation of the Translational Energy of Fragments of Ion Decomposition," S.H. Lin, *J. Phys. Chem.*, **75**, 2548 (1971).
47. "A PMR Investigation of Some Weak Interactions between C<sub>10</sub>H<sub>8</sub> and Alkyl Iodides-in CCl<sub>4</sub>," R. Sahai and S. H. Lin, *J. Chem.*, **49**, 1771 (1971).
48. "Theoretical Calculation of External Heavy-Atom Effect on the Spin-Orbit Coupling of Benzene Molecules," K.C. Lin and S.H. Lin, *Mol. Phys.*, **21**, 1105 (1971).
49. "Theory of Thermal Delayed Fluorescence," S.H. Lin, *Theor. Chim. Acta*, **23**, 98 (1971).
50. "Calculation of Potential Energy Surfaces of Reactions between Halogen Atoms and Halogen Molecules," H. Eyring, L. Dalla Riva and S.H. Lin, In: *Schumacher Volume, 'Anales, Asoc. Quim. Argentina*, **59**, 133 (1971).
51. "Spectral Band Shape and Absorption Coefficients of Electronic Transitions," C.O. Hill and S.H. Lin, *Trans. Faraday Soc.*, **67**, 2833 (1971).
52. "Absolute Reaction Rate Constants and Chemical Reaction Cross Sections of Bimolecular Reactions," S.H. Lin, K.H. Lau and H. Eyring, *J. Chem. Phys.*, **55**, 5657 (1971).
53. "Angular Distribution of Products from Photodissociation of Diatomic Molecules," S.H. Lin and C.J. Koizumi, *Can. J. Phys.*, **49**, 2425 (1971).
54. "Calculation of Chemical Reaction Cross Sections in Truncated Rotator-Oscillator Approximation," S.H. Lin, *Mol. Phys.*, **22**, 375 (1971).
55. "Isotope Effect, Energy Gap Law and Temperature Effect in Resonance Energy Transfer," S.H. Lin, *Mol. Phys.*, **21**, 853 (1971).
56. "Band Shape of Circular Dichroism," S.H. Lin, *J. Chem. Phys.*, **55**, 3546 (1971).

57. "Theoretical Analysis of Emission Spectra of Electronic Transitions of Molecules in Dense Media," S.H. Lin, L. Colangelo and H. Eyring, *Proc. Natl. Acad. Sci. U.S.A.*, **68**, 2135 (1971).
58. "Temperature Effect on Radiationless Transitions," S.H. Lin, *J. Chem. Phys.*, **56**, 2645 (1972).
59. "Stochastic Model of Molecular Luminescence," S.H. Lin, *J. Chem. Phys.*, **56**, 1972 (1972).
60. "Potential Energy Surfaces and Reaction Rates," H. Eyring and S.H. Lin, In: *International Conference on Potential Energy Surfaces*, Santa Cruz, p 150 (1970).
61. "Stochastic Model of Unimolecular Reactions and the RRKM Theory," S.H. Lin, K.H. Lau, W. Richardson, L. Volk and H. Eyring, *Proc. Natl. Acad. Sci. U.S.A.*, **69**, 2778 (1972).
62. "Magnetic Circular Dichroism of Molecules in Dense Media II. Benzene," D. J. Shieh, S.H. Lin and H. Eyring, *Proc. Natl. Acad. Sci. U.S.A.*, **69**, 2000 (1972).
63. "Magnetic Circular Dichroism of Molecules in Dense Media I. Theory," D. J. Shieh, S.H. Lin and H. Eyring, *J. Phys. Chem.*, **76**, 1844 (1972).
64. "Quantum Statistical Theory of Rate Processes," S.H. Lin and H. Eyring, *Proc. Natl. Acad. Sci. U.S.A.*, **69**, 3192 (1972).
65. "Magnetic Circular Dichroism of Molecules in Dense Media III. Substituted Benzenes," D. J. Shieh, S.H. Lin and H. Eyring, *J. Phys. Chem.*, **77**, 1031 (1973).
66. "Application of the Singular Perturbation Method to Reaction Kinetics," W. Richardson, L. Volk, K.H. Lau, S.H. Lin and H. Eyring, *Proc. Natl. Acad. Sci. U.S.A.*, **70**, 1588 (1973).
67. "Radiationless Transitions in Isolated Molecules," S.H. Lin, *J. Chem. Phys.*, **58**, 5760 (1973).
68. "Absolute Reaction Rate Constants and Chemical Reaction Cross Sections for Bimolecular Reactions. II. Numerical Results," K.H. Lau, S.H. Lin and H. Eyring, *J. Chem. Phys.*, **58**, 1261 (1973).
69. "Radiative Lifetimes of Single Vibronic States," G.R. Fleming, O.L.J. Gijzeman and S.H. Lin, *Chem. Phys. Lett.*, **21**, 527 (1973).
70. "On the Theory of Non-radiative Energy Transfer of Electronic Excitation," S.H. Lin, *Proc. Roy. Soc.*, **335A**, 51 (1973).

71. "Effect of High Pressures on Molecular Electronic Spectra and Electronic Relaxation," S.H. Lin, *J. Chem. Phys.*, **59**, 4458 (1973).
72. "Potential Energy Surfaces," S.H. Lin and H. Eyring, In: *Physical Chemistry: An Advanced Treatise*, **Vol. VI**, W. Jost, ed. (Academic Press), p 121 (1974).
73. "Nuclear Magnetic Resonance Investigation of Molecular Complexes," R. Sahai, G.L. Loper and S.H. Lin, *Proc. Natl. Acad. Sci. U.S.A.*, **71**, 1449 (1974).
74. "Theory of Intramolecular Vibrational Relaxation of Large Systems," G.R. Fleming, O.L. J. Gijzeman and S.H. Lin, *Faraday Trans., II*, **70**, 37 (1974).
75. "Magnetic Circular Dichroism of Molecules in Dense Media IV. Effect of Chemical Substitution on Absorption Spectra and MCD," D. J. Shieh, Y.C. Fu, S.H. Lin and H. Eyring, *Proc. Natl. Acad. Sci. U.S.A.*, **71**, 209 (1974).
76. "Stochastic Processes in Physical Chemistry," S.H. Lin and H. Eyring, *Ann. Rev. Phys. Chem.*, **25**, 39 (1974).
77. "Time Resolved Absorption Spectra," G.R. Fleming, O.L.J. Gijzeman and S.H. Lin, *Faraday Trans., II*, **70**, 1074 (1974).
78. "On the Master Equation Approach of Vibrational Relaxation in Condensed Media," S.H. Lin, *J. Chem. Phys.*, **61**, 3810 (1974).
79. "Study of Vibronic and Born-Oppenheimer Couplings," S.H. Lin and H. Eyring, *Proc. Natl. Acad. Sci. U.S.A.*, **71**, 3415 (1974)
80. "Study of the Franck-Condon and Herzberg-Teller Approximations," S.H. Lin and H. Eyring, *Proc. Natl. Acad. Sci. U.S.A.*, **71**, 3802 (1974)
81. "The Resonance Inverse Raman Effect," S.H. Lin, E.S. Reid and C.J. Treadwell, *Chem. Phys. Lett.*, **29**, 389 (1974).
82. "Statistical Study of Optical Rotation for Synthetic D.L.-Copolyptide Solutions," H. Gotoh, S.H. Lin and H. Eyring, *Proc. Natl. Acad. Sci. U.S.A.*, **71**, 4675 (1974).
83. "Theory of Reaction Rates in Condensed Phases," S.H. Lin, K.P. Li and H. Eyring, In: *Physical Chemistry: An Advanced Treatise*, **Vol. VII**, H. Eyring, ed. (New York: Academic Press), p. 1 (1975).
84. "MCD of Molecules in Dense Media V. Relation between MCD and Hammett's Constants," D.J. Shieh, S.T. Lee, Y.C. Yim, S.H. Lin and H. Eyring, *Proc. Natl. Acad. Sci. U.S.A.*, **72**, 452 (1975).

85. "Theory of Time Resolved Emission Spectra," G.R. Fleming, O.L.J. Gijzeman, K.F. Freed and S.H. Lin, *Faraday Trans. II*, **71**, 773 (1975).
86. "Theory of Electric Field Effect on Electronic Spectra and Electronic Relaxation with Applications to F Centers," S.H. Lin, *J. Chem. Phys.*, **62**, 4500 (1975).
87. "Study of Collisional Energy Transfer and Quenching of Electronic Excitation," S.H. Lin and H. Eyring, *Proc. Natl. Acad. Sci. U.S.A.*, **72**, 4205 (1975).
88. "Nuclear Coordinate Dependence of Electronic Matrix Elements for Radiationless Transition," K.F. Freed and S.H. Lin, *Chem. Phys.*, **11**, 409 (1975).
89. "Theory of Vibrational Relaxation and IR Absorption in Condensed Media," S.H. Lin, *J. Chem. Phys.*, **65**, 1053 (1976).
90. "Effect of Temperature and Quencher Concentration on Vibrational Relaxation in Condensed Media," S.H. Lin, H.P. Lin and D. Knittel, *J. Chem. Phys.*, **64**, 441 (1976).
91. "Study of Vibronic, Spin-Orbit and Vibronic-Spin-Orbit Couplings of Formaldehyde with Application to Radiative and Non-Radiative Processes," S.H. Lin, *Proc. Roy. Soc.*, **A352**, 57 (1976).
92. "Significant Structure Theory of Liquids Applied to Critical Phenomena: Calculation of Critical Point Exponents," S.M. Ma, S.H. Lin and H. Eyring, *Chem. Phys. Lett.*, **43**, 420 (1976).
93. "MCD of Spin-Forbidden Transitions of Formaldehyde," Y.H. Yoon, S.T. Lee and S.H. Lin, *Proc. Natl. Acad. Sci. U.S.A.*, **73**, 2964 (1976).
94. "Oxygen Transport in Polycrystals and Single Crystals of  $\text{Pr}_7\text{O}_{12\pm 8}$ ," K.H. Lau, D.L. Fax, S.H. Lin and L. Eyring, *High Temp. Sci.*, **8**, 129 (1976).
95. "Medium-induced Radiationless Transitions and Effect of Solvent on Radiationless Transitions," S.H. Lin and S.T. Lee and Y.H. Yoon, *Proc. Natl. Acad. Sci. U.S.A.*, **73**, 2533 (1976).
96. "Magnetic Circular Dichroism of Molecules in Dense Media VI. Dimerization of Benzoic Acids," Y.H. Yoon, S.T. Lee, D.J. Shieh and S.H. Lin, *Chem. Phys. Lett.*, **38**, 24 (1976).
97. "Effect of Temperature on Radiationless Transitions II," D. Knittel, H.P. Lin, H. Raiszadeh and S.H. Lin, *JCS Faraday Trans. II*, **73**, 120 (1977).
98. "Theoretical Investigation of Symmetry-Forbidden Transitions in MCD and Electronic Spectra of Benzene," S.T. Lee, Y.H. Yoon and S.H. Lin, *J. Chem. Phys.*, **66**, 4349 (1977).

99. "Investigation of Steady State and Equilibrium Approximations in Reaction Kinetics," L.J. Volk, W.B. Richardson, K.H. Lau, M. Hall and S.H. Lin, *J. Chem. Ed.*, **54**, 95 (1977).
100. "General Treatment of Relaxation Phenomena," S.H. Lin, *Proc. Natl. Acad. Sci. U.S.A.*, **74**, 3623 (1977).
101. "Quantum Statistical Theory of Optical Phenomena," S.H. Lin, *Proc. Natl. Acad. Sci. U.S.A.*, **74**, 3105 (1977).
102. "A Thermodynamic Model of Hysteresis in Phase Transitions and its Application to Rare Earth Oxide Systems," D.R. Knittel, S.P. Pack, S.H. Lin and L. Eyring, *J. Chem. Phys.*, **67**, 134 (1977).
103. "Participation of Rotational Motion in Vibrational Relaxation of Molecules in Condensed Media," D.R. Knittel and S.H. Lin, *Mol. Phys.*, **36**, 893 (1978).
104. "Calculation of Rates of Radiationless Transitions in Matrix-Isolated CN," D. Fletcher, Y. Fujimura and S.H. Lin, *Chem. Phys. Lett.*, **57**, 400 (1978).
105. "Ion Flow through a Membrane: Concentration and Current Responses to a Step Potential Change," T.R. Hays, C.Q. Buckwalter, S.H. Lin and H. Eyring, *Proc. Natl. Acad. Sci. U.S.A.*, **75**, 1612 (1978).
106. "Ion Flow through a Membrane: Effect of Chemical Reaction on Time Dependence," T.R. Hays and S.H. Lin, *Proc. Natl. Acad. Sci. U.S.A.*, **75**, 2064 (1978).
107. "Theory of Vibrational Energy Transfer Among Diatomic Molecules in Inert Matrices," A. Blumen, S.H. Lin and J. Manz, *J. Chem. Phys.*, **69**, 881 (1978).
108. "Temperature Dependence of Rate Constants of Thermal Activated Processes and Vibrational Relaxation in Starvation Kinetics," S.M. Ma, S.H. Lin, D. Wutz, Y. Fujimura and H. Eyring, *Chem. Phys. Lett.*, **58**, 159 (1978).
109. "Thermodynamic Study of Hysteresis in Phase Transitions of Solid Methanes," S.M. Ma, S.H. Lin and H. Eyring, *Proc. Natl. Acad. Sci. U.S.A.*, **75**, 4664 (1978).
110. "Effect of Magnetic Field on Molecular Luminescence," S.H. Lin and Y. Fujimura, In: *Excited State*, **Vol. 4** (New York: Academic Press), pp 237-280 (1979).
111. "A Theoretical Study of Resonance Raman Scattering from Molecules," Y. Fujimura and S.H. Lin, *J. Chem. Phys.*, **70**, 247 (1979).



112. "Application of the Collision Complex Model to Collision-induced Intersystem Crossing and Collisional Magnetic Quenching of Polyatomic Molecules," H.L. Selzle, S.H. Lin and E.W. Schlag, *Chem. Phys. Lett.*, **62**, 230 (1979).
113. "A Theoretical Study of Light-induced Explosion," S.H. Lin and W.B. Richardson, *Proc. Natl. Acad. Sci. U.S.A.*, **76**, 4162 (1979).
114. "A Thermal Diffusion Model of Photothermal Spectroscopy," R. Tom, T.A. Moore, D. Benin and S.H. Lin, *Chem. Phys. Lett.*, **66**, 390 (1979).
115. "Resonance Raman Scattering from Molecules with Vibronically Coupled Excited States," Y. Fujimura and S.H. Lin, *Chem. Phys. Lett.*, **63**, 199 (1979).
116. "A Theoretical Study of Resonance Raman Scattering from Molecules II Temperature Effect," Y. Fujimura and S.H. Lin, *J. Chem. Phys.*, **71**, 3733 (1979).
117. "Time-evolution of the Triplet after a Radiationless Transition: Theory and Experimental Results," Y. Fujimura, S.H. Lin, H. Schröder, H.J. Neusser and E.W. Schlag, *Chem. Phys.*, **43**, 205 (1979).
118. "Time-evolution of the Triplet after a Radiationless Transition: Effect of Initial Distributions," Y. Fujimura, T. Nakajima, S.H. Lin and E.W. Schlag, *Chem. Phys. Lett.*, **67**, 299 (1979).
119. "Effect of Molecular Rotation on Vibrational Energy Transfer in Condensed Phases," S.H. Lin, T. Hays and H. Eyring, *Proc. Natl. Sci. U.S.A.*, **76**, 3571 (1979).
120. "On the Mechanisms of Triboluminescence," S.H. Lin, D. Wutz, Z.Z. Ho and H. Eyring, *Proc. Natl. Acad. Sci. U.S.A.*, **77**, 1245 (1980).
121. "Some Considerations of Theory and Experiment in Ultrafast Processes, S.H. Lin, In: *Radiationless Transitions*, S.H. Lin, ed. (New York: Academic Press) (1980).
122. "Theory of Vibrational Relaxation in Isolated Molecules," S.H. Lin, *Chem. Phys. Lett.*, **70**, 492 (1980).
123. "Calculation of Raman Spectra of Pyrazine Resonant to the S<sub>2</sub> State," Y. Fujimura, T. Nakajima and S.H. Lin, *Chem. Phys. Lett.*, **70**, 97 (1980).
124. "A Theoretical Study of Resonance Raman Scattering from Molecules: High Pressure Effect," Y. Fujimura, S.H. Lin and H. Eyring, *Proc. Natl. Acad. Sci. U.S.A.*, **77**, 5032 (1980).
125. "Random Distribution Statistical Analysis of Surface Activities of Aromatic Amine Local Anesthetics at Air/Water Interface in the Presence and Absence of Phospholipid

- Monolayers," H.C. Lin, I. Ueda, S.H. Lin, D.D. Shien, H. Kamaya and H. Eyring, *Biochim. Biophys. Acta(M)*, **598**, 51 (1980).
126. "Theory of Time-resolved Level Anti-crossing Experiment," R. Haberkorn, H.L. Selzle, W. Dietz, S.H. Lin and E.W. Schlag, *Chem. Phys.*, **52**, 363 (1980).
127. "A Kinetic Study of Oxidation of Praseodymium Oxides:  $\text{PrO}_{1.778}$ ," H. Inaba, S.P. Pack, S.H. Lin and L. Eyring, *J. Solid State Chem.*, **33**, 295 (1980).
128. "Physical Chemistry of the Interaction of Local Anesthetics with Model and Natural Membranes," I. Ueda, H. Yasuhara, D.D. Shieh, H.C. Lin and S.H. Lin, *Prog. Anesthesiology*, **2**, 285 (1980).
129. "Wavelength Regulation in Rhodopsin: Effect of Dipoles and Amino Acid Side Chains," T.R. Hays and S.H. Lin, *Proc. Natl. Acad. Sci. U.S.A.*, **77**, 6314 (1980).

## 1981 – 1990

130. "Theory of Time-resolved Level Anti-crossing Experiment: Effect of Excitation Radiation," H.L. Selzle, R. Haberkorn, W. Dietz, S.H. Lin and E.W. Schlag, In: *European Conference on Dynamics of Excited States*, 1980 Nuovo Cimento, **63B**, 420 (1981).
131. "Resonance Effects on Two-photon Absorption processes of Molecules," Y. Fujimura and S.H. Lin, *J. Chem. Phys.*, **74**, 3726 (1981).
132. "A Kinetic Study of the Oxidation and Reduction of Praseodymium Oxides:  $\frac{1}{7}\text{Pr}_7\text{O}_{12} + \left(\frac{1}{7} - \frac{x}{2}\right)\text{O}_2 \xrightleftharpoons{\leftarrow} \text{PrO}_{2-x}$ ," H. Inaba, S.H. Lin and L. Eyring, *J. Solid State Chem.*, **37**, 58 (1981).
133. "Effect of Collision and Magnetic Field on Quantum Beat in Biacetyl," W. Henke, H.L. Selzle, T.R. Hays, S.H. Lin and E.W. Schlag, *Chem. Phys. Lett.*, **77**, 448 (1981).
134. "Pressure Dependence of the Absorption Spectra of  $\beta$ -Carotene," Z.Z. Ho, T.A. Moore, S.H. Lin and R.C. Hanson, *J. Chem. Phys.*, **74**, 873 (1981).
135. "On the Density Matrix Approach of Intramolecular Relaxation Process," S.H. Lin, and H. Eyring, *Proc. Natl. Acad. Sci. U.S.A.*, **78**, 2013 (1981).

136. "A Theoretical Study of Resonance Raman Scattering from Molecules, III. Resonance Raman Scattering and Resonance Fluorescence," Y. Fujimura, H. Kono, T. Nakajima and S.H. Lin, *J. Chem. Phys.*, **75**, 99 (1981).
137. "Quantum Statistical Mechanical Theory of Diffusion and Diffusion with Interaction," S.H. Lin, A. Ziv and H. Eyring, *Proc. Natl. Acad. Sci. U.S.A.*, **78**, 3989 (1981).
138. "A Theoretical Study of the Resonant Multiphoton Ionization from a Molecular System," Y. Fujimura and S.H. Lin, *J. Chem. Phys.*, **75**, 5110 (1981).
139. "Theory of Quantum Beats: Master Equation Approach," H. Kono, Y. Fujimura and S.H. Lin, *J. Chem. Phys.*, **75**, 2569 (1981).
140. "The Kinetics of the Oxidation of Phi Phase Terbium Oxide:  

$$\frac{7}{2}\text{Tb}_2\text{O}_{3+\delta} + \left(\frac{3}{4} - \frac{7}{4}\delta\right)\text{O}_2 \rightarrow \text{Tb}_7\text{O}_{12}$$
," T. Sugihara, S.H. Lin and L. Eyring, *J. Solid State Chem.*, **40**, 189 (1981).
141. "A Kinetic Study of the Oxidation of Zeta Phase Praseodymium Oxide:  

$$\frac{10}{9}\text{Pr}_9\text{O}_{16} + \frac{1}{9}\text{O}_2 \rightarrow \text{Pr}_{10}\text{O}_{18}$$
," T. Sugihara, S.H. Lin and L. Eyring, *J. Solid State Chem.*, **40**, 226 (1981).
142. "Analysis of the Molecular Electronic Absorption Spectra of Shock Heated Aromatic Compounds," W.B. Richardson, S.H. Lin and D.L. Evans, *JCS Faraday Trans., II*, **78**, 1 (1982).
143. "Rotational Fine Structure in Photophysical Processes," E.W. Schlag, W.E. Henke and S.H. Lin, *Int. Rev. Phys. Chem.*, **2**, 1 (1982).
144. "Rate Constant of Vibrational Redistribution in Molecules Using Adiabatic Approximation Model," S.H. Lin, X.-G. Zhang, Z.-D. Qian, X.-W. Li and H. Eyring, *Proc. Natl. Acad. Sci. U.S.A.*, **79**, 1356 (1982).
145. "Single Rotational Lifetimes of Formaldehyde in a Hypersonic Jet," W.E. Henke, H.L. Selzle, T.R. Hays, E.W. Schlag and S.H. Lin, *J. Chem. Phys.*, **76**, 1327 (1982).
146. "Theoretical Study of Rotational Fine Structure in Radiationless Transitions," W.E. Henke, H.L. Selzle, T.R. Hays, E.W. Schlag and S.H. Lin, *J. Chem. Phys.*, **76**, 1335 (1982).
147. "Application of the Density Matrix Method to Vibrational Relaxation in Isolated Molecules," S.H. Lin, *Chem. Phys. Lett.*, **86**, 533 (1982).
148. "A Model for Multiphoton Ionization Mass Spectroscopy with Application to Benzene," W. Dietz, H.J. Neusser, D. Boesl, S.H. Lin and E.W. Schlag, *Chem. Phys.*, **66**, 105 (1982).

149. "Effect of Formation of van der Waals Complexes on Molecular Physical Properties." K. Godzik, T.R. Hays, W.E. Henke, H.L. Selzle, E.W. Schlag and S.H. Lin, *Laser Chem.*, **1**, 45 (1982).
150. "Theory of Time-resolved X-ray Scattering and its Application to Solid State Reaction Kinetics," T. Groy, S. Porter, R. Von Dreele, S.H. Lin and L. Eyring, *J. Mol. Sci.*, **2**, 105 (1982).
151. "Experimental and Theoretical Studies of Resonance Raman Scattering: Temperature Effects in  $\beta$ -Carotene," Z.Z. Ho, R.C. Hanson and S.H. Lin, *J. Chem. Phys.*, **77**, 3414 (1982).
152. "Theory of Transient Narrowing," A.A. Villaeys, K.F. Freed and S.H. Lin, *J. Mol. Sci.*, **2**, 31 (1982).
153. "Rotational Effect on SRVL Nonradiative Transitions: Line Width and Coriolis Coupling," H. Kono, S.H. Lin and E.W. Schlag, *J. Chem. Phys.*, **77**, 4474 (1982).
154. "Application of the Adiabatic Approximation to Coupled Oscillators," Z.-D. Qian, X.-G. Zhang, X.-W. Li, H. Kono and S.H. Lin, *Mol. Phys.*, **47**, 713 (1982).
155. "Dephasing Analysis of the Spin Motion on the Recombination of Solute-Ion Pairs in Solution," A.A. Villaeys, S.H. Lin, A. Boeglin and J. Klein, *Chem. Phys. Lett.*, **93**, 293 (1982).
156. "Theory of Inelastic Processes in Energetic Ion Impact on Solid Surfaces," A.R. Ziv, S.H. Lin, M. Skiff, B.P. Nigam, C.M. Loxton and I.S.T. Tsong, *J. Mol. Sci.*, **1**, 55 (1983).
157. "Application of Singular Perturbation Method to Master Equation Approach," T. Ohmae, Y. Fujimura, T. Nakajima and S.H. Lin, *J. Mol. Sci.*, **1**, 33 (1983).
158. "Interdependence of Radiative and Nonradiative Decay Rates of the Lowest Excited States as Revealed by the Fluorescence of Dinaphthylalkanes," B.T. Lim, S.H. Lin and E.C. Lim, *J. Chem. Phys.*, **78**, 1112 (1983).
159. "Spectroscopic Properties and Relaxation Processes of Impurity Molecules in Solids. I. Rotational Spectra," H. Kono and S.H. Lin, *J. Chem. Phys.*, **78**, 2607 (1983).
160. "A Theory of Visible/UV Multiphoton Processes in Molecules. I. Resonance Effect on Three-Photon Absorption," Y. Fujimura and S.H. Lin, *J. Chem. Phys.*, **78**, 6468 (1983).
161. "Theory of Multiphoton Magnetic Circular Dichroism: Two Identical Photon Case," S.H. Lin, Y. Fujimura and M. Saito, *J. Phys. Chem.*, **87**, 2895 (1983).
162. "Theoretical Studies of Non-Cascade Sputtering Processes," S.H. Lin, I.S.T. Tsong, A.R. Ziv, M. Szymorsk and C.M. Loxton, In: *Fourth International Workshop on Inelastic Ion-Surface Collisions*, Denmark, 1982, *Physica Scripta*, **T6**, 106 (1983).

163. "Spectroscopic Properties and Relaxation Processes of Impurity Molecules in Solids. II. Vibrational Relaxation," H. Kono and S.H. Lin, *J. Chem. Phys.*, **79**, 2748 (1983).
164. "Dynamical Effect of Vibrational Relaxation on Electronic Relaxation," A. Boeglin, A.A. Villaeys, R. Voltz and S.H. Lin, *J. Chem. Phys.*, **79**, 3819 (1983).
165. "Kinetic Energy Distributions of Sputtered Particles in Non-Cascade Sputtering Processes," A.R. Ziv, B.V. King, S.H. Lin and I.S.T. Tsong, presented at: *Sixth International Conference on Ion Beam Analysis*, Arizona State University, Tempe, Arizona, May 23-27, 1983, *Nuclear Instruments and Methods*, **218**, 742 (1983).
166. "<sup>2</sup>E Relaxation in Mixed-Ligand Cr(NH<sub>3</sub>)<sub>6-n</sub>X<sub>n</sub> Complexes," A.F. Fucaloro, L.S. Forster, J.V. Rund and S.H. Lin, *J. Phys. Chem.*, **87**, 1796 (1983).
167. "Intramolecular Vibrational Relaxation in Electronically Excited States," R. Voltz, A. Boeglin, A.A. Villaeys and S.H. Lin, *Laser Chem.*, **2**, 253 (1983).
168. "Theoretical Studies of Molecules Adsorbed on Solid Surfaces. I. Electronic Spectra," H. Kono, A.R. Ziv and S.H. Lin, *Surface Sci.*, **134**, 614 (1983).
169. "Photoacoustic Spectroscopy of Rare Earth Oxides," J.R. Schoonover, Y.L. Lee, S.N. Su, S.H. Lin and L. Eyring, *Appl. Spect.*, **38**, 154 (1984).
170. "Intramolecular Vibrational Relaxation of Benzene," E. Riedle, H.J. Neusser, E.W. Schlag and S.H. Lin, *J. Phys. Chem.*, **88**, 198 (1984).
171. "A Theoretical Study of Resonance Raman Scattering from Molecules IV. Anharmonic Effect," H. Kono, Z.Z. Ho and S.H. Lin, *J. Chem. Phys.*, **80**, 1760 (1984).
172. "Nonequilibrium Phonons in Nonradiative Rate Processes," B. Fain and S.H. Lin, *Physica*, **128A**, 164 (1984).
173. "A Theoretical Model of Solid State Phase Reactions: Hysteresis and Kinetics," A. Moren, S.H. Lin, R.H. Langley and L. Eyring, *J. Solid State Chem.*, **53**, 329 (1984).
174. "Raman and Resonance Raman Spectroscopy of Rare Earth Oxides," L. Tucker, F. Carney, P. McMillan, S.H. Lin and L. Eyring, *Appl. Spect.*, **38**, 857 (1984).
175. "Theoretical Studies of Laser-Stimulated Surface Processes. I. General Formalism," B. Fain and S.H. Lin, *Surf. Sci.*, **147**, 497 (1984).
176. "Theoretical Studies of Laser-Stimulated Surface Processes. II. Desorption," G.S. Wu, B. Fain, A.R. Ziv and S.H. Lin, *Surf. Sci.*, **147**, 537 (1984).

177. "Luminescence of Quadrate Cr(III) Amine Complexes. 2. Nonradiative Excited-state Relaxation Rates," L.S. Forster, I.V. Rund, A.F. Fucaloro and S.H. Lin, *J. Phys. Chem.*, **88**, 5017 (1984).
178. "Theory of Laser-Stimulated Surface Processes: Master Equation Approach," B. Fain, A.R. Ziv, G.S. Wu and S.H. Lin, In: *Advances in Multiphoton Processes and Spectroscopy*, **Vol. 1**, (Singapore: World Scientific Publishing), pp 425-514 (1984).
179. "Excess Energy Dependence in Radiationless Transitions. Triplet to Ground State Non-radiative Rate Calculations in Benzene," H. Hornberger, H. Kono and S.H. Lin, *J. Chem. Phys.*, **81**, 3554 (1984).
180. "Role of Viscosity Effect on Photoisomerization," A.A. Villaeys, A. Boeglin and S.H. Lin, *J. Lumin.*, **31**, 579 (1984).
181. "Theory of IR Absorption Spectra of Molecules," S.H. Lin, X. Li, X. Zhang and Z. Qian, *Acta Mathematica Scientia*, **4**, 173 (1984).
182. "Spectral Shifts of Anthrocene Argon Complexes," W.J. Yu, W.E. Henke, H.L. Selzle, E.W. Schlag, D. Wutz and S.H. Lin, *Chem. Phys.*, **92**, 182 (1985).
183. "Si<sub>L</sub> Core Edge Fine Structure in an Oxidation Series of Silicon Compounds: A Comparison of Micro Electron Energy Loss Spectra with Theory," W. M. Skiff, R.W. Carpenter and S.H. Lin, *J. Appl. Phys.*, **58**, 3463-3469 (1985).
184. "Resonance Raman Scattering from Molecules with a Non-equilibrium Vibronic Distribution," Y. Fujimura, Y. Ohtsuki, M. Arai and S.H. Lin, *J. Chem. Phys.*, **82**, 1246 (1985).
185. "Experimental and Theoretical Studies of Interaction between Anesthetics and Phospholipid Membranes: Inhalation Anesthetics," A. Shibata, T. Mori, I. Ueda, H.C. Lin, S.M. Ma and S.H. Lin, *J. Mol. Sci.*, **3**, 15-27 (1985).
186. "Effect of Vibrational Energy Transfer on Laser-induced Desorption," B. Fain and S.H. Lin, *Chem. Phys. Lett.*, **114**, 497-502 (1985).
187. "Studies of Resonance Raman Scattering: High Pressure Effects in  $\beta$ -Carotene," Z.Z. Ho, R.C. Hanson and S.H. Lin, *J. Phys. Chem.*, **89**, 1544-1552 (1985).
188. "Evaluation of the Isomerization Rates in the Overdamped Case," A.A. Villaeys, A. Boeglin and S.H. Lin, *Chem. Phys. Lett.*, **116**, 210-216 (1985).

189. "Mass Distribution of Ejected Molecules and Clusters in Non-cascade Sputtering Processes," B.V. King, A.R. Ziv, S.H. Lin, and I.S.T. Tsong, *J. Chem. Phys.*, **82**, 3641-3645 (1985).
190. "Viscosity Effect on Non Adiabatic Isomerization and Electronic Relaxation of Molecules in Liquids," A.A. Villaeys, A. Boeglin and S.H. Lin, *J. Chem. Phys.*, **82**, 4044-4053 (1985).
191. "Application of the Electron Gas Model to the Calculation of the Geometries of van der Waals Complexes," G.S. Wu, D. Wutz and S.H. Lin, *Mol. Phys.*, **54**, 1437-1452 (1985).
192. "Calculation of Crystal Field Parameters of Praseodymium Ethylsulfate and Praseodymium Trichloride," Y.Q. Jia, S.H. Lin and L.S. Forster, *J. Solid State Chem.*, **60**, 289-296 (1985).
193. "Theory of Multiphoton Ionization of Atoms and Molecules," B. Fain, H. Kono, S.H. Lin, W.E. Henke, H.L. Selzle and E.W. Schlag, *J. Chinese Chem. Soc.*, **32**, 187-199 (1985) (invited paper).
194. "Relativistic Configuration Interaction Calculations on the Low-lying Electronic States of HI," D. Chapman, K. Balasubramanian and S.H. Lin, *Chem. Phys. Lett.*, **118**, 192-198 (1985).
195. "Shifts Fluorescence Excitation Spectra of Anthracene-Argon van der Waals Complexes," W. E. Henke, W. Yu, H.L. Selzle, E.W. Schlag, D. Wutz and S.H. Lin, *Chem. Phys.*, **92**, 187 (1985).
196. "Theoretical Study of Electronic Spectral Shifts of van der Waals Complexes," W.J. Yu, W.E. Henke, H.L. Selzle, E.W. Schlag, D. Wutz and S.H. Lin, *Chem. Phys.*, **97**, 205 (1985).
197. "Magnetic Circular Dichroism," S.H. Lin and D.D. Shieh, In: *Treatise on Analytical Chemistry*, **Vol. 8**, P.J. Elving and E.J. Meehan, eds. (Wiley-Interscience), Chap. 12, pp 149-207 (1986).
198. "Resonance Raman Overtone Intensity Calculations of a Matrix-Isolated I<sub>2</sub> Molecule by the Symmetrized Split Operator Fast Fourier Transform Method," H. Kono and S.H. Lin, *J. Chem. Phys.*, **84**, 1071-1079 (1986).
199. "Non-Markoffian Theory of Quantum Beats in Molecular Fluorescence," Y. Fujimura, T. Akiyama, T. Nakajima and S.H. Lin, *J. Chem. Phys.*, **84**, 2112-2119 (1986).

200. "Interpretation of the Mass Distribution of Ejected  $(C_sI)_n C_s^+$  Ion Clusters by the Non-Cascade Sputtering Model," B.V. King, A.R. Ziv, S.H. Lin and I.S.T. Tsong, *Surface Sci.*, **167**, 18-27 (1986).
201. "Application of the Density Matrix Method to Multiphoton Ionization of Molecules," A. Boeglin, B. Fain and S.H. Lin, *J. Chem. Phys.*, **84**, 4838 (1986).
202. "Theoretical Studies of Laser-Stimulated Surface Processes. III. Effect of Vibrational Energy Transfer on Desorption," B. Fain and S.H. Lin, *Physica*, **138B**, 63 (1986).
203. "On the Microscopic Approach of the Mean Field Kinetic Ising Model," X.-G. Zhang and S.H. Lin, *Physica*, **139A**, 439 (1986).
204. "Theory of Photoisomerization of Impurity Molecules in Solids," S.H. Lin, X.-G. Zhang and G.Y.C. Wu, *J. Chem. Phys.*, **85**, 221 (1986).
205. "Anesthetic Dissolution of Unfreezable and Bound Water in Phospholipid Vesicle Membranes and Elevation of the Main Phase-Transition Temperature," I. Ueda, H.S. Tseng, Y. Kaminoh, S.M. Ma, H. Kamaya and S.H. Lin, *Mole. Pharmacol.*, **29**, 582 (1986).
206. "Theory of Laser-stimulated Phase Transition Kinetics in Solids," A. Boeglin, K. Lin, S.H. Lin and B. Fain, *Chem. Phys. Lett.*, **129**, 493 (1986).
207. "Instability of Desorption Mode in Laser-stimulated Desorption," B. Fain, A. Boeglin and S.H. Lin, *Physica*, **142B**, 165 (1986).
208. "Photodesorption via Stimulated Raman Emission of Coherent Surface Phonons," B. Fain, and S.H. Lin, *Physica*, **142B**, 1 (1986).
209. "Lose-Dependent Non-linear Response of the Main Phase-Transition Temperature of Phospholipid Membranes to Alcohols," H. Kamaya, S.M. Ma and S.H. Lin, *J. Membrane Biol.*, **90**, 157 (1986).
210. "Ab Initio Configuration Interaction Calculations for Five States of  $ArHe^+$ ," M.Z. Liao, K. Balasubramanian, D. Chapman and S.H. Lin, *Chem. Phys.*, **111**, 423 (1987).
211. "Theory of Laser-stimulated Desorption Spectroscopy," S.H. Lin, A. Boeglin and B. Fain, *J. Opt. Soc. Amer.*, **4B**, 211 (1987).
212. "Theory of Laser-stimulated Desorption of Molecules via Electronic Excitation of Adsorbed Molecules," S.H. Lin, A. Boeglin, B. Fain and C.Y. Yeh, *Surface Sci.*, **180**, 289 (1987).



213. "Ion-induced Desorption of  $(\text{H}_2\text{O})_n^+ \text{H}$  Ion Clusters," J.W. Christiansen, I.S.T. Tsong and S.H. Lin, *J. Chem. Phys.*, **86**, 3516 (1987).
214. "Time-resolved X-ray Diffraction by Synchrotron Radiation: The Thermal Decomposition of  $\text{C}_d(\text{OH})_2$  Powders," Ö. Sorborg, J.R. Schoonover, S.H. Lin and L. Eyring, *J. Solid State Chem.*, **68**, 214 (1987).
215. "A Theoretical Investigation of the Mechanism of Electron Transfer in Condensed Media," Z.T. Chu, Y.Y. Lin and S.H. Lin, *J. Mol. Sci.*, **5**, 127 (1987).
216. "Relativistic Configuration Interaction Calculations for Electronic States of  $\text{KrHe}^+$ ," K. Balasubramanian, M.Z. Liao and S.H. Lin, *Chem. Phys. Lett.*, **138**, 49 (1987).
217. "A Theoretical Study of Two-Color Photoionization and Autoionization of Molecules," S.H. Lin, A. Boeglin and S.M. Lin, *J. Photochem.*, **39**, 173 (1987).
218. "Multiphoton Spectroscopy," S.H. Lin and Y. Fujimura, In: *The Encyclopedia of Physical Science and Technology*, R.A. Meyers, ed. (New York: Academic Press), **Vol. 8**, p 592-619 (1987).
219. "Mechanisms of Ion-induced Desorption of Large Molecules and Clusters," B.V. King, I.S.T. Tsong and S.H. Lin, *Intern. J. Mass Spectry. and Ion Processes*, **78**, 341-356 (1987).
220. "Nonlinear Response of Membrane Potential to Sudden Perturbation of External pH in a Liquid Membrane with Mobile Ion-Carrier," K. Nomura, S. M. Ma, S.H. Lin, H. Kamaya and I. Ueda, *Bioelectrochem. Bioenerg.*, **17**, 193 (1987).
221. "Magnetic Susceptibility and Fluorescence Spectra of  $\text{S}_m\text{I}_2$  in THF," S.H. Wang, G. King, S.H. Lin and T.M. Brown, *J. Solid State Chem.*, **69**, 224 (1987).
222. "CASSCF/CI Calculations of Potential Energy Surfaces of  $\text{He}_3^+$  and  $\text{He}_2^+$ ," K. Balasubramanian, M.Z. Liao and S.H. Lin, *Chem. Phys. Lett.*, **142**, 349 (1987).
223. "Electronic Dipole and Transition Moments from the Relativistic CI Wavefunction: Application to HI," D.A. Chapman, K. Balasubramanian and S.H. Lin, *J. Chem. Phys.*, **87**, 5325 (1987).
224. "A Theoretical Study of Spectroscopic Properties and Transition Moments of  $\text{HBr}$ ," D.A. Chapman, K. Balasubramanian and S.H. Lin, *Chem. Phys.*, **118**, 333 (1987).
225. "Theoretical Investigation of the Electronic States of  $\text{He}_r^+$ ," K. Balasubramanian, M. Z. Liao and S.H. Lin, *J. Phys. Chem.*, **91**, 5836 (1987).

226. "Near-edge Fine Structure Analysis of Core Shell Electronic Absorption Edges in Si and its Refractory Compounds Using Electron Energy Loss Microscopy," W. M. Skiff, R.W. Carpenter and S.H. Lin, *J. Appl. Phys.*, **62**, 2439 (1987).
227. "IR-Laser-Induced Photodesorption: Analysis of Theoretical Models," B. Fain and S.H. Lin, *Physica*, **146B**, 324 (1987).
228. "Theoretical and Experimental Study of the Quenching of Singlet Oxygen by Solvent," Y.Y. Lin, Z.T. Chu and S.H. Lin, *J. Photochem. Photobiol.*, **44A**, 229 (1988).
229. "Theory of Vibrational Predissociation Spectroscopy of Weak Complexes," S.H. Lin, A. Boeglin, Y. Fujimura and B. Fain, *Chem. Phys. Lett.*, **145**, 334 (1988).
230. "Intermolecular Energy Transfer in IR-Laser-Induced Desorption," B. Fain, V. Fleurov and S.H. Lin, *Chem. Phys.*, **122**, 17 (1988).
231. "K,L,M,N,O and P Ionization Cross Sections for Electron Energy Loss Spectroscopy," W.M. Skiff, R.W. Carpenter and S.H. Lin, *Ultramicroscopy*, **25**, 47 (1988).
232. "Theory of Photoionization Threshold Spectroscopy of Molecules and Clusters," S.H. Lin, H.L. Selzle, K.O. Börnsen and E.W. Schlag, *J. Phys. Chem.*, **92**, 1469 (1988).
233. "Theory of Multiphoton Processes," B. Fain, A. Boeglin and S.H. Lin, *J. Chem. Phys.*, **88**, 7559 (1988).
234. "Monte Carlo Calculation of the Quantum Partition Function via Path Integral Formulations," H. Kono, A. Takasaka and S.H. Lin, *J. Chem. Phys.*, **88**, 6390 (1988).
235. "On the Role of Low Frequency Modes in the Energy or Temperature Dependence of Intersystem Crossing," H. Kono, S.H. Lin and E.W. Schlag, *Chem. Phys. Lett.*, **145**, 280 (1988).
236. "Time-resolved X-ray Diffraction by Synchrotron Radiation: The Thermal Decomposition of  $\text{CaCO}_3$  Powder," J.R. Schoonover and S.H. Lin, *J. Solid State Chem.*, **76**, 143 (1988).
237. "Extraction of Ground State Properties by Discretized Path Integral Formulations," H. Kono, A. Takasaka and S.H. Lin, *J. Chem. Phys.*, **89**, 3233 (1988).
238. "Production and Unimolecular Decay Rate of Rotationally Selected Polyatomic Molecular Ions," A. Kiermeier, H. K. Lewind, H.J. Neusser, E.W. Schlag and S.H. Lin, *J. Chem. Phys.*, **88**, 6881 (1988).

239. "A Microscopic Form of the Extended Kramers Equations," S.B. Zhu, G.W. Robinson, J. Lee and S.H. Lin, *Chem. Phys. Lett.*, **148**, 164 (1988).
240. "Quantum Mechanical Calculation of Decomposition of H<sub>2</sub>O<sub>2</sub>," K. Nishikawa and S.H. Lin, *Chem. Phys. Lett.*, **149**, 243 (1988).
241. "Stark Effect on Dynamics and Spectroscopy of Isolated Molecules," S.H. Lin, A. Boeglin, H.L. Dai and E.W. Schlag, *J. Phys. Chem.*, **92**, 5398 (1988).
242. "Coherence-Population Interdependence in Nonlinear Optics," J.P. Lavone, a. Boeglin, S.H. Lin and A.A. Villaeys, *Phys. Rev.*, **A38**, 2896 (1988).
243. "Ion-beam-induced Desorption of Ar<sub>n</sub><sup>+</sup> Ion Clusters," J.W. Christiansen, I.S.T. Tsong and S.H. Lin, *J. Vac. Sci. Tech.*, **A6**, 699 (1988).
244. "Analysis of Valence Shell Electronic Excitations in Si and its Refractory Compounds Using Electron Energy Loss Microspectroscopy," W.M. Skiff, R.W. Carpenter and S.H. Lin, *J. Appl. Phys.*, **64**, 6328 (1988).
245. "Resonances in Molecular Photoionization. IV. Theory of One-color and Two-color Photoionization of Molecules," W. Domcke, A.L. Sobolewski and S.H. Lin, *J. Chem. Phys.*, **89**, 6209 (1988).
246. "Membrane-Buffer Partition Coefficients of Tetracaine for Liquid-crystal and Solid-gel Membrane Estimated by Direct UV-Spectrophotometry," Q.T. Inoue, Y. Kaminoh, S.M. Ma, I. Ueda and S.H. Lin, *Biochem. Biophys. Acta*, **946**, 337 (1988).
247. "Effect of Surface Ionization of Dimyristoylphosphatidic Acid Vesicle Membranes on the Main Phase-Transition Enthalpy and Temperature," Y. Kaminoh, F. Kano, J.S. Chiou, H. Kamaya, S.H. Lin and I. Ueda, *Biochem. Biophys. Acta*, **943**, 522 (1988).
248. "Spike Membrane Potential in a Liquid Membrane System Induced by pH-Jump. II. Theory for Relaxation of the Peak Potential," S. M. Ma, K. Nomura, H. Kamaya, I. Ueda and S.H. Lin, *Bioelectrochem. Bioenerg.*, **19**, 301 (1988).
249. "Theoretical Study of the Negative Ions of HBr and HI," D.A. Chapman, K. Balasubramanian and S.H. Lin, *Phys. Rev.*, **A38**, 6098 (1988).
250. "Time-resolved X-ray Diffraction of Solid-state Reactions: The Effect of Atmosphere on Product Particle Growth," J.R. Schoonover and S.H. Lin, *Materials Lett.*, **7**, 274 (1988).

251. "Experimental and Theoretical Study of Laser-enhanced Ionization and Dual Laser Ionization of Sodium Vapor," K.C. Lin, S.H. Lin, P.M. Hunt, G.E. Leroi and S.R. Crouch, *Appl. Spectroscopy*, **43**, 66 (1989).
252. "Theory of Photo-induced Intramolecular Electron Transfer in Dense Media," S.H. Lin, *J. Chem. Phys.*, **90**, 7103 (1989).
253. "Application of the Theory of Two-dimensional Spectroscopy to the Real-time Femtosecond Transition State Spectroscopy," S.H. Lin and B. Fain, *Chem. Phys. Lett.*, **155**, 216 (1989).
254. "Spectra of Isotopically Mixed Benzene Trimers," K.O. Börnsen, S.H. Lin, H.W. Selzle and E.W. Schlag, *J. Chem. Phys.*, **90**, 1299 (1989).
255. "Rate Processes Affected by Ultrashort-pulse Fields," B. Fain, S.H. Lin and W.X. Wu, *Phys. Rev.*, **A40**, 824 (1989).
256. "Experimental and Theoretical Studies of Energy Transfer in F-Center/OH<sup>-</sup>(OD<sup>-</sup>) Defect Pairs in KCl," G. Halama, K.T. Tsen, S.H. Lin, F. Luty and J.B. Page, *Phys. Rev. B*, **B39**, 13457 (1989).
257. "Two-dimensional Spectroscopy: Theory of Non-stationary, Time-dependent Absorption and Its Application to Femtosecond Processes," B. Fain, S.H. Lin and H. Hamer, *J. Chem. Phys.*, **91**, 4485 (1989).
258. "Avalanche Phenomena in UV Laser-induced Desorption," B. Fain and S.H. Lin, *Chem. Phys. Lett.*, **157**, 233 (1989).
259. "Laser-induced Explosive Desorption," B. Fain and S.H. Lin, *J. Chem. Phys.*, **91**, 2726 (1989).
260. "Theoretical Aspects of Laser Induced Desorption," B. Fain, S.H. Lin and Z.W. Gortel, *Surface Sci.*, **213**, 531 (1989).
261. "Splitting of High Temperature X-ray Diffraction Profiles During the PbO Tetragonal  $\leftrightarrow$  Orthorhombic Phase Transitions," J.R. Schoonover, T.L. Groy and S.H. Lin, *J. Solid State Chem.*, **83**, 207 (1989).
262. "Theory of Photothermal Spectroscopy Applied to Solid State Reaction Kinetics," J.R. Schoonover and S.H. Lin, *Appl. Spectroscopy*, **43**, 1265 (1989).
263. "Theory of Real-time Femtosecond Transition Spectroscopy," S.H. Lin, B. Fain and N. Hamer, *Adv. Chem. Phys.*, **79**, 133 (1990).

264. "Theory of Non-stationary, Time-dependent Emission and Its Application to Ultrafast Processes," S.H. Lin, B. Fain, N. Hamer and C.Y. Yeh, *Chem. Phys. Lett.*, **162**, 73 (1990).
265. "Theory of Multiphoton Processes by the Fourier-Expansion Density Matrix Method," S.H. Lin, Y. Nomura and Y. Fujimura, *J. Chem. Phys.*, **92**, 2910 (1990).
266. "General Asymptotic Behavior for Amplitude and Frequency Dependence of Multiphoton Ionization Rates," B. Fain and S.H. Lin, *Chem. Phys. Lett.*, **165**, 229 (1990).
267. "Generalized Susceptibility Approach to Transient Nonlinear Optical Processes," A.A. Villaeys, J.C. Vallet and S.H. Lin, *Phys. Rev.*, **A41**, 2796 (1990).
268. "A Theoretical Study of the Electric Field Effect on Intramolecular Electron Transfer in Dense Media," S.H. Lin, C.Y. Yeh and G.Y.C. Wu, *Chem. Phys. Lett.*, **166**, 195 (1990).
269. "Experimental and Theoretical Studies of Energy Transfer in F-center-CN<sup>-</sup> Defect Pairs in KCl," G. Halama, K.T. Tsen, S.H. Lin, F. Luty and J.B. Page, *Phys. Rev.*, **B40**, 11524 (1990).
270. "Ultrafast Time-resolve Fluorescence Spectroscopy," S.H. Lin, B. Fain and C.Y. Yeh, *Phys. Rev.*, **A41**, 2718 (1990).
271. "Application of the Density Matrix Method to the Primary Electron Transfer in Photosynthetic Reaction Centers," M. Sugawara, Y. Fujimura, C.Y. Yeh and S.H. Lin, *J. Photochem. Photobiol.*, **54A**, 321 (1990).
272. "Band Structure of Stationary Emission Spectra from a Three-level Molecule Pumped by Strong Radiation Fields," Y. Ohtsuki, Y. Fujimura and S.H. Lin, *J. Chem. Phys.*, **93**, 3012 (1990).
273. "Space-time Coherences Induced by Ultrashort Electromagnetic Pulses," B. Fain and S.H. Lin, *J. Chem. Phys.*, **93**, 6387 (1990).
274. "Theoretical Comparison of Electron Energy-Loss and X-ray Absorption Near-edge Fine Structure of SiL<sub>2,3</sub> Edge," H. Ma, S.H. Lin, R.W. Carpenter and O.F. Sankey, *J. Appl. Phys.*, **68**, 288 (1990).
275. "Particle Coarsening Kinetics During Thermal Decompositions: CdO from CdCO<sub>3</sub>," J.R. Schoonover and S.H. Lin, *J. Materials Sci.*, **25**, 4518 (1990).
276. "Study of the Interfacial Concentration Profile of Two Component Systems in the Solid-Solid Interface," N. Tapia, H. Ma, S.H. Lin and R.W. Carpenter, *Materials Lett.*, **10**, 256 (1990).

277. "Effect of Antioxidants on Asphalt Durability," R.F. Ju, S.H. Lin and W. Burke, *Oxidation Comm.*, **13**, 198 (1990).

## 1991 – 2000

278. "Theory of Ultrafast Time-resolved Absorption Spectroscopy," C.Y. Yeh, W.L. Chang, H. Ma and S.H. Lin, *Int. J. Quantum Chem.*, **39**, 353 (1991).

279. "Interfacial Dehydration by Alcohols: Hydrogen Bonding of Alcohols to Phospholipids," J.S. Chiou, C.C. Kuo, S.H. Lin, H. Kamaya and I. Ueda, *Alcohol*, **8**, 143 (1991).

280. "Femtosecond Time-resolved Resonance Raman Scattering," S.H. Lin, R.G. Alden, A.A. Villaeys and B. Fain, *J. Mol. Structure*, **249**, 11 (1991).

281. "Application of the Collision-Complex Model to the Photophysical Processes of Singlet Oxygen in Liquids," S.H. Lin, J. Lewis and T.A. Moore, *J. Photochem. Photobio.*, **56A**, 25 (1991).

282. "A Unified Transformation of the Complete Molecular Hamiltonian," R. Islampour and S.H. Lin, *J. Mol. Spectry.*, **147**, 1 (1991).

283. "Infrared Studies on Hydrogen Bonding of Alcohols. Self Association," J.S. Chiou, S.M. Ma, C.C. Kuo, G. Sandling, H. Ma, H. Kamaya, S.H. Lin and I. Ueda, *Trends in Chem. Physics*, **1**, 1-15 (1991).

284. "Effects of Anharmonicity on Intramolecular Electron Transfer Rates," R. Islampour and S.H. Lin, *Chem. Phys. Lett.*, **179**, 147 (1991).

285. "Non-Markovian Effects on Optical Absorption," A.A. Villaeys, J.C. Vallet and S.H. Lin, *Phys. Rev. A*, **43**, 5030 (1991).

286. "Studies of Energy Transfer Processes in F-center/ $\text{CN}^-$  Defect Pairs in KBr," G. Halomo, K.T. Tsen, S.H. Lin, F. Luty and J.B. Page, *Phys. Rev. B*, **44**, 2040 (1991).

287. "Ultrafast Pump-probe Absorption Spectroscopy of Bacterial Photosynthetic Reaction Centers," S.H. Lin, In: *Advances in Multiphoton Processes and Spectroscopy*, **Vol. 7**, 237-310 (1991).

288. "On the Theory of Photoinduced Intramolecular Electron Transfer," S.H. Lin, *J. Phys. Chem.*, **95**, 10261 (1991).

289. "Dynamics of Stochastic Systems in Nonlinear Optics I. General Formalism," A.A. Villaeys, A. Boeglin, and S.H. Lin, *Phys. Rev. A*, **44A**, 4660 (1991).
290. "Dynamics of Stochastic Systems in Nonlinear Optics II," A.A. Villaeys, A. Boeglin, and S.H. Lin, *Phys. Rev. A*, **44A**, 4671 (1991).
291. "Ab initio Study of the Valence-electron Relaxation Effect on X-ray Emission Spectra and the Excitonic Effect on Electron-energy-loss Spectra of the SiL<sub>2,3</sub> Edge," H. Ma, S.H. Lin, R.W. Carpenter and O.F. Sankey, *Phys. Rev.*, **44B**, 13393 (1991).
292. "Femto-second Processes and Ultrafast Biological Electron Transfer," S.H. Lin, R.G. Alden, C.K. Tang, Y. Fujimura and M. Sugawara, in *Mode Selective Chemistry*, edited by J. Jortner et al. (Dordrecht, The Netherlands: Kluwer) p 467-484 (1991).
293. "Theories of Electronic Spectral Bandshape Functions of Molecules," R. Islampour and S.H. Lin, In: *Trends in Chemical Physics*, **1**, 244 (1991).
294. "A Modified Parametrization Scheme for the Complete Neglect of Differential Overlap Method with Relativistic Correction of Orbital Exponents and Energy Levels with Particular Applications to Rare Earth Compounds," G.S. Wu, H. Ma and S.H. Lin, *J. Chem. Phys.*, **96**, 4518 (1992).
295. "Theory of Spectroscopy and Energy Transfer of Oligomeric Pigments in Chlorosome Antennas of Green Photosynthetic Bacteria," R.G. Alden, S.H. Lin and R.E. Blankenship, *J. Lumin.*, **51**, 51 (1992).
296. "Theory of Femtosecond Time-resolved Infrared Absorption Spectroscopy with Application to Ligand Dissociation in Haemoglobin," R.G. Alden, S.H. Lin, W.Z. Xiao, B. Fain and R. Islampour, *Mol. Phys.*, **75**, 1375 (1992).
297. "Theory of Optical Properties in Non-stationary Media Created by Femtosecond Pulse: Linear Case," B. Fain and S.H. Lin, *Chem. Phys.*, **161**, 515 (1992).
298. "Collective Spontaneous Emission in CS<sub>2</sub>," H.T. Liou, B. Fain and S.H. Lin, *Appl. Spectry.*, **46**, 940 (1992).
299. "Vibrational Relaxation and Coherence and Primary Electron Transfer in Photosynthetic Reaction Centers," R.G. Alden, W.D. Cheng and S.H. Lin, *Chem. Phys. Lett.*, **194**, 318 (1992).

300. "Theoretical Study of Laser Heating and Dissociation Reactions in Solids Using Ultrafast Time-resolved X-ray Diffraction," H. Ma, S.H. Lin and P. Rentzepis, *J. Appl. Phys.*, **72**, 2174 (1992).
301. "Rate of Reaction of Electron Transfer Over a Long Range and Mediated by a Solvent," J. M. Chen, C.Y. Mou and S.H. Lin, *J. Chinese Chem. Soc.*, **39**, 529 (1992).
302. "Multiphoton Spectroscopy," Y. Fujimura and S.H. Lin in *Encyclopedia of Physical Science and Technology*, **Vol. 10** (New York: Academic Press) p 495-523 (1992).
303. "General Theory of Temperature Dependent Ultrafast Transient Hole Burning," A.A. Villaeys, J.C. Vallet, H. Ma and S.H. Lin, *Phys. Rev.*, **A46**, 5959 (1992).
304. "Molecular Dynamics Study of Thermal Desorption of Xe from Ag (111) Surfaces," S.B. Zhu, G.W. Robinson and S.H. Lin, *Surface Sci.*, **279**, 99 (1992).
305. "A Theoretical Study of Laser Desorption of Molecules Induced by a Ultrashort Pulse," B. Fain, S.H. Lin, J. Grotemeyer and E.W. Schlag, *Chem. Phys. Lett.*, **202**, 357 (1993).
306. "Limitations of Pump-probe Femtosecond Time-resolved Experiments: Time-dependent Absorption and Dispersion Lineshapes," B. Fain and S.H. Lin, *Phys. Rev.*, **A47**, 3222 (1993).
307. "Experimental and Theoretical Studies of Matrix-assisted Laser Desorption of Neutral Organic Molecules," J. Grotemeyer, E.W. Schlag and S.H. Lin, *Chem. Phys. Lett.*, **209**, 499 (1993).
308. "Effect of Temperature, Energy Gap and Distortion of Potential Surfaces on Photo-induced Intramolecular Electron Transfer," R. Islampour, R.G. Alden, G.Y.C. Wu and S.H. Lin, *J. Phys. Chem.*, **97**, 6793 (1993).
309. "Generalized Förster-Dexter Theory of Photo-induced Intramolecular Energy Transfer," S.H. Lin, W.Z. Xiao and W. Dietz, *Phys. Rev.*, **47E**, 3698 (1993).
310. "Ab Initio Calculation of Band Structure, X-ray Emission, Quantum Yield and Electron-Energy-Loss Spectra of Hexagonal Boron Nitride," H. Ma, S.H. Lin, R.W. Carpenter, P. Rice and O.F. Sankey, *J. Appl. Phys.*, **73**, 7422 (1993).
311. "Experimental and Theoretical Studies of Femtosecond Time-resolved Three-Dimensional Spectra of Photosynthetic Reaction Centers," R.G. Alden, M. Hayashi, J.P. Allen, N.W. Woodbury, H. Murchison and S.H. Lin, *Chem. Phys. Lett.*, **208**, 350 (1993).



312. "Theory of Second Harmonic Generation of Molecular Systems. Steady-State Case," S.H. Lin, R.G. Alden, A.A. Villaeys and V. Pflumio, *Phys. Rev.*, **A48**, 3137 (1993).
313. "Phase Dependent Absorption and Stimulated Emission in Femtosecond Pump-probe Experiments," B. Fain and S.H. Lin, *Chem. Phys. Lett.*, **207**, 287 (1993).
314. "Vibrational Relaxation of Bulk Modes Perturbed by Electronic State of Dilute Impurities," T.C. Chang, S.H. Chou, H.W. Li and S.H. Lin, *J. Chem. Phys.*, **99**, 2781 (1993).
315. "Theoretical Analysis of the Bond-shape Function of a Molecular System Imbedded in a Host Crystal--Application to F-Center," J. West, S.H. Lin and K.T. Tsen, *J. Chem. Phys.*, **99**, 7574 (1993).
316. "The Calculation of Single-vibronic Level Rate Constants for Displaced-distorted Potential Surfaces," M. Hayashi, R. Islampour and S.H. Lin, *Chem. Phys. Lett.*, **213**, 465 (1993).
317. "Theoretical Calculation of Femtosecond Time-resolved Spectra of Initial Electron Transfer in Photosynthetic Reaction Centers," S.H. Lin, R.G. Alden, M. Hayashi, S. Suzuki and H.A. Murchison, *J. Phys. Chem.*, **97**, 12566 (1993).
318. "Dual-frequency Pump-probe Time-resolved Spectroscopy," B. Fain, T.C. Chang, H.T. Liou, D.Y. Yang and S.H. Lin, *Chem. Phys. Lett.*, **216**, 551 (1993).
319. "Nitroxyl Free Radical Enhancement of the Forbidden  $O_2\left(^3\Sigma_g^-\right) \leftarrow O_2\left(^1\Delta_g\right)$  Radiative Transition in Chlorinated Hydrocarbon Solvents," R.E. Belford, G. Seely, D. Gust, T.A. Moore, A. Moore, N.J. Cherepy, S. Ekbundit, J.E. Lewis and S.H. Lin, *J. Photochem. Photobiol.*, **70A**, 125 (1993).
320. "The Kinetics of Reactions in Condensed Media by Time-resolved Photothermal Spectroscopy," J.R. Schoonover, S.H. Lin and Lauri A. Tucker, *Trends in Appl. Spectroscopy*, **1**, (1993).
321. "Phase-dependent Amplification in Pump-probe Experiments," B. Fain, V. Khidekel and S.H. Lin, *Phys. Rev.*, **49A**, 1498 (1994).
322. "Theoretical Description of Steady-state Sum-frequency Generation in Molecular Adsorbates," S. H. Lin and A.A. Villaeys, *Phys. Rev.*, **A50**, 5134 (1994).

323. "Effect of Temperature and Inhomogeneities on Binding of a Ligand to Haeme Proteins," D.W. Liao, D.-Y. Yang, S.Y. Sheu, M. Hayashi, C.K. Tang, S. Suzuki, R.G. Alden, and S.H. Lin, *J. Chin. Chem. Soc.*, **41**, 401 (1994).
324. "Theory of Second-harmonic Generation of Molecular Systems: The Case of Coincident Pulses," A.A. Villaeys, V. Pflumio and S.H. Lin, *Phys. Rev.*, **A49**, 4996 (1994).
325. "Laser-driven Spontaneous Emission: Calculation by Fourth Order Approximation," Benjamin Fain and Sheng H. Lin, *Chem. Phys. Lett.*, **228**, 191 (1994).
326. "On Absorption Line Shape Model for F-Center/ $\text{CN}^-$  Molecule Defect Pairs in CsCl" J. West, K.T. Tsen and S.H. Lin, *Phys. Rev.*, **B50**, 9759 (1994).
327. "Molecular Orbital Calculations of Electronic Excited States of PPV" J. Yu, W.S. Fann, F.J. Kao, D.Y. Yang and S.H. Lin, *Synthetic Metals*, **66**, 134 (1994).
328. "Breakdown of the Born-Oppenheimer Approximation in ZEKE States of  $\text{Ag}_2$ " C. Yeretian, H.L. Selzle, E.W. Schlag and S.H. Lin, *Chem. Phys. Lett.*, **239**, 61(1995).
329. "Vibrational Coherence and Relaxation Dynamics in the Primary Donor State of the Mutant Reaction Center of Rhodobacter Capsalutus: Theoretical Analysis of Pump-probe Stimulated Emission" X.Z. Gu, M.Hayashi, S. Suzuki and S.H. Lin, *Biochim. Biophys. Acta*, **1229**, 215 (1995).
330. "Theoretical Analyses on Femtosecond Time-resolved Spectra of Initial Electron Transfer of Photosynthetic Reaction Centers at Low Temperatures" S.H. Lin, M. Hayashi, W.Z. Xiao, S. Suzuki, X.Z. Gu and M. Sugawara, *Chem. Phys.*, **197**, 435-455 (1995).
331. "Experimental and Theoretical Studies of Absorption and Photoluminescence Excitation Spectra of Poly (p-phenylene vinylene)", J. Yu, J.H. Hsu, K.R. Chuang, C.I. Chao, S.A. Chen, F.J. Kao, W.S. Fann and S.H. Lin, *Synthetic Metals*, **74**, 7-13 (1995).
332. "Ultrafast Electron Transfer and Spectroscopy of Photosynthetic Reaction Centers," S.H. Lin, M. Hayashi, R.G. Alden, S. Suzuki, X.Z. Gu and Y.Y. Lin, In: *Femtosecond Chemistry* Edited by J. Manz and L. Waste (Berlin: Verlag Chemie), p 633, (1995).
333. "Effect of Intermolecular Vibronic Coupling on Non-radiative Transitions and Optical Absorption of Dimers," A. Pakhomov, S. Ekbundit, C. Huie Lin, R.G. Alden, R.E. Blankenship and S.H. Lin, *J. of Luminescence*, **63**, 129 (1995).

334. "Theoretical Studies of IR—UV Sum-frequency Generation Applied to Adsorbed Molecules," S.H. Lin, M. Hayashi, C.H. Lin, J. Yu, A.A. Villaeys and George Y.C. Wu, *Molecular Physics*, **84**, 453 (1995).
335. "Effect of Distortion and Displaced of Potential Surfaces on Resonance Raman scattering" R. Islampour, M. Hayashi and S.H. Lin, *Chem. Phys. Lett.*, **234**, 7 (1995).
336. "Omission in CS<sub>2</sub> Vapor Stimulated by a Counterintuitive Sequence of Pulses", V. Khidekel, B. Fain, H.T. Liou, S.H. Lin, *Chem. Phys. Lett.*, **234**, 39 (1995).
337. "On Theoretical Treatments of Electronic Excitation Energy Transfer", D.W. Liao, W.D. Cheng, J. Bigman, Y. Karni, S. Speiser and S.H. Lin, *J. Chin. Chem. Soc.*, **42**, 177 (1995).
338. "On the Investigation of the Preparation of Inorganic Ionic Clusters by Laser Desorption Ionization", H.M. Hung, C.C. Han and S.H. Lin, *J. Cluster Sci.*, **6**, 533-548 (1995).
339. "Theory of Ultrafast Time-resolved X-ray Diffraction and Applications to Vaporization Kinetics of Finite Systems", S.H. Lin, C.H. Chao, H. Ma and P.M. Rentzepis, *Proc. SPIE*, **2521**, 258-268 (1995).
340. "Femtosecond Process and Ultrafast Biological Electron Transfer", S. Suzuki, H.C. Sung, M. Hayashi, and S.H. Lin, Proceedings of Second IUPAP Topical Conference: Nonlinear and Random Processes, *Physica A*, **221**, 15-29 (1995).
341. "Lifetime Determination for High-Lying Excited States Using Z-scan". T.H. Wei, T.H. Huang, H-D. Lin and S.H. Lin, *App. Phys. Lett.*, **67**, 2266-2268 (1995).
342. "Study of the Absorption Spectrum of F-center/OH-defect pairs in CsCl, CsI and CsBr", J. West, K.T. Tsen and S.H. Lin, *Modern Physics Letters*, **9**, 26/27, 1759-1769 (1995).
343. "Molecular Theory of Second-order Sum-frequency Generation", S.H. Lin, M. Hayashi, R. Islampour, J. Yu, D.Y. Yang, and George Y.C. Wu, *Physica B*, **222**, 191-208 (1996).
344. "Theoretical Wave Packet Study on Pump-probe Stimulated Emission Signals from Electron Transfer Systems in Condensed Phases", M. Sugawara, M. Hayashi, S. Suzuki and S.H. Lin, *Mol. Phys.*, **87**, 3, 637-650 (1996).
345. "A Vibronic Theory of Steady-State Third Harmonic Generation", S.H. Lin, J. Yu, M. Hayashi, W.S. Fann, F. Guo and A.A. Villaeys, *Chem. Phys. Lett.*, **249**, 20-28 (1996).
346. " $\pi$ -bonded-trimer Formation on the Clean Diamond C(111) Surface", M. -H. Tsai, J.C. Jiang and S.H. Lin, *Phys. Rev. B*, **54**, 16, 11141 (1996).

347. "Oscillations and Non-exponential Decays in Electron-transfer Reactions", Jau Tang and S.H. Lin, *Chem. Phys. Lett.*, **254**, 1,6-12 (1996).
348. "Transient Degenerate Four-wave Mixing in Molecular Systems", A. Pakhomov, Chung-Jen Wu, Yit-Tsong Chen and S.H. Lin, *Optical and Quantum Electronics*, **28**, 1477-1493 (1996).
349. " $\pi$ - $\pi^*$  Vibronic Spectrum of Ethylene from Ab Initio Calculations of the Franck-Condon Factors", A.M. Mebel, Y.-T. Chen and S.H. Lin, *Chem. Phys. Lett.*, **258**, 53-62 (1996).
350. "Temperature Effect on the Electronic Spectra of Poly(p-phenylene vinylene)", Jenwei Yu, M. Hayashi, S.H. Lin, K.-K. Liang, J.H. Hsu, W.S. Fann, Ching-Ian Chao, Kuen-Ru Chuang, Show-An Chen, *Synthetic Metals*, **82**, 159-166 (1996).
351. "Two-dimensional Near-field Intensity Distribution of Tapered Fiber Probes", P.K. Wei, R.L. Chang, J. H. Hsu, S.H. Lin, W.S. Fann and B.R. Hsieh, *Optics Lett.*, **21**,23, 1876-1878 (1996).
352. "Resonance Fluorescence of a Single Molecule Under Near Field Excitation", R. Chang, W.S. Fann and S.H. Lin, *Applied Physics Letter*, **69** (16), 2338-2340 (1996).
353. "Stochastic Gating in Diffusion-influenced Ligand Binding to Proteins: Gated Protein versus Gated Ligands", A. M. Berezhkovskii, Dah-Yen Yang, Sheh-Yi Sheu, and Sheng Hsien Lin, *Physical Review E*, **54**, 4, 4462 (1996).
354. "On the Theoretical Investigation of Vibronic Spectrum of Ethylene by ab initio Calculations of the Franck-Condon Factors", A.M. Mebel, Y.-T. Chen, S.H. Lin, *J. Chem. Phys.*, **105**, 9007-9020 (1996).
355. "Quantum Mechanical Calculation of Line Shape Parameters for the Depolarized Raman Q branch of D<sub>2</sub> in He", R. Brezina, S.H. Lin, and W.K. Liu, *Chem. Phys. Lett.*, **262**, 437-441 (1996).
356. "Theory and Experiment of Degenerate Four-wave Mixing In Molecular Systems", A.A. Pakhomov, Yit-Tsong Chen and S.H. Lin, *Trends in Chemical Physics*, **4**, 243-268 (1996).
357. "Excitonic Energy Transfer in Light Emitting Polymers", K.K. Liang, J.H. Hsu, W.S. Fann, S.H. Lin, K.H. Lee, M.K. Leung, K.R. Chuang and S.A. Chen, *Synthetic Metals*, **84**, 953-954 (1997).

358. "Theoretical Study of Vibronic Spectra and Photodissociation Pathways of Methane", A.M. Mebel, S.H. Lin, C.-H. Chang, *J. Chem. Phys.*, **106 (7)**, 2612-2620 (1997).
359. "Excited Electronic States of the Methyl Radical. Ab Initio Molecular Orbital Study of Geometries, Excitation Energies and Vibronic Spectra", A.M. Mebel, S.H. Lin, *Chem. Phys.*, **215**, 329-341 (1997).
360. "Ab initio Molecular Orbital Study of Excited Electronic States of the Vinyl Radical", A.M. Mebel, Y.-T. Chen, S.H. Lin, *Chem. Phys. Lett.*, **275**, 19-27 (1997).
361. "Adiabatic Theory of Laser-induced Vibrational Predesorption of Physisorbed Molecules: Application to a CO/NaCl System", Y. Ohtsuki, T. Kato, Y. Fujimura and S.H. Lin, *J. Chem. Phys.*, **106 (10)**, 4339 (1997).
362. "On the Calculation of Resonance Raman Spectra", R. Islampour, M. Hayashi, and S.H. Lin, *J. Raman Spectroscopy*, **28**, 331-338 (1997).
363. "Theory of Gas-phase Time-resolved Ultrafast Electron Diffraction", W.-K. Liu and S.H. Lin, *Physical Review A*, **55**, 1, 641-647 (1997).
364. "Comment on the Spontaneous Emission Rates of ZEKE States", Sheng Der Chao, S.H. Lin, H.L. Selzle, E.W. Schlag, *Chemical Physics Letters*, **265**, 445-448 (1997).
365. "Theoretical Study on Surface Vibrational Infrared-visible Sum-frequency Generation Spectroscopy", T. Kato, M. Hayashi, A.A. Villaeys, and S.H. Lin, *Physical Review A*, **56**, 1, 980-993 (1997).
366. "Satellite Hole Investigations of the Hole-burning Mechanism and Vibrational Mode Coupling of 9-aminoacridine Doped in Glycerol-water Glasses at Different pH Values", Chien-Chih Chiang, Bor-Chyuan Hwang, Jenwei Yu, Ji-Yen Chen, Chung-Yuan Mou, Sheng-Hsien Lin and Ta-Chau Chang, *J. Chem. Soc., Faraday Trans.*, **93(7)**, 1297-1304 (1997).
367. "On the Theoretical Investigation on Spectroscopy of the Electron Donor-Acceptor Complex TCNE-HMB", M. Hayashi, T.-S. Yang, J. Yu, A. Mebel, and S.H. Lin, *J. Physical Chemistry A*, **101**, No. 23, 4156-4162 (1997).
368. "Vibronic and Vibrational Coherence and Relaxation Dynamics of Molecules in Condensed Phases", M. Hayashi, T.-S. Yang, A. Mebel, C.H. Chang, S.H. Lin, N.F. Scherer, *Chemical Physics*, **217**, 259-273 (1997).

369. "Effect of Magnetic Field on Photophysical Processes of Molecules", S.H. Lin, M. Hayashi, H. Abe and S. Ikeda, *J. of Chinese Chemical Society*, **44**, 203-210 (1997).
370. "Theoretical Modeling of the Electronic Spectra of Poly\*p-phenylene vinylene", Jenwei Yu, S.H. Lin, *Synthetic Metals*, **85**, 1115-1116 (1997).
371. "Theoretical Study on the Mechanism of the Dissociation of Benzene. The C<sub>5</sub>H<sub>3</sub>+CH<sub>3</sub> Product Channel", A. Mebel, S.H. Lin, X. M. Yang, and Y.T. Lee, *J. Phys. Chem., A*, **101**, 6638-6646 (1997).
372. "A sing ab initio MO Calculations to Understand the Photodissociation Dynamics of CH<sub>2</sub>CCH<sub>2</sub> and CH<sub>2</sub>C<sub>2</sub>", W. Jackson, A.M. Mebel, S.H. Lin, and Y.T. Lee, *J. Phys. Chem., A*, **101**, 6781-6789 (1997).
373. "Ab initio Calculations of Vibronic Coupling. Applications to Symmetry-Forbidden Vibronic Spectra and Internal Conversion in Ethylene", A.M. Mebel, M. Hayashi and S.H. Lin, *Chem. Phys. Lett.*, **274**, 281-292 (1997).
374. "Smoluchowski-type Theory of Stochastically gated Diffusion-influenced reactions", A. M. Berezhkovskii, Dah-Yen Yang, Sheng Hsien Lin, Yu A. Makhnovskii, and Sheh-Yi Sheu, *J. Chem. Phys.*, **106**(17), 6985-6998 (1997).
375. "Ab initio Molecular Orbital Study of Excited Electronic States of the Vinyl Radical", Alexander M. Mebel, Yit-Tsung Chen, and Sheng-Hsien Lin, *Chem. Phys. Lett.*, **275**, 19-27 (1997).
376. "Effect of Temperature on the Infrared and Sum-frequency Generation Spectra of Adsorbates", W.-K. Liu, M. Hayashi, J.-C. Lin, H.-C. Chang, and S.H. Lin, *J. Chem. Phys.*, **106**(14), 5920-5927 (1997).
377. "The Effect of Environment Induced Pure Decoherence on the Generalized Jaynes-Cummings Model", Gautam Gangopadhyay and S.H. Lin, *Pramana, J. of Physics*, **49** (4), 399-416 (1997).
378. "Lower Dependence of Transient Degenerate four-wave Mixing in Molecular Systems", A. Pakhomov, Chung-Jen Wu, Yit-Tsong Chen and S. H. Lin, *Physcial Review A*, **55**(4), 3086-3091 (1997).
379. "Quantum-tunneling versus Thermally Activated Electron Transfer in Ohmic and non-ohmic Heat Baths", Jau Tang and S. H. Lin, *J. Chem. Phys.*, **107** (9), 3485-3491 (1997).
380. "Identifying 2- and 3-coordinated H<sub>2</sub>O in Protonated Ion-water Clusters by Vibrational pre-dissociation spectroscopy and ab initio Calculations", Y.-S. Wang, J.C.

- Jiang and C.L. Cheng, S. H. Lin, Y.T. Lee, and H.-C. Chang, *J. Chem. Phys.*, **107**(22), 9695-9698 (1997).
381. "Theoretical Study of the Structure, Energetics, and the  $n-\pi^*$  Electronic Transition of the Acetone +  $n\text{H}_2\text{O}$  ( $n=1-3$ ) Complexes", Dai-Wei Liao, Alexander M. Mebel, Yit-Tsong Chen and Sheng-Hsien Lin, *J. Physical Chemistry A*, **101**, 51, 9925-9934 (1997).
382. "Kramers Theory of Chemical Reactions in a Slowly Adjusting Environment", A. M. Berezhkovskii, V. Yu Zitserman, S. Y. Sheu, D.-Y. Yang, J. Kuo and S. H. Lin, *J. Chem. Phys.*, **107** (24), 10539-10554 (1997)
383. "The Effect of Pure decoherence on the Jaynes-Cummings Model", G. Gangopadhyay and S. H. Lin, *Physica Scripta*, **55**, 425-430 (1997).
384. "Ab initio Calculations of Spectroscopy and Dynamics of Polyatomic Molecules", A. M. Mebel, M. Hayashi and S. H. Lin, *Trends in Physical Chemistry*, **6**, 315-341 (1997).
385. "Theories of Photo-induced Electronic Energy Transfer in Biological Systems", X.Z. Gu, M. Hayashi, K. K. Liang, R. L. Chang, C. H. Chang and S. H. Lin, *Trends in Photochemistry & Photobiology*, **4**, 183-211 (1997).
386. "Kinetic Theory of Ligand Recombination of Myoglobin: a Model for a Combination of Entropic and Enthalpic Effects", Dah-Yen Yang, Wen-Shyan Sheu, Sheh-Yi Sheu and S. H. Lin, *Molecular Physics*, **93**, 1, 159-172 (1998).
387. "Ab initio Calculations of Radiationless Transitions between Excited and Ground Singlet Electronic States of Ethylene", M. Hayashi, A.M. Mebel, K. K. Liang, and S. H. Lin, *J. Chem. Phys.*, **108**, 5, 2044-2055 (1998).
388. "Stochastic Gating Influence on the Kinetics of Diffusion-limited Reactions", Yurii A. Makhnovskii, Alexander M. Berezhkovskii, Sheh-Yi Sheu, Dah-Yen Yang, Jimmy Kuo and Sheng Hsien Lin, *J. Chem. Phys.*, **108** (3), 971-983 (1998).
389. "A Theoretical Study of Ultrafast Biological Electron Transfer", Michi-toshi Hayashi, T.-S. Yang, C. H. Chang, R. Chang, K. K. Liang and S. H. Lin, *J. of the Korean Physical Society*, **32**, 3, 217-223 (1998).
390. "A Vibronic Theory of Sum-Frequency Generation and its Application to Surface Science", D. W. Liao, M. Hayashi, W.-K. Liu, R. Islampour, T.-S. Yang George Y.C. Wu, J. Yu and S. H. Lin, *J. of the Korean Physical Society*, **32**, 3, 320-325 (1998).

391. "Potential Energy Surfaces of Excited States of  $H_2^-$ ", A. M. Mebel, S. H. Lin, L. A. Pinnaduwaage, *Chem. Phys. Lett.*, **285**, 114–120 (1998).
392. "Theoretical Studies of Coherent Phonon Generations in Dense Media", Sheng Hsien Lin, Railing Chang, Kuo Kan Liang, Jui-Hung Hsu, Jenwei Yu, Michitoshi Hayashi and Wunshain Fann, *Proceedings of SPIE*, **3277**, 56–65 (1998).
393. "Dynamical Principles in Biological Processes", E. W. Schlag, S. H. Lin, R. Weinkauff and P. M. Rentzepis, *Proc. Natl. Acad. Sci. U.S.A.*, **95**, 1358–1362 (1998).
394. "Dissipationless States in Dissipative Systems: Spin-boson Systems", Benjamin Fain, Sheng H. Lin, *Physica A*, **252**, 461–476 (1998).
395. "Ab initio Calculations of Potential Energy Surface and Rate Constants for Ethylene Photodissociation at 193 and 157 nm", A.H.H. Chang, A.M. Mebel, X.-M. Yang, S. H. Lin, Y. T. Lee, *Chem. Phys. Lett.*, **287**, 301–306 (1998).
396. "Photodissociation Dynamics of Propyne and Allene: A view from ab initio Calculations of the  $C_3H_n$  ( $n=1-4$ ) Species and the Isomerization Mechanism for  $C_3H_2$ ", A. M. Mebel, W. M. Jackson, A. H. H. Chang, and S. H. Lin, *J. of American Chemical Society*, **120**, 23, 5751–5763 (1998).
397. "Vibrotational Investigation of DODC Cation for Recognition of Guanine Dimeric Hairpin Quadruplex Studied by Satellite Holes", Ji-Yen Cheng, Sheng-Hsien Lin, and Ta-Chau Chang, *J. of Physical Chemistry B*, **102**, 28, 5542–5546 (1998).
398. "On the Electric Field on the Dynamics of High Rydberg States of Hydrogen Atom and the Model of ZEKE Spectroscopy", S.D. Chao, M. Hayashi, S. H. Lin and E. W. Schlag, *J. of Chin. Chem. Soc.*, **45**, 491–501 (1998).
399. "Ab initio/RRKM Approach Toward the Understanding of Ethylene Photodissociation", A. H. H. Chang, A. M. Mebel, X-M. Yang, S. H. Lin, and Y. T. Lee, *J. Chem. Phys.*, **109**, 7, 2748–2761 (1998).
400. "The Free-OH Stretching Frequencies of 3 Coordinated  $H_2O$  in Water Clusters and on Ice Surfaces", J. C. Jiang, J.-C. Chang, B. C. Wang, S. H. Lin, Y. T. Lee, and H.-C. Chang, *Chem. Phys. Lett.*, **289**, 373–82 (1998).
401. "Vibronic and Vibrational Coherence and Relaxation Dynamics in the TCNE-HMB Complex", M. Hayashi, T.-S. Yang, J. Yu, A. Mebel, R. Chang, S. H. Lin, Igor V. Rubtsov, and K. Yoshihara, *J. Phys. Chem. A*, **102 (23)**, 4256–4265 (1998).



402. "I-mixing Dynamics of Rydberg States of Hydrogen Atom in a Static Electric Field", S. D. Chao, M. Hayashi, S. H. Lin and E. W. Schlag, *J. Phys. B: At Mol. Opt. Phys.*, **31**, 2007-2021 (1998).
403. "Reversible Chemical Reactions in Slowly Relaxing Environments: Kramers' Turnover of the Rate Constant", A. M. Berezhkovskii, V. Yu. Zitserman, D.-Y. Yang, S. H. Lin, *Chem. Phys.*, **235**, 201-212 (1998).
404. "Effect of Trap Clustering on Brownian Particle Trapping Rate", Yu. A. Makhnovskii, D. -Y. Yang, A. M. Berezhkovskii, Sheh-Yi Sheu, and S. H. Lin, *Physical Review E*, **58**, 4, 4340-4343 (1998).
405. "Picosecond Hard X-ray Pulses and their Application to Time-resolved Diffraction", I. V. Tomov, P. Chen, S. H. Lin and P. M. Rentzepis, in "Time-resolved Diffraction" edited by J. R. Helliwell and P. M. Rentzepis (Oxford Science Publications), p 1 (1998).
406. "Theory of Ultrafast Time-resolved X-ray and Electron Diffraction", C. H. Chao, S. H. Lin, W. -K. Liu, In "Time-resolved Diffraction" edited by J. R. Helliwell and P. M. Rentzepis (Oxford Science Publications), p 260-283 (1998).
407. "Structures and Isomeric Transitions of  $\text{NH}_4^+(\text{H}_2\text{O})_{3-6}$ : From Single to Double Rings", Y. -S. Wang, J.-C. Jiang, S. H. Lin, Y. T. Lee and H. C. Chang, *J. Am. Chem. Soc.*, **120**, 8777 (1998).
408. "Activated Rate Processes in Many Dimensions: Energy Diffusion under Slow Adjustment of the Nonreactive Mode", *Physica A*, **251**, 399 (1998).
409. "Multiphoton-excited Luminescence from Diamond Nanoparticles and an Evolution to Emission Accompany the Laser Vaporization Process", Yu D. Glinka, K. -W. Lin, and S. H. Lin, *Applied Physics Letters*, 74(2), 236-238 (1999).
410. "A New Expression for Multidimensional Franck-Condon Integrals", R. Islampour, M. Dehestani, and S. H. Lin, *J. Molecular Spectroscopy*, **194**, 179-184 (1999).
411. "Quantum Dynamics of Chirped excitation of Multimode Systems", J. M. Yuan, W.-K. Liu, M. T. Hayashi and S. H. Lin, *J. Chem. Phys.*, **110**, 8, 3823-3834 (1999).
412. "Crossed-beam Reaction of Carbon Atoms with Hydrocarbon Molecules V: Chemical Dynamics of n-C<sub>4</sub>H<sub>3</sub> Formation from Reaction of C(<sup>3</sup>P<sub>j</sub>) with allene, H<sub>2</sub>CCCH<sub>2</sub> (X<sup>1</sup>A<sub>1</sub>), *J. Chem. Phys.*, **110**, 10330-10344 (1999).

413. "Isomeric Transitions between Linear and Cyclic  $H^+(CH_3OH)_{4,5}$ : Implications for Proton Migration in Liquid Methanol", J. C. Jiang, S. H. Lin, Y. T. Lee and H. -C. Chang, *J. Phys. Chem., A*, **103**, 2941-2944 (1999).
414. "Ab initio Studies of  $NH_4^+(H_2O)_{1-5}$  and the Influence of Hydrogen-bonding Nonadditivity on Geometries and Vibrations", J. C. Jiang, H.-C. Chang, Y. T. Lee and S. H. Lin, *J. Phys. Chem., A* **103**, 3123-3135 (1999).
415. " Ab Initio Molecular Orbital and Density Functional Study of the C<sub>6</sub>H<sub>6</sub>.I<sub>2</sub> Complex in the Ground and Excited Electronic States", A. M. Mebel, H. L. Lin , S. H. Lin, *Int. J. Quantum Chem.*, **72**, 307-318 (1999).
416. "Enhanced Electron Attachment to Rydberg States in Molecular Hydrogen Volume Discharges" L. A. Pinnaduwa, W. X. Ding, D. L. McCorkle, S. H. Lin, A. M. Mebel, A. Garscadden, *J. Appl. Phys.*, **85**, 7064-7069 (1999).
417. "Toward Understanding of Ethylene Photodissociation: Theoretical Study of Energy Partition in Products and Rate Constants", A. H. H. Chang, D. W. Hwang, X. M. Yang, A. M. Mebel, S. H. Lin, Y. T. Lee, *J. Chem. Phys.*, **110**, 10810-10820 (1999).
418. "Migration of an Excess Proton Upon Asymmetric Hydration:  $H^+[(CH_3)_2O](H_2O)_n$  as a Model System", J. C. Jiang, I. Hahndorf, S. H. Lin, Y. T. Lee, and H.-C. Chang, *J. Am. Chem. Soc.*, **121**, 4443-4450 (1999).
419. "Role of Trap Clustering in the Trapping Kinetics", Yu. Makhnovskii, A. M. Berezhkovskii, Sheh-Yi Sheu, D. Y. Yang and S. H. Lin, *J. Chem. Phys.*, **111**, 711-720 (1999).
420. "Multiphoton-excited Luminescence from Diamond Nanoparticles", Yu. D. Glinka, K.-W. Lin, H.-C. Chang, and S. H. Lin, *J. Physical Chem. B*, **103**, 21, 4251-4263 (1999).
421. "Local Vibrations in Systems of Interacting Adsorbed Molecules", V. M. Rozenbaum and S. H. Lin, *J. Chem. Phys.*, **110**, 12, 5919-5932 (1999).
422. "Femtosecond Pump-probe Study of Molecular Vibronic Structures and Dynamics of a Cyanine Dye in Solution", T.-S. Yang, M.-S. Chang, R. Chang, M. Hayashi, and S. H. Lin, P. Vohringer, W. Dietz, N. F. Scherer, *J. Chem. Phys.*, **110**, 24, 12070-12081 (1999).
423. "Ab initio Study of the n- $\pi^*$  Electronic Transition in Acetone: Symmetry-Forbidden Vibronic Spectra", D. W. Liao, A. M. Mebel, M. Hayashi, Y. J. Shiu, Y. T. Chen, S. H. Lin, *J. Chem. Phys.*, **111**, 1, 205-215 (1999).

424. "Crossed Beam of Cyano Radicals with Hydrocarbon Molecules. I. Chemical Dynamics of Cyanobenzene ( $C_6H_5CN; X^1A_1$ ) and Perdeutero Cyanobenzene ( $C_6D_5CN; X^1A_1$ ) Formation from Reaction of  $CN(X^2\Sigma^+)$  with benzene  $C_6H_6(X^1A_{1g})$ , and d<sub>6</sub>-benzene  $C_6D_6(X^1A_{1g})$ , N. Balucani, O. Asvany, A. H. H. Chang, S. H. Lin, Y. T. Lee, and R. I. Kaiser, H. F. Bettinger, P.v.R. Schleyer, and H. F. Schaefer III, *J. Chem. Phys.*, **111**, 16, 7457-7471 (1999).
425. "Excitation of the NO Molecule by Chirped Infrared Laser Pulses", J. T. Lin, M. Hayashi, and S. H. Lin, *Physical Review A*, **60**, 5, 3911-3915 (1999).
426. "Crossed Beam Reaction of Cyano Radicals with Hydrocarbon Molecules. II. Chemical Dynamics of 1-Cyano-1-methylallene ( $CNCH_3CCCH_2; X^1A'$ ) Formation from Reaction of  $CN(X^2\Sigma^+)$  with Dimethylacetylene  $CH_3CCCH_3(X^1A'_1)$ , N. Balucani, O. Asvany, A. H. H. Chang, S. H. Lin, Y. T. Lee, and R. I. Kaiser, H. F. Bettinger, P.v.R. Schleyer, and H. F. Schaefer III, *J. Chem. Phys.*, **111**, 16, 7472-7479 (1999).
427. "Excitation energy-transfer processes between two trimers in C-phycocyanin hexamer from the cyanobacterium *Anabaena variabilis*. Investigation by group theory and time-resolved fluorescence spectroscopy", J. M. Zhang, F. L. Zhao, X. G. Zheng, H. Z. Wang, T. S. Yang, M. Hayashi, and S. H. Lin, *J. Photochem. Photobiol., B-Biology*, **53**, 128-135 (1999).
428. "Molecular-dynamics study of the C-H vibrational spectra on diamond (111) and (100) surfaces", M. H. Tsai, J. C. Jiang, and S. H. Lin, *Phys. Rev. B*, **60**, 16972-16976 (1999).
429. "An asymptotic series solution to the Schrodinger equation for a model potential", S. D. Chao, and S. H. Lin, *Eur. Phys. J. D*, **7**, 475-478 (1999).
430. "Effects of displacement and distortion of potential surfaces on absorption and emission spectra of MPV oligomer in solutions", C. H. Chang, J. C. Chang, R. Chang, J. H. Hsu, W. S. Fann, M. Hayashi, J. Yu, J. C. Jiang, S. H. Lin, Y. Z. Lee, K. R. Chuang, and S. A. Chen, *Synth. Met.*, **106**, 139-144 (1999).
431. "Ab initio calculations of vibronic spectra and dynamics for small polyatomic molecules: Role of Duschinsky effect", A. M. Mebel, M. Hayashi, K. K. Liang, and S. H. Lin, *J. Phys. Chem. A*, **103**, 10674-10690 (1999).

432. "Effect of a cyclic fragment in a polymethine chain on absorption region and intensity", M. L. Dekhtyar, V. M. Rozenbaum, and S. H. Lin, *J. Mol. Struct.-Theochem*, **490**, 263-267 (1999).
433. "A theoretical study of photocurrent in conjugated polymer systems", R. Chang, and S. H. Lin, *J. Chin. Chem. Soc.*, **46**, 651-658 (1999).
434. "Calculation of the cross sections for the n, l-changing collisions of Rydberg hydrogen", S. D. Chao, and S. H. Lin, *Chin. J. Phys.*, **37**, 442-448 (1999).
435. "Photoionization of methanol dimer using a tunable vacuum ultraviolet laser", S. T. Tsai, J. C. Jiang, Y. T. Lee, A. H. Kung, S. H. Lin, and C. K. Ni, *J. Chem. Phys.*, **111**, 3434-3440 (1999).
436. "Classical dynamics of multiphoton excitation and dissociation of diatomic molecules by infrared laser pulses", W. K. Liu, J. M. Yuan, and S. H. Lin, *Phys. Rev. A*, **60**, 1363-1370 (1999).
437. "A numerical study on vibronic and vibrational dynamics generated by chirped laser pulses in the presence of relaxation processes", K. Mishima, M. Hayashi, J. T. Lin, K. Yamashita, and S. H. Lin, *Chem. Phys. Lett.*, **309**, 279-286 (1999).
438. "The photoluminescence from hydrogen-related species in composites of SiO<sub>2</sub> nanoparticles", Y. D. Glinka, S. H. Lin, and Y. T. Chen, *Appl. Phys. Lett.*, **75**, 778-780 (1999).
439. "On theoretical study of a molecular dimer system", M. Hayashi, Y. J. Shiu, C. H. Chang, K. K. Liang, R. Chang, T. S. Yang, R. Islampour, J. Yu, and S. H. Lin, *J. Chin. Chem. Soc.*, **46**, 381-393 (1999).
440. "Molecular vibronic structures of HDITC in solutions studied by femtosecond wavelength-resolved pump-probe spectroscopy", T. S. Yang, P. Vohringer, W. Dietz, N. F. Scherer, and S. H. Lin, *J. Chin. Chem. Soc.*, **46**, 409-416 (1999).
441. "Theory of vibrational predissociation spectroscopy", R. Chang, J. C. Jiang, P. J. Hsieh, H. C. Chang, and S. H. Lin, *J. Chin. Chem. Soc.*, **46**, 417-426 (1999).
442. "On the search for H<sub>5</sub>O<sub>2</sub><sup>+</sup>-centered water clusters in the gas phase", H. C. Chang, J. C. Jiang, H. C. Chang, Y. S. Wang, S. H. Lin, and Y. T. Lee, *J. Chin. Chem. Soc.*, **46**, 427-434 (1999).

443. "Relaxation times of a dissipative two-state system for a resonance treatment. Application to electron transfer reactions", T. Cheche, and S. H. Lin, *Chem. Phys.*, **243**, 123-135 (1999).
444. "Investigation of the validity conditions of using an isolated-line approximation to the level-mixing model", S. D. Chao, M. Hayashi, S. H. Lin, and E. W. Schlag, *Chem. Phys. Lett.*, **302**, 255-261 (1999).
445. "The I-mixing dynamics of high Rydberg states and the high resolution principle of ZEKE spectroscopy", S. D. Chao, M. Hayashi, S. H. Lin, and E. W. Schlag, *Abstr. Pap. Am. Chem. Soc.*, **217**, U363-U363 (1999).
446. Y. D. Glinka, K. W. Lin, H. C. Chang, S. H. Lin, and Y. T. Chen, In: *Defects and Diffusion in Ceramics*, p 37-44 (2000).
447. "Time-resolved phase transitions of the nanocrystalline cubic to submicron monoclinic phase in zirconia", M. Lajavardi, D. J. Kenney, and S. H. Lin, *J. Chin. Chem. Soc.*, **47**, 1043-1053 (2000).
448. "Time-resolved phase transitions of the nanocrystalline cubic to submicron monoclinic phase in  $\text{Mn}_2\text{O}_3\text{-ZrO}_2$ ", M. Lajavardi, D. J. Kenney, and S. H. Lin, *J. Chin. Chem. Soc.*, **47**, 1055-1063 (2000).
449. "Time-resolved high and low temperature phase transitions of the nanocrystalline cubic phase in the  $\text{Y}_2\text{O}_3\text{-ZrO}_2$  and  $\text{Fe}_2\text{O}_3\text{-ZrO}_2$  system", M. Lajavardi, D. J. Kenney, and S. H. Lin, *J. Chin. Chem. Soc.*, **47**, 1065-1075 (2000).
450. "Photoluminescence from mesoporous silica: Similarity of properties to porous silicon", Y. D. Glinka, S. H. Lin, L. P. Hwang, and Y. T. Chen, *Appl. Phys. Lett.*, **77**, 3968-3970 (2000).
451. "A combined crossed beam and ab initio investigation on the reaction of carbon species with  $\text{C}_4\text{H}_6$  isomers. I. The 1,3-butadiene molecule,  $\text{H}_2\text{CCHCHCH}_2(\text{X}(1)\text{A}')$ ", I. Hahndorf, H. Y. Lee, A. M. Mebel, S. H. Lin, Y. T. Lee, and R. I. Kaiser, *J. Chem. Phys.*, **113**, 9622-9636 (2000).
452. "A combined crossed beam and ab initio investigation on the reaction of carbon species with  $\text{C}_4\text{H}_6$  isomers. II. The dimethylacetylene molecule,  $\text{H}_3\text{CCCCH}_3(\text{X}(1)\text{A}(1\text{g}))$ ", L. C. L. Huang, H. Y. Lee, A. M. Mebel, S. H. Lin, Y. T. Lee, and R. I. Kaiser, *J. Chem. Phys.*, **113**, 9637-9648 (2000).

453. "Application of the density matrix method to spectroscopy and dynamics of photosynthetic reaction centers", M. Hayashi, T. S. Yang, C. H. Chang, K. K. Liang, R. L. Chang, and S. H. Lin, *Int. J. Quantum Chem.*, **80**, 1043-1054 (2000).
454. "Crossed beam reaction of cyano radicals with hydrocarbon molecules. III. Chemical dynamics of vinylcyanide ( $C_2H_3CN$ ;  $X1A'$ ) formation from reaction of  $CN(X(2)\Sigma(+))$  with Ethylene,  $C_2H_4(X(1)A(g))$ ", N. Balucani, O. Asvany, A. H. H. Chang, S. H. Lin, Y. T. Lee, R. I. Kaiser, and Y. Osamura, *J. Chem. Phys.*, **113**, 8643-8655 (2000).
455. "Crossed beam reaction of cyano radicals with hydrocarbon molecules. IV. Chemical dynamics of cyanoacetylene ( $HCCCN$ ;  $X(1)\Sigma(+)$ ) formation from reaction of  $CN(X(2)\Sigma(+))$  with acetylene,  $C_2H_2(X(1)\Sigma(+)(g))$ ", L. C. L. Huang, O. Asvany, A. H. H. Chang, N. Balucani, S. H. Lin, Y. T. Lee, R. I. Kaiser, and Y. Osamura, *J. Chem. Phys.*, **113**, 8656-8666 (2000).
456. "Simulation of the Wiener sausage", D. Y. Yang, Y. A. Makhnovskii, S. Y. Sheu, and S. H. Lin, *Phys. Rev. E*, **62**, 3116-3120 (2000).
457. "Extended approximated Born-Oppenheimer equation - I. Theory", M. Baer, S. H. Lin, A. Alijah, S. Adhikari, and G. D. Billing, *Phys. Rev. A*, **62** (2000).
458. "Extended approximated Born-Oppenheimer equation. II. Application", S. Adhikari, G. D. Billing, A. Alijah, S. H. Lin, and M. Baer, *Phys. Rev. A*, **62** (2000).
459. "Photoluminescence spectroscopy of silica-based mesoporous materials", Y. D. Glinka, S. H. Lin, L. P. Hwang, and Y. T. Chen, *J. Phys. Chem. B*, **104**, 8652-8663 (2000).
460. "Generalised master equation for the spin-boson Hamiltonian by the projection operator technique", T. O. Cheche, M. Hayashi, and S. H. Lin, *J. Chin. Chem. Soc.*, **47**, 729-739 (2000).
461. "Models of ultrafast energy and electron transfers in bacterial reaction centers", M. Hayashi, T. S. Yang, K. K. Liang, C. H. Chang, and S. H. Lin, *J. Chin. Chem. Soc.*, **47**, 741-752 (2000).
462. "Homogeneous line-width of optical transitions and multiple electron-LO-phonon scattering in quantum dots", K. Kral, Z. Khas, C. Y. Lin, and S. H. Lin, *J. Chin. Chem. Soc.*, **47**, 753-757 (2000).
463. "A theoretical analysis of absorption spectra and dynamics of photosynthetic reaction centers", C. H. Chang, M. Hayashi, R. Chang, K. K. Liang, T. S. Yang, and S. H. Lin, *J. Chin. Chem. Soc.*, **47**, 785-797 (2000).

464. "Dynamical principles in biological processes: A model of charge migration in proteins and DNA", E. W. Schlag, D. Y. Yang, S. Y. Sheu, H. L. Selzle, S. H. Lin, and P. M. Rentzepis, *Proceedings of the National Academy of Sciences of the United States of America*, **97**, 9849–9854 (2000).
465. "Two-photon-excited luminescence and defect formation in SiO<sub>2</sub> nanoparticles induced by 6.4-eV ArF laser light", Y. D. Glinka, S. H. Lin, and Y. T. Chen, *Phys. Rev. B*, **62**, 4733–4743 (2000).
466. "Surface-enhanced Raman scattering at cryogenic substrate temperatures", R. Chang, P. T. Leung, S. H. Lin, and W. S. Tse, *Phys. Rev. B*, **62**, 5168–5173 (2000).
467. "Theory of charge transport in polypeptides", E. W. Schlag, S. Y. Sheu, D. Y. Yang, H. L. Selzle, and S. H. Lin, *J. Phys. Chem. B*, **104**, 7790–7794 (2000).
468. "Heats of formation of small bicyclic hydrocarbons, spiropentadiene (C<sub>5</sub>H<sub>4</sub>), spiropentane (C<sub>5</sub>H<sub>8</sub>) and bicyclo[1.1.0]but-1(3)-ene (C<sub>4</sub>H<sub>4</sub>): a theoretical study by the G2M(RCC,MP2) method", T. L. Nguyen, T. N. Le, A. M. Mebel, and S. H. Lin, *Chem. Phys. Lett.*, **326**, 468–476 (2000).
469. "Novel approach of calculating the optical spectra of molecules with Duschinsky effects", K. K. Liang, M. Hayashi, and S. H. Lin, *Abstr. Pap. Am. Chem. Soc.*, **219**, U612–U612 (2000).
470. "A high-pressure FT-IR study of the isotope effects on water and high-pressure ices", H. C. Chang, K. H. Huang, Y. L. Yeh, and S. H. Lin, *Chem. Phys. Lett.*, **326**, 93–100 (2000).
471. "Ab initio study of H photodetachment from the ethyl radical", A. S. Zyubin, A. M. Mebel, and S. H. Lin, *Chem. Phys. Lett.*, **323**, 441–447 (2000).
472. "Optical line-shape and the time-domain photon echo measurement in semiconductor quantum dots", K. Kral, Z. Khas, C. Y. Lin, and S. H. Lin, *Opt. Commun.*, **180**, 271–275 (2000).
473. "Probing the nature of surface intersection by ab initio calculations of the nonadiabatic coupling matrix elements: A conical intersection due to bending motion in C<sub>2</sub>H", A. M. Mebel, M. Baer, and S. H. Lin, *J. Chem. Phys.*, **112**, 10703–10706 (2000).
474. "Trapping by clusters of traps", Y. A. Makhnovskii, A. M. Berezhkovskii, D. Y. Yang, S. Y. Sheu, and S. H. Lin, *Phys. Rev. E*, **61**, 6302–6307 (2000).

475. "Determining the structure of trimethylphosphine bound to the Bronsted acid site in zeolite HY: Double-resonance NMR and ab initio studies", H. M. Kao, H. M. Liu, J. C. Jiang, S. H. Lin, and C. P. Grey, *J. Phys. Chem. B*, **104**, 4923-4933 (2000).
476. "Orientational states, phase transitions, and spectra of vibrational excitations for two-dimensional systems with quadrupole interactions", V. M. Rozenbaum, and S. H. Lin, *J. Chem. Phys.*, **112**, 9083-9091 (2000).
477. "Dipolar dispersion laws and their contribution to dephasing of high-frequency collective vibrations in surface molecular ensembles", V. M. Rozenbaum, and S. H. Lin, *Surf. Sci.*, **452**, 67-78 (2000).
478. "The absorption and emission spectra of 1,4-di(2-phenylvinyl)benzene. A theoretical analysis", J. W. Yu, W. S. Fann, and S. H. Lin, *Theor. Chem. Acc.*, **103**, 374-379 (2000).
479. "Dissociation dynamics of  $\text{HeRh}_2^+$  in field-ion microscopy", J. T. Lin, J. M. Yuan, S. C. Smith, and S. H. Lin, *Phys. Rev. B*, **61**, 9419-9426 (2000).
480. "A theoretical study of the reactions of  $\text{S(D-1)}+\text{H-2}$ , HD, D-2", A. H. H. Chang, and S. H. Lin, *Chem. Phys. Lett.*, **320**, 161-168 (2000).
481. "Dissociation and dynamics of the high-vibrational-state HF molecules under intense half-cycle and few-cycle pulses", J. T. Lin, S. H. Lin, and T. F. Jiang, *Phys. Rev. A*, **61**, 033407 (2000).
482. "Ultrafast dynamics probed by the time-resolved anisotropy measurements", M. Hayashi, T. S. Yang, K. K. Liang, C. H. Chang, R. L. Chang, and S. H. Lin, *J. Chin. Chem. Soc.*, **47**, 117-127 (2000).
483. "Infrared spectra of  $\text{H}^+(\text{H}_2\text{O})(5-8)$  clusters: Evidence for symmetric proton hydration", J. C. Jiang, Y. S. Wang, H. C. Chang, S. H. Lin, Y. T. Lee, G. Niedner-Schatteburg, and H. C. Chang, *J. Am. Chem. Soc.*, **122**, 1398-1410 (2000).
484. "Charge conductivity in peptides: Dynamic simulations of a bifunctional model supporting experimental data", E. W. Schlag, S. Y. Sheu, D. Y. Yang, H. L. Selzle, and S. H. Lin, *Proceedings of the National Academy of Sciences of the United States of America*, **97**, 1068-1072 (2000).
485. "Experimental and theoretical investigations of absorption and emission spectra of the light-emitting polymer MEH-PPV in solution", R. Chang, J. H. Hsu, W. S. Fann, K. K. Liang, C. H. Chiang, M. Hayashi, J. Yu, S. H. Lin, E. C. Chang, K. R. Chuang, and S. A. Chen, *Chem. Phys. Lett.*, **317**, 142-152 (2000).



486. "Aggregated states of luminescent conjugated polymers in solutions", R. Chang, J. H. Hsu, W. S. Fann, J. Yu, S. H. Lin, Y. Z. Lee, and S. A. Chen, *Chem. Phys. Lett.*, **317**, 153-158 (2000).
487. "Calculation of resonance Raman excitation profiles", R. Islampour, M. Dehestani, and S. H. Lin, *Mol. Phys.*, **98**, 101-110 (2000).
488. "Behaviors of an excess proton in solute-containing water clusters: A case study of  $H^+(CH_3OH)(H_2O)(1-6)$ ", C. C. Wu, J. C. Jiang, D. W. Boo, S. H. Lin, Y. T. Lee, and H. C. Chang, *J. Chem. Phys.*, **112**, 176-188 (2000).

## 2001 – 2010

489. "Photodissociation and photoisomerization of small aromatic molecules in a molecular beam", C. L. Huang, J. C. Jiang, S. H. Lin, Y. T. Lee, and C. K. Ni, *Aust. J. Chem.*, **54**, 561-571 (2001).
490. "A theory of coulomb explosion of molecules", S. H. Lin, K. Mishima, M. Hayashi, A. H. H. Chang, J. Yi, and A. M. Mebel, *J. Chin. Chem. Soc.*, **48**, 963-969 (2001).
491. "Product branching ratios of the  $C(P-3)+C_2H_3((2)A')$  and  $CH((2)Pi)+C_2H_2(1\Sigma^+(+)(g))$  reactions and photodissociation of  $H_2CCCH(B-2(1))$  at 193 and 242 nm: an ab initio/RRKM study", T. L. Nguyen, A. M. Mebel, S. H. Lin, and R. I. Kaiser, *J. Phys. Chem. A*, **105**, 11549-11559 (2001).
492. "Dissipative dynamics and electronic coherence", T. O. Cheche, and S. H. Lin, *Chem. Phys.*, **274**, 165-173 (2001).
493. "Dynamics of the spin-boson Hamiltonian by the projection operator technique: Applications to electron transfer reactions", T. O. Cheche, and S. H. Lin, *Phys. Rev. E*, **64**, art no. 061103 (2001).
494. "Intermolecular potential and equilibrium orientational states for dimers of non-polar molecules", V. M. Rozenbaum, A. M. Mebel, and S. H. Lin, *Mol. Phys.*, **99**, 1883-1897 (2001).
495. "Photoluminescence properties of silica-based mesoporous materials similar to those of nanoscale silicon", Y. D. Glinka, A. S. Zyubin, A. M. Mebel, S. H. Lin, L. P. Hwang, and Y. T. Chen, *Eur. Phys. J. D*, **16**, 279-283 (2001).

496. "Pressure-dependent studies on hydration of the C-H group in formic acid", H. C. Chang, J. C. Jiang, M. C. Chao, M. S. Lin, S. H. Lin, H. Y. Chen, and H. C. Hsueh, *J. Chem. Phys.*, **115**, 8032-8037 (2001).
497. "Investigations of ultrafast exciton dynamics in allophycocyanin trimer", J. M. Zhang, Y. J. Shiu, M. Hayashi, K. K. Liang, C. H. Chang, V. Gulbinas, C. M. Yang, T. S. Yang, H. Z. Wang, Y. T. Chen, and S. H. Lin, *J. Phys. Chem. A*, **105**, 8878-8891 (2001).
498. "Computational formulas for symmetry-forbidden vibronic spectra and their application to n- $\pi^*$  transition in neat acetone", Y. J. Shiu, M. Hayashi, A. M. Mebel, Y. T. Chen, and S. H. Lin, *J. Chem. Phys.*, **115**, 4080-4094 (2001).
499. "Ultrafast dynamics of excitations in conjugated polymers: A spectroscopic study", R. Chang, M. Hayashi, S. H. Lin, J. H. Hsu, and W. S. Fann, *J. Chem. Phys.*, **115**, 4339-4348 (2001).
500. "Size effect in self-trapped exciton photoluminescence from SiO<sub>2</sub>-based nanoscale materials", Y. D. Glinka, S. H. Lin, L. P. Hwang, Y. T. Chen, and N. H. Tolk, *Phys. Rev. B*, **6408**, 085421 (2001).
501. "High-pressure and concentration-dependent studies on C-H...O interactions of binary aqueous mixtures: Formic acid/D<sub>2</sub>O and acetone/D<sub>2</sub>O", M. C. Chao, N. H. Weng, H. C. Chang, J. C. Jiang, and S. H. Lin, *J. Chin. Chem. Soc.*, **48**, 603-607 (2001).
502. "Sum frequency vibrational spectroscopy of the liquid-air interface of aqueous solutions of ethanol in the OH region", S. S. Ju, T. D. Wu, Y. L. Yeh, T. H. Wei, J. Y. Huang, and S. H. Lin, *J. Chin. Chem. Soc.*, **48**, 625-629 (2001).
503. "Theory of medium-induced optical activities", F. C. Hsu, Y. T. Kuo, Y. J. Shiu, K. K. Liang, M. Hayashi, T. C. Chang, and S. H. Lin, *J. Chin. Chem. Soc.*, **48**, 631-639 (2001).
504. "Investigations of ultrafast dynamics in light-emitting polymers", R. Chang, M. Hayashi, K. K. Liang, and S. H. Lin, *J. Chin. Chem. Soc.*, **48**, 641-649 (2001).
505. "Evidence for C-H-O interaction of acetone and deuterium oxide probed by high-pressure", H. C. Chang, J. C. Jiang, S. H. Lin, N. H. Weng, and M. C. Chao, *J. Chem. Phys.*, **115**, 3215-3218 (2001).
506. "The role of the ground and excited potential energy surfaces in the O(D-1 and P-3)+SiH<sub>4</sub> reactions: A theoretical study", T. L. Nguyen, A. M. Mebel, and S. H. Lin, *J. Chem. Phys.*, **114**, 10816-10834 (2001).

507. "Branching ratios of C-2 products in the photodissociation of C<sub>2</sub>H at 193 nm", A. M. Mebel, M. Hayashi, W. M. Jackson, J. Wrobel, M. Green, D. D. Xu, and S. H. Lin, *J. Chem. Phys.*, **114**, 9821-9831 (2001).
508. "Time-resolved extended x-ray absorption fine structure (EXAFS) studies by means of an energy dispersive spectrometer", D. A. Oulianov, I. V. Tomov, S. H. Lin, and P. M. Rentzepis, *J. Chin. Chem. Soc.*, **48**, 127-132 (2001).
509. "Ab initio molecular orbital/Rice-Ramsperger-Kassel-Marcus theory study of multichannel rate constants for the unimolecular decomposition of benzene and the H+C<sub>6</sub>H<sub>5</sub> reaction over the ground electronic state", A. M. Mebel, M. C. Lin, D. Chakraborty, J. Park, S. H. Lin, and Y. T. Lee, *J. Chem. Phys.*, **114**, 8421-8435 (2001).
510. "Ab initio study of nonadiabatic coupling matrix elements between excited 2(2)A' and 3(2)A' electronic states of C<sub>2</sub>H", A. M. Mebel, M. Baer, V. M. Rozenbaum, and S. H. Lin, *Chem. Phys. Lett.*, **336**, 135-142 (2001).
511. "Influence of the transverse velocity on TC-RFWM spectra of jet-cooled CH", A. A. Villaeys, K. K. Liang, and S. H. Lin, *Chem. Phys. Lett.*, **336**, 268-277 (2001).
512. "Degenerate conical intersections: The interaction between the 3 (2)A(') and 4 (2)A(') electronic states of C<sub>2</sub>H as a case study", A. M. Mebel, M. Baer, and S. H. Lin, *J. Chem. Phys.*, **114**, 5109-5112 (2001).
513. "A theoretical analysis of absorption spectra of photosynthetic reaction centers: Mechanism of temperature dependent peak shift", C. H. Chang, M. Hayashi, K. K. Liang, R. Chang, and S. H. Lin, *J. Phys. Chem. B*, **105**, 1216-1224 (2001).
514. "Structure of the acetone liquid/vapor interface", Y. L. Yeh, C. Zhang, H. Held, A. M. Mebel, X. Wei, S. H. Lin, and Y. R. Shen, *J. Chem. Phys.*, **114**, 1837-1843 (2001).
515. "Xanthophylls as possible IRBP Ligands", E. D. Gonzalez-Fernandez, Y. J. Shiu, S. H. Lin, and F. Gonzalez-Fernandez, *Invest. Ophthalmol. Vis. Sci.*, **43**, U1005-U1005 (2002).
516. "The Crude Born-Oppenheimer Adiabatic Approximation of Molecular Potential Energies", K. K. Liang, J. C. Jiang, V. V. Kislov, A. M. Mebel, S. H. Lin, and M. Hayashi, *Adv. Chem. Phys.*, **124**, 505 (2002).
517. "A transient absorption study of allophycocyanin", Y. J. Shiu, J. M. Zhang, M. Hayashi, V. Gulbinas, C. M. Yang, and S. H. Lin, *Proc. Indian Acad. Sci.-Chem. Sci.*, **114**, 611-621 (2002).

518. "Theoretical studies of the long-range Coulomb potential effect on photoionization by strong lasers", K. Mishima, M. Hayashi, J. Yi, S. H. Lin, H. L. Selzle, and E. W. Schlag, *Phys. Rev. A*, **66** (2002).
519. "Tunneling ionization rates of atoms and molecules", K. Mishima, M. Hayashi, J. Yi, S. H. Lin, H. L. Selzle, and E. W. Schlag, *J. Chin. Chem. Soc.*, **49**, 639-649 (2002).
520. "Intermolecular interactions in aqueous dimethyl sulphoxide and acetic acid probed by high-pressure FTIR", C. M. Feng, H. E. Kao, C. C. Su, J. C. Jiang, S. H. Lin, and H. C. Chang, *J. Chin. Chem. Soc.*, **49**, 663-667 (2002).
521. "Theory of the Stark effect on single molecular spectroscopy", M. Hayashi, C. H. Chiang, K. K. Liang, Y. J. Shiu, C. H. Chang, D. Y. Wu, F. Y. Li, T. C. Chang, U. Wild, T. Y. Latychevskaia, and S. H. Lin, *J. Chin. Chem. Soc.*, **49**, 797-804 (2002).
522. "Generalization of Keldysh's theory", K. Mishima, M. Hayashi, J. Yi, S. H. Lin, H. L. Selzle, and E. W. Schlag, *Phys. Rev. A*, **66**, 053408 (2002).
523. "Prediction of absolute rate coefficients and product branching ratios for the C(P-3) plus allene reaction system", H. W. Schranz, S. C. Smith, A. M. Mebel, and S. H. Lin, *J. Chem. Phys.*, **117**, 7055-7067 (2002).
524. "An ab initio/Rice-Ramsperger-Kassel-Marcus study of photo dissociation of carbonyl cyanide", H. Y. Lee, A. M. Mebel, and S. H. Lin, *Int. J. Quantum Chem.*, **90**, 566-574 (2002).
525. "Molecular twisting and relaxation in the excited state of triarylpyrylium cations", D. Abramavicius, V. Gulbinas, L. Valkunas, Y. J. Shiu, K. K. Liang, M. Hayashi, and S. H. Lin, *J. Phys. Chem. A*, **106**, 8864-8869 (2002).
526. "A theoretical study of the O(D-1)+CH<sub>4</sub> reaction I", A. H. H. Chang, and S. H. Lin, *Chem. Phys. Lett.*, **363**, 175-181 (2002).
527. "Correlation between optical properties and chain-length in a quasi-one-dimensional electronic polymer", J. H. Hsu, M. T. Hayashi, S. H. Lin, W. S. Fann, L. J. Rothberg, G. Y. Perng, and S. A. Chen, *J. Phys. Chem. B*, **106**, 8582-8586 (2002).
528. "Ab initio study of excited electronic states and vibronic spectra of phenyl radical", G. S. Kim, A. M. Mebel, and S. H. Lin, *Chem. Phys. Lett.*, **361**, 421-431 (2002).

529. "Time-resolved photoluminescence study of silica nanoparticles as compared to bulk type-III fused silica", Y. D. Glinka, S. H. Lin, and Y. T. Chen, *Phys. Rev. B*, **66**, 035404 (2002).
530. "On the search for C-H-O hydrogen bonding in aqueous acetic acid: Combined high-pressure infrared spectroscopy and ab initio calculations study", H. C. Chang, J. C. Jiang, M. S. Lin, H. E. Kao, C. M. Feng, Y. C. Huang, and S. H. Lin, *J. Chem. Phys.*, **117**, 3799-3803 (2002).
531. "Polaron model in self-assembled InAs/GaAs quantum dots - A perturbative approach", P. Lelong, and S. H. Lin, *Appl. Phys. Lett.*, **81**, 1002-1004 (2002).
532. "Theory of single molecule fluorescence in large molecular systems", A. A. Villaeys, and S. H. Lin, *J. Lumines.*, **98**, 97-105 (2002).
533. "Hydrophobic hydration in aqueous acetic acid and formic acid solutions probed by high pressure", M. S. Lin, C. M. Feng, H. E. Kao, Y. C. Huang, H. C. Chang, J. C. Jiang, and S. H. Lin, *J. Lumines.*, **98**, 177-182 (2002).
534. "Doubly-resonant sum-frequency generation spectroscopy for surface studies", M. B. Raschke, M. Hayashi, S. H. Lin, and Y. R. Shen, *Chem. Phys. Lett.*, **359**, 367-372 (2002).
535. "Charge-enhanced C-H - O interactions of a self-assembled triple helical spine probed by high-pressure", H. C. Chang, K. M. Lee, J. C. Jiang, M. S. Lin, J. S. Chen, I. J. B. Lin, and S. H. Lin, *J. Chem. Phys.*, **117**, 1723-1728 (2002).
536. "Dissociation pathways of benzene trication", T. S. Zyubina, G. S. Kim, S. H. Lin, A. M. Mebel, and A. D. Bandrauk, *Chem. Phys. Lett.*, **359**, 253-261 (2002).
537. "Effect of polydispersity on Brownian-particle trapping by clusters of traps", Y. A. Makhnovskii, S. Y. Sheu, D. Y. Yang, and S. H. Lin, *J. Chem. Phys.*, **117**, 897-901 (2002).
538. "Photoluminescence from mesoporous silica akin to that from nanoscale silicon: the nature of light-emitters", Y. D. Glinka, A. S. Zyubin, A. M. Mebel, S. H. Lin, L. P. Hwang, and Y. T. Chen, *Chem. Phys. Lett.*, **358**, 180-186 (2002).
539. "Ab initio and DFT study of the formation mechanisms of polycyclic aromatic hydrocarbons: The phenanthrene synthesis from biphenyl and naphthalene", V. V. Kislov, A. M. Mebel, and S. H. Lin, *J. Phys. Chem. A*, **106**, 6171-6182 (2002).

540. "Photoluminescence of silanone and dioxasilyrane groups in silicon oxides: A theoretical study", A. S. Zyubin, A. M. Mebel, S. H. Lin, and Y. D. Glinka, *J. Chem. Phys.*, **116**, 9889-9896 (2002).
541. "Photodissociation of ethylbenzene at 248 nm", C. L. Huang, J. C. Jiang, S. H. Lin, Y. T. Lee, and C. K. Ni, *J. Chem. Phys.*, **116**, 7779-7782 (2002).
542. "Ultrafast Dynamics and Spectroscopy of Bacterial Photosynthetic Reaction Centers" S. H. Lin, C. H. Chang, K. K. Liang, R. Chang, Y. J. Shiu, J. M. Zhang, T. S. Yang, M. Hayashi, and F. C. Hsu, *Adv. Chem. Phys.*, **121**, 1 (2002).
543. "Experimental and theoretical studies of the effects of collisions and magnetic fields on quantum beat", C. H. Chang, C. L. Huang, C. K. Ni, H. L. Dai, M. Hayashi, K. K. Liang, A. Kung, I. C. Chen, and S. H. Lin, *Mol. Phys.*, **100**, 1117-1128 (2002).
544. "Photoisomerization and photodissociation of toluene in molecular beam", C. K. Lin, C. L. Huang, J. C. Jiang, A. H. H. Chang, Y. T. Lee, S. H. Lin, and C. K. Ni, *J. Am. Chem. Soc.*, **124**, 4068-4075 (2002).
545. "A molecular theory for doubly resonant IR-UV-vis sum-frequency generation", M. Hayashi, S. H. Lin, M. B. Raschke, and Y. R. Shen, *J. Phys. Chem. A*, **106**, 2271-2282 (2002).
546. "Ab initio study of the ammoniated ammonium ions  $\text{NH}_4^+(\text{NH}_3)(0-6)$ ", B. C. Wang, J. C. Chang, J. C. Jiang, and S. H. Lin, *Chem. Phys.*, **276**, 93-106 (2002).
547. "Self-organization of triple-stranded carbon nanoropes", C. J. Su, D. W. Hwang, S. H. Lin, B. Y. Jin, and L. P. Hwang, *PhysChemComm*, 34-36 (2002).
548. "Red and near-infrared photoluminescence from silica-based nanoscale materials: Experimental investigation and quantum-chemical modeling", A. S. Zyubin, Y. D. Glinka, A. M. Mebel, S. H. Lin, L. P. Hwang, and Y. T. Chen, *J. Chem. Phys.*, **116**, 281-294 (2002).
549. "Ab initio/RRKM study of dissociation mechanism of benzene trication", T. S. Zyubin, G. S. Kim, A. M. Mebel, S. H. Lin, and A. D. Bandrauk, *J. Theor. Comput. Chem.*, **2**, 205-231 (2003).
550. "Surface interface effects upon the conformational stability of a peripheral membrane protein", S. A. Hocker, K. M. Gligorich, K. Brocksmith, Y. Y. Cheng, S. H. Lin, H. C. Chang, M. C. Su, and G. C. Hoops, *Abstr. Pap. Am. Chem. Soc.*, **226**, U187-U187 (2003).
551. "Attenuated total internal reflection study in conformational changes of cytochrome C on fused silica surfaces", K. M. Gligorich, S. A. Hocker, K. Brocksmith, M. C. Su, G. Hoops,

- Y. Y. Cheng, S. H. Lin, and H. C. Chang, *Abstr. Pap. Am. Chem. Soc.*, **226**, U329-U329 (2003).
552. "Thermodynamics and kinetics of protein folding: A mean field theory", K. K. Liang, M. Hayashi, Y. J. Shiu, Y. Mo, J. S. Shao, Y. J. Yan, and S. H. Lin, *Phys. Chem. Chem. Phys.*, **5**, 5300-5308 (2003).
553. "Probing adsorption, orientation and conformational changes of cytochrome c on fused silica surfaces with the soret band", Y. Y. Cheng, S. H. Lin, H. C. Chang, and M. C. Su, *J. Phys. Chem. A*, **107**, 10687-10694 (2003).
554. "Evidence of charge-enhanced C-H-O interactions in aqueous protonated imidazole probed by high pressure infrared spectroscopy", C. C. Su, H. C. Chang, J. C. Jiang, P. Y. Wei, L. C. Lu, and S. H. Lin, *J. Chem. Phys.*, **119**, 10753-10758 (2003).
555. "Orientational regularities in two-dimensional quasidipole system with degenerate ground states", V. M. Rozenbaum, A. N. Morozov, and S. H. Lin, *Phys. Rev. B*, **68**, 155405 (2003).
556. "A quantum chemical study of bonding interaction, vibrational frequencies, force constants, and vibrational coupling of pyridine-M-n (M = Cu, Ag, Au; n=2-4)", D. Y. Wu, M. Hayashi, Y. J. Shiu, K. K. Liang, C. H. Chang, Y. L. Yeh, and S. H. Lin, *J. Phys. Chem. A*, **107**, 9658-9667 (2003).
557. "Quantum chemical modeling of photoabsorption and photoluminescence of the [AlO<sub>4</sub>](0) defect in bulk SiO<sub>2</sub>", A. S. Zyubin, A. M. Mebel, and S. H. Lin, *J. Chem. Phys.*, **119**, 11408-11414 (2003).
558. "Influence of distortion and Duschinsky effects on Marcus-type theories of electron transfer rate", K. K. Liang, A. M. Mebel, S. H. Lin, M. Hayashi, H. L. Selzle, E. W. Schlag, and M. Tachiya, *Phys. Chem. Chem. Phys.*, **5**, 4656-4665 (2003).
559. "C-H---Ohydrogen bonds in beta-sheetlike networks: Combined X-ray crystallography and high-pressure infrared study", K. M. Lee, H. C. Chang, J. C. Jiang, J. C. C. Chen, H. E. Kao, S. H. Lin, and I. J. B. Lin, *J. Am. Chem. Soc.*, **125**, 12358-12364 (2003).
560. "Effects of the Duschinsky mode-mixing mechanism on temperature dependence of electron transfer processes", J. Tang, M. T. Lee, and S. H. Lin, *J. Chem. Phys.*, **119**, 7188-7196 (2003).
561. "Field and size dependence of exciton-LO-phonon interaction in a semiconductor quantum dot", R. L. Chang, and S. H. Lin, *Phys. Rev. B*, **68**, 045326 (2003).

562. "Femtosecond spectroscopy study of electronically excited states of Chlorophyll a molecules in ethanol", Y. J. Shiu, Y. Shi, M. Hayashi, C. Su, K. L. Han, and S. H. Lin, *Chem. Phys. Lett.*, **378**, 202–210 (2003).
563. "Single molecule spectroscopy", T. Y. Latychevskaya, K. K. Liang, M. Hayashi, C. H. Chang, A. Renn, U. P. Wild, J. H. Hsu, T. C. Chang, and S. H. Lin, *J. Chin. Chem. Soc.*, **50**, 477–516 (2003).
564. "Density-functional-theory calculation of semiconducting carbon nanotubes under an external electric field", L. G. Tien, T. M. Liaw, F. Y. Li, S. H. Lin, M. H. Lee, and S. Clark, *J. Chin. Chem. Soc.*, **50**, 627–629 (2003).
565. "Theoretical study of the fragmentation of glycine radical cation", H. F. Lu, F. Y. Li, and S. H. Lin, *J. Chin. Chem. Soc.*, **50**, 729–734 (2003).
566. "Theoretical calculations on vibrational frequencies and absorption spectra of S-1 and S-2 states of pyridine", D. Y. Wu, M. Hayashi, Y. J. Shiu, K. K. Liang, C. H. Chang, and S. H. Lin, *J. Chin. Chem. Soc.*, **50**, 735–744 (2003).
567. "Coherence control between two quantum systems using spatial phase", K. Mishima, M. Hayashi, and S. H. Lin, *Phys. Lett. A*, **315**, 16–22 (2003).
568. "Uniform carbon spheres of high purity prepared on kaolin by CCVD", J. Y. Miao, D. W. Hwang, C. C. Chang, S. H. Lin, K. V. Narasimhulu, and L. P. Hwang, *Diam. Relat. Mat.*, **12**, 1368–1372 (2003).
569. "Application of the generalized kinetic Ising model to the kinetics of protein folding", K. K. Liang, M. Hayashi, Y. J. Shiu, Y. Mo, J. S. Shao, Y. J. Yan, and S. H. Lin, *J. Chin. Chem. Soc.*, **50**, 335–338 (2003).
570. "Effects of confinement on protein folding and protein stability", G. Ping, J. M. Yuan, M. Vallieres, H. Dong, Z. Sun, Y. Wei, F. Y. Li, and S. H. Lin, *J. Chem. Phys.*, **118**, 8042–8048 (2003).
571. "Quasi-one-dimensional approximation in the HMO model of polymethine dyes", M. Dekhtyar, V. Rozenbaum, and S. H. Lin, *Match-Commun. Math. Comput. Chem.*, 71–78 (2003).
572. "Ab initio/RRKM study of the potential energy surface of triplet ethylene and product branching ratios of the C(P-3)+CH<sub>4</sub> reaction", G. S. Kim, T. L. Nguyen, A. M. Mebel, S. H. Lin, and M. T. Nguyen, *J. Phys. Chem. A*, **107**, 1788–1796 (2003).



573. "Bonding interaction, low-lying states and excited charge-transfer states of pyridine-metal clusters: Pyridine-M-n (M=Cu, Ag, Au; n=2-4)", D. Y. Wu, M. Hayashi, C. H. Chang, K. K. Liang, and S. H. Lin, *J. Chem. Phys.*, **118**, 4073-4085 (2003).
574. "An ab initio/RRKM study of product branching ratios in the photodissociation of buta-1,2-and-1,3-dienes and but-2-yne at 193 nm", H. Y. Lee, V. V. Kislov, S. H. Lin, A. M. Mebel, and D. M. Neumark, *Chem.-Eur. J.*, **9**, 726-740 (2003).
575. "Adiabatic theory of infrared laser-induced predesorption of CO from a NaCl (100) surface", K. Nakagami, Y. Ohtsuki, Y. Fujimura, and S. H. Lin, *Phys. Chem. Chem. Phys.*, **5**, 528-537 (2003).
576. "High-pressure spectroscopic probe of hydrophobic hydration of the methyl groups in dimethyl sulfoxide", H. C. Chang, J. C. Jiang, C. M. Feng, Y. C. Yang, C. C. Su, P. J. Chang, and S. H. Lin, *J. Chem. Phys.*, **118**, 1802-1807 (2003).
577. "Reversible mechanical unfolding of single ubiquitin molecules", C. L. Chyan, F. C. Lin, H. B. Peng, J. M. Yuan, C. H. Chang, S. H. Lin, and G. L. Yang, *Biophys. J.*, **87**, 3995-4006 (2004).
578. "Chirped pulse control of long range electron transfer", B. D. Fainberg, V. A. Gorbunov, and S. H. Lin, *Chem. Phys.*, **307**, 77-90 (2004).
579. "Theoretical interpretation of the fragments generated from a glycine radical cation", H. F. Lu, F. Y. Li, and S. H. Lin, *J. Phys. Chem. A*, **108**, 9233-9243 (2004).
580. "Time-resolved entanglement of bound and dissociative atoms and molecules", K. Mishima, M. Hayashi, and S. H. Lin, *Chem. Phys.*, **306**, 219-227 (2004).
581. "Ab initio study of the isomerization and photodissociation of the C<sub>3</sub>H<sub>6</sub>O+center dot cation radicals", K. Mishima, M. Hayashi, and S. H. Lin, *Int. J. Mass Spectrom.*, **238**, 1-15 (2004).
582. "Evidence for hydrogen bond-like C-H-O interactions in aqueous 1,4-dioxane probed by high pressure", H. C. Chang, J. C. Jiang, C. W. Chuang, and S. H. Lin, *Chem. Phys. Lett.*, **397**, 205-210 (2004).
583. "Catalytic wheel as a Brownian motor", V. M. Rozenbaum, D. Y. Yang, S. H. Lin, and T. Y. Tsong, *J. Phys. Chem. B*, **108**, 15880-15889 (2004).

584. "Theoretical study of oxygen isotope exchange and quenching in the  $O(D-1)+CO_2$  reaction", A. M. Mebel, M. Hayashi, V. V. Kislov, and S. H. Lin, *J. Phys. Chem. A*, **108**, 7983-7994 (2004).
585. "Applications of molecular theory of sum-frequency generations to study molecular chirality", M. Hayashi, S. H. Lin, and Y. R. Shen, *J. Phys. Chem. A*, **108**, 8058-8076 (2004).
586. "Dissociation pathways of cyclohexane trication", T. S. Zyubina, S. H. Lin, A. D. Bandrauk, and A. M. Mebel, *Chem. Phys. Lett.*, **393**, 470-477 (2004).
587. "Rate constant for H-atom tunneling in the fluorene-acridine system based on DFT potential energy surface", L. I. Trakhtenberg, A. A. Fokeyev, S. P. Dolin, A. M. Mebel, and S. H. Lin, *Chem. Phys.*, **303**, 107-113 (2004).
588. "Photoisomerization and photodissociation of aniline and 4-methylpyridine", C. M. Tseng, Y. A. Dyakov, C. L. Huang, A. M. Mebel, S. H. Lin, Y. T. Leet, and C. K. Ni, *J. Am. Chem. Soc.*, **126**, 8760-8768 (2004).
589. "Probing C-H center dot center dot center dot X hydrogen bonds in amide-functionalized imidazolium salts under high pressure", K. M. Lee, H. C. Chang, J. C. Jiang, L. C. Lu, C. J. Hsiao, Y. T. Lee, S. H. Lin, and I. J. B. Lin, *J. Chem. Phys.*, **120**, 8645-8650 (2004).
590. "Synthesis and properties of carbon nanospheres grown by CVD using Kaolin supported transition metal catalysts", J. Y. Miao, D. W. Hwang, K. V. Narasimhulu, P. I. Lin, Y. T. Chen, S. H. Lin, and L. P. Hwang, *Carbon*, **42**, 813-822 (2004).
591. "Photodissociation of benzene under collision-free conditions: An ab initio/Rice-Ramsperger-Kassel-Marcus study", V. V. Kislov, T. L. Nguyen, A. M. Mebel, S. H. Lin, and S. C. Smith, *J. Chem. Phys.*, **120**, 7008-7017 (2004).
592. "Mechanical unfolding of individual ubiquitin molecules", G. L. Yang, C. L. Chyan, H. B. Peng, F. C. Lin, J. M. Yuan, C. H. Chang, and S. H. Lin, *Biophys. J.*, **86**, 621A-621A (2004).
593. "Flashing ratchet model with high efficiency", Y. A. Makhnovskii, V. M. Rozenbaum, D. Y. Yang, S. H. Lin, and T. Y. Tsong, *Phys. Rev. E*, **69**, 021102 (2004).
594. "A theoretical study of the  $O(D-1)+CH_4$  reaction II", A. H. H. Chang, and S. H. Lin, *Chem. Phys. Lett.*, **384**, 229-235 (2004).

595. "Theoretical differential Raman scattering cross-sections of totally-symmetric vibrational modes of free pyridine and pyridine-metal cluster complexes", D. Y. Wu, M. Hayashi, S. H. Lin, and Z. Q. Tian, *Spectroc. Acta Pt. A-Molec. Biomolec. Spectr.*, **60**, 137-146 (2004).
596. "Theoretical studies of high-power laser ionization of molecules in the tunneling region", K. Mishima, K. Nagaya, M. Hayashi, and S. H. Lin, *Phys. Rev. A*, **70**, 063414 (2004).
597. "Entanglement in scattering processes", K. Mishima, M. Hayashi, and S. H. Lin, *Phys. Lett. A*, **333**, 371-377 (2004).
598. "Alcohol-induced conformational changes of Cytochrome c on fused silica surfaces", M. C. Su, H. C. Chang, K. M. Gligorich, G. C. Hoops, T. A. Hopkins, S. A. Hocker, S. H. Lin, S. Mistry, and Y. Y. Cheng, *Abstr. Pap. Am. Chem. Soc.*, **227**, U321-U321 (2004).
599. "Pressure-enhanced C-H center dot center dot center dot O interactions in aqueous tert-butyl alcohol", H. C. Chang, J. C. Jiang, C. C. Su, L. C. Lu, C. J. Hsiao, C. W. Chuang, and S. H. Lin, *J. Phys. Chem. A*, **108**, 11001-11005 (2004).
600. "Experimental and theoretical studies of protein folding-unfolding", Y. J. Shiu, C. Su, Y. L. Yeh, K. K. Liang, M. Hayashi, Y. Mo, Y. J. Yan, and S. H. Lin, *J. Chin. Chem. Soc.*, **51**, 1161-1173 (2004).
601. "Atomic force microscopic and theoretical studies of poly-ubiquitin proteins", Y. L. Yeh, C. H. Chang, K. K. Liang, Y. J. Shiu, C. Su, M. Hayashi, C. L. Chyan, G. Yang, Y. Mo, Y. J. Yan, and S. H. Lin, *Chem. Phys. Lett.*, **399**, 440-445 (2004).
602. "Quantum interference and laser pulse phase effect on the photoionization rates of excited hydrogen atoms in the tunneling region", K. Mishima, M. Hayashi, and S. H. Lin, *J. Theor. Comput. Chem.*, **4**, 1153-1163 (2005).
603. "Quantum-chemical simulation of the optical properties of O=X and O<sub>2</sub>X point defects in silicon and germanium oxides", A. S. Zyubin, A. M. Mebel, and S. H. Lin, *Russ. J. Inorg. Chem.*, **50**, 1912-1920 (2005).
604. "High-pressure Raman studies on aqueous protonated thiazole: Presence of charge-enhanced C-H center dot center dot center dot O hydrogen bonds", H. C. Chang, J. C. Jiang, W. W. Lai, J. S. Lin, G. C. Chen, W. C. Tsai, and S. H. Lin, *J. Phys. Chem. B*, **109**, 23103-23107 (2005).
605. "Fragmentation of heme and hemin(+) with sequential loss of carboxymethyl groups: A DFT and mass-spectrometry study", O. P. Charkin, N. M. Klimenko, P. T.

- Nguyen, D. O. Charkin, A. M. Mebel, S. H. Lin, Y. S. Wang, S. C. Wei, and H. C. Chang, *Chem. Phys. Lett.*, **416**, 362–369 (2005).
606. "Quantum state-to-state rate constants for the rotationally inelastic collision of CH(B (2)Sigma(-), nu=0, N -> N') with Ar", S. D. Chao, S. H. Lin, and M. H. Alexander, *J. Chem. Phys.*, **123**, 194304 (2005).
607. "Theoretical study of isomerization and dissociation of acetylene dication in the ground and excited electronic states", T. S. Zyubina, Y. A. Dyakov, S. H. Lin, A. D. Bandrauk, and A. M. Mebel, *J. Chem. Phys.*, **123**, 194304 (2005).
608. "Distortion effects of the initial electronic states on tunneling photo-ionization of hydrogen atom", K. Nagaya, K. Mishima, M. Hayashi, and S. H. Lin, *Chem. Phys. Lett.*, **414**, 438–443 (2005).
609. "Photodissociation of Azulene at 193 nm: Ab initio and RRKM study", Y. A. Dyakov, C. K. Ni, S. H. Lin, Y. T. Lee, and A. M. Mebel, *J. Phys. Chem. A*, **109**, 8774–8784 (2005).
610. "Theoretical study of fragmentation of heme and its ion with successive removal of carboxymethyl groups", O. P. Charkin, N. M. Klimenko, T. P. Nguyen, D. O. Charkin, Y. S. Wang, S. C. Wei, H. C. Chang, and S. H. Lin, *Russ. J. Inorg. Chem.*, **50**, 1398–1407 (2005).
611. "Temperature and pressure dependences of tunneling rate constant: Density-functional theory potential-energy surface for H-atom transfer in the fluorene-acridine system", L. I. Trakhtenberg, A. A. Fokeyev, S. P. Dolin, A. M. Mebel, and S. H. Lin, *J. Chem. Phys.*, **123**, 114508 (2005).
612. "Hydrogen abstraction acetylene addition and Diels–Alder mechanisms of PAH formation: A detailed study using first principles calculations", V. V. Kislov, N. I. Islamova, A. M. Kolker, S. H. Lin, and A. M. Mebel, *Journal of Chemical Theory and Computation*, **1**, 908–924 (2005).
613. "Intermolecular hydrogen bonding and structures in 1,3-dioxane/D2O mixtures studied by high-pressure Raman spectroscopy", J. S. Lin, J. C. Jiang, C. M. Chang, W. W. Lai, J. W. Fang, S. H. Lin, and H. C. Chang, *J. Chin. Chem. Soc.*, **52**, 625–630 (2005).
614. "Theoretical studies of distyrylbenzene and its optical properties", H. W. Wang, C. Chen, F. C. Hsu, H. C. Shieh, J. K. Wang, S. H. Lin, and M. Hayashi, *J. Chin. Chem. Soc.*, **52**, 665–675 (2005).
615. "Photodissociation dynamics of pyridine", M. F. Lin, Y. A. Dyakov, C. M. Tseng, A. M. Mebel, S. H. Lin, Y. T. Lee, and C. K. Ni, *J. Chem. Phys.*, **123**, 054309 (2005).

616. "Excited-state dynamics of trans, trans-distyrylbenzene: A femtosecond transient absorption study", F. C. Hsu, S. H. Lin, and J. K. Wang, *Chem. Phys. Lett.*, **411**, 103-107 (2005).
617. "Photoluminescence of oxygen-containing surface defects in germanium oxides: A theoretical study", A. S. Zyubin, A. M. Mebel, and S. H. Lin, *J. Chem. Phys.*, **123** (2005).
618. "Hydrogen bond-like equatorial C-H center dot center dot center dot O interactions in aqueous 1,3-dioxane: A combined high-pressure infrared and Raman spectroscopy study", H. C. Chang, J. C. Jiang, C. W. Chuang, J. S. Lin, W. W. Lai, Y. C. Yang, and S. H. Lin, *Chem. Phys. Lett.*, **410**, 42-48 (2005).
619. "Photodissociation dynamics of ethyltoluene and p-fluoroethylbenzene at 193 and 248 nm", C. L. Huang, Y. A. Dyakov, S. H. Lin, Y. T. Lee, and C. K. Ni, *J. Phys. Chem. A*, **109**, 4995-4999 (2005).
620. "Keldysh-type photoionization rate of large polyatomic molecules in the tunneling region", K. Mishima, M. Hayashi, and S. H. Lin, *Phys. Rev. A*, **71**, 053411 (2005).
621. "Bond lengths and diameters of armchair single wall carbon nanotubes", M. F. Budyka, T. S. Zyubina, A. G. Ryabenko, S. H. Lin, and A. M. Mebel, *Chem. Phys. Lett.*, **407**, 266-271 (2005).
622. "Two approaches toward a high-efficiency flashing ratchet", V. M. Rozenbaum, T. Y. Korochkova, D. Y. Yang, S. H. Lin, and T. Y. Tsong, *Phys. Rev. E*, **71**, 041102 (2005).
623. "Photodissociation dynamics of  $C_6H_xF_{6-x}$  ( $x=1-4$ ) at 193 nm", M. F. Lin, Y. A. Dyakov, S. H. Lin, Y. T. Lee, and C. K. Ni, *J. Phys. Chem. B*, **109**, 8344-8349 (2005).
624. "Effect of quantum interference on tunneling photoionization rates of N-2 and O-2 molecules", K. Mishima, K. Nagaya, M. Hayashi, and S. H. Lin, *J. Chem. Phys.*, **122**, 104312 (2005).
625. "Potential energy surfaces in coulomb explosion of polyatomic molecules: Benzene and cyclohexane trications and acetylene dication", A. M. Mebel, T. S. Zyubina, Y. A. Dyakov, A. D. Bandrauk, and S. H. Lin, *Int. J. Quantum Chem.*, **102**, 506-519 (2005).
626. "Local structure dependence of the charge transfer band in nanocrystalline  $Y_2O_3:Eu^{3+}$ ", J. W. Wang, Y. M. Chang, H. C. Chang, S. H. Lin, L. C. L. Huang, X. L. Kong, and M. W. Kang, *Chem. Phys. Lett.*, **405**, 314-317 (2005).
627. "Effect of displacement and distortion of potential energy surfaces and overlapping resonances of electronic transitions on surface-enhanced Raman scattering: Models

- and ab initio theoretical calculation", M. T. Lee, D. Y. Wu, Z. Q. Tian, and S. H. Lin, *J. Chem. Phys.*, **122**, 084719 (2005).
628. "Towards the realization of the quantum chemistry approach to tunneling photoionization processes in strong laser fields", K. Mishima, K. Nagaya, M. Hayashi, and S. H. Lin, *J. Chem. Phys.*, **122**, 094719 (2005).
629. "Electron-phonon interaction in absorption and photoluminescence spectra of quantum dots", T. O. Cheche, M. C. Chang, and S. H. Lin, *Chem. Phys.*, **309**, 109-114 (2005).
630. "High temperature effect on photo-induced electron transfer", M. T. Lee, K. Mishima, M. Hayashi, and S. H. Lin, *Mol. Phys.*, **103**, 83-88 (2005).
631. "Theoretical study of the structure and stability of the ferriporphyrin dimer (Fe(III)C<sub>34</sub>H<sub>31</sub>N<sub>4</sub>O<sub>4</sub>)(2)", O. P. Charkin, N. M. Klimenko, D. O. Charkin, Y. S. Wang, S. C. Wei, H. C. Chang, and S. H. Lin, *Russ. J. Inorg. Chem.*, **51**, 89-98 (2006).
632. "Theoretical study of "deep" fragmentation of hemin ion with successive loss of methyl and vinyl groups", O. P. Charkin, N. M. Klimenko, T. P. Nguyen, D. O. Charkin, Y. S. Wang, H. C. Chang, and S. H. Lin, *Russ. J. Inorg. Chem.*, **51**, 1613-1622 (2006).
633. "Quantum-chemical study of crystal formation of supramolecular silver compounds with trans-1,2-bis(4-pyridyl)ethylene and their electronic absorption spectra", T. S. Zyubina, V. F. Razumov, S. B. Brichkin, V. Anisimov, S. H. Lin, and A. M. Mebel, *Russ. J. Inorg. Chem.*, **51**, 925-940 (2006).
634. "Control of nonadiabatic dissociation dynamics with the use of laser-induced wave packet interferences", K. Nagaya, S. H. Lin, and H. Nakamura, *J. Chem. Phys.*, **125**, 214311 (2006).
635. "The effect of pressure on charge-enhanced C-H...O interactions in aqueous triethylamine hydrochloride probed by high pressure Raman spectroscopy", H. C. Chang, J. C. Jiang, W. C. Tsai, G. C. Chen, C. Y. Chang, and S. H. Lin, *Chem. Phys. Lett.*, **432**, 100-105 (2006).
636. "The structures, conversions and fragmentations of C<sub>2</sub>H<sub>6</sub>O<sub>2</sub><sup>+</sup> isomers: An ab initio study", H. F. Lu, F. Y. Li, K. Nagaya, M. Hayashi, and S. H. Lin, *J. Mol. Struct.-Theochem*, **773**, 71-79 (2006).

637. "Conformations of 1-butyl-3-methylimidazolium chloride probed by high pressure Raman spectroscopy", H. C. Chang, C. Y. Chang, J. C. Su, W. C. Chu, J. C. Jiang, and S. H. Lin, *Int. J. Mol. Sci.*, **7**, 417-424 (2006).
638. "Theoretical treatments of ultrafast electron transfer from adsorbed dye molecule to semiconductor nanocrystalline surface", K. K. Liang, C. K. Lin, H. C. Chang, M. Hayashi, and S. H. Lin, *J. Chem. Phys.*, **125**, 154706 (2006).
639. "The empirical correlation between size and two-photon absorption cross section of CdSe and CdTe quantum dots", S. C. Pu, M. J. Yang, C. C. Hsu, C. W. Lai, C. C. Hsieh, S. H. Lin, Y. M. Cheng, and P. T. Chou, *Small*, **2**, 1308-1313 (2006).
640. "Modeling of folding and unfolding mechanisms in alanine-based alpha-helical polypeptides", A. N. Morozov, and S. H. Lin, *J. Phys. Chem. B*, **110**, 20555-20561 (2006).
641. "Photodissociation and photoisomerization of alpha-fluorotoluene and 4-fluorotoluene in a molecular beam", C. L. Huang, J. C. Jiang, Y. A. Dyakov, M. F. Lin, C. M. Tseng, S. H. Lin, Y. T. Lee, and C. K. Ni, *J. Chem. Phys.*, **125**, 133305 (2006).
642. "Theoretical investigation of the photoinitiated folding of HP-36", S. Jang, N. Sreerama, V. H. C. Liao, S. H. F. Lu, F. Y. Li, S. Shin, R. W. Woody, and S. H. Lin, *Protein Sci.*, **15**, 2290-2299 (2006).
643. "The role of charge-enhanced C-H center dot center dot center dot O interactions in gel-like mixtures prepared from ionic liquids and tungsten(VI) oxide nanoparticles", H. C. Chang, J. C. Jiang, W. C. Tsai, G. C. Chen, and S. H. Lin, *Chem. Phys. Lett.*, **427**, 310-316 (2006).
644. "Photoluminescence of oxygen-deficient defects in germanium oxides: A quantum chemical study", A. S. Zyubin, A. M. Mebel, and S. H. Lin, *J. Chem. Phys.*, **125**, 064701 (2006).
645. "Reciprocating nanoengine", Y. A. Makhnovskii, V. M. Rozenbaum, D. Y. Yang, S. H. Lin, and T. Y. Tsong, *Eur. Phys. J. B*, **52**, 501-505 (2006).
646. "Unified semiclassical theory for the two-state system: An analytical solution for general nonadiabatic tunneling", C. Y. Zhu, and S. H. Lin, *J. Chem. Phys.*, **125**, 044104 (2006).
647. "Distance versus energy fluctuations and electron transfer in single protein molecules", J. Tang, and S. H. Lin, *Phys. Rev. E*, **73**, 061108 (2006).

648. "Theoretical studies on tunneling ionizations of ethylene and benzene in high-power lasers", K. Nagaya, K. Mishima, H. F. Lu, M. Hayashi, and S. H. Lin, *Chem. Phys. Lett.*, **424**, 34-41 (2006).
649. "Compact photo-ionization rate based on Keldysh theory", K. Nagaya, K. Mishima, M. Hayashi, and S. H. Lin, *J. Phys. Soc. Jpn.*, **75**, 044302 (2006).
650. "Fragmentations of singly charged ethanol cation: An ab initio/RRKM study", H. F. Lu, F. Y. Li, K. Nagaya, M. Hayashi, K. Mishima, and S. H. Lin, *J. Mol. Struct.-Theochem*, **761**, 159-169 (2006).
651. "Solvent effect on photophysical properties of a fluorescence probe: BMVC", C. C. Chang, J. F. Chu, H. H. Kuo, C. C. Kang, S. H. Lin, and T. C. Chang, *J. Lumines.*, **119**, 84-90 (2006).
652. "Theoretical studies on tunneling ionizations of helium atom in intense laser fields", K. Nagaya, K. Mishima, M. Hayashi, and S. H. Lin, *J. Chem. Phys.*, **124**, 144303 (2006).
653. "Energy losses different in a flashing ratchet with different potential well shapes", V. M. Rozenbaum, D. Y. Yang, S. H. Lin, and T. Y. Tsong, *Physica A*, **363**, 211-216 (2006).
654. "Ab initio and RRKM study of photodissociation of azulene cation", Y. A. Dyakov, C. K. Ni, S. H. Lin, Y. T. Lee, and A. M. Mebel, *Phys. Chem. Chem. Phys.*, **8**, 1404-1415 (2006).
655. "Transient absorption of the Chlorophyll a in ethanol", Y. Shi, Y. J. Shiu, C. Su, S. H. Lin, and K. I. Han, *Chin. J. Chem. Phys.*, **19**, 6-10 (2006).
656. "The role of seven-membered ring in the photoisomerization and photodissociation of small aromatic molecules", C. M. Tseng, Y. A. Dyakov, C. L. Huang, Y. T. Lee, S. H. Lin, and C. K. Ni, *J. Chin. Chem. Soc.*, **53**, 33-40 (2006).
657. "Theoretical treatments of radiationless transitions", C. H. Chin, H. Y. J. Shiu, H. W. Wang, Y. L. Chen, C. C. Wang, S. H. Lin, and M. Hayashi, *J. Chin. Chem. Soc.*, **53**, 131-152 (2006).
658. "Acetylene elimination in photodissociation of neutral azulene and its cation: An ab initio and RRKM study", Y. A. Dyakov, A. M. Mebel, S. H. Lin, Y. T. Lee, and C. K. Ni, *J. Chin. Chem. Soc.*, **53**, 161-168 (2006).
659. "Photodissociation dynamics of pyrimidine", M. F. Lin, Y. A. Dyakov, C. M. Tseng, A. M. Mebel, S. H. Lin, Y. T. Lee, and C. K. Ni, *J. Chem. Phys.*, **124**, 084303 (2006).



660. "Hydrogen bond stabilization in 1,3-dimethylimidazolium methyl sulfate and 1-butyl-3-methylimidazolium hexafluorophosphate probed by high pressure: The role of charge-enhanced C-H center dot center dot center dot O interactions in the room-temperature ionic liquid", H. C. Chang, J. C. Jiang, W. C. Tsai, G. C. Chen, and S. H. Lin, *J. Phys. Chem. B*, **110**, 3302-3307 (2006).
661. "A modified Ising model for the thermodynamic properties of local and global protein folding unfolding observed by circular dichroism and small-angle X-ray scattering", Y. J. Shiu, U. S. Jeng, C. Su, Y. S. Huang, M. Hayashi, K. K. Liang, Y. L. Yeh, and S. H. Lin, *J. Appl. Crystallogr.*, **40**, S195-S199 (2007).
662. "Rigorous contour integral analysis of generalized Keldysh theory of strong laser photoionization", H. Mineo, S. D. Chao, K. Nagaya, K. Mishima, M. Hayashi, and S. H. Lin, *Chem. Phys. Lett.*, **439**, 224-230 (2007).
663. "Aggregate versus excimer emissions from poly(2,5-di-n-octyloxy-1,4-phenylenevinylene)", Y. F. Huang, Y. J. Shiu, J. H. Hsu, S. H. Lin, A. C. Su, K. Y. Peng, S. A. Chen, and W. S. Fann, *J. Phys. Chem. C*, **111**, 5533-5540 (2007).
664. "Reply to 'Comment on 'Generalization of Keldysh's theory' '"', H. Mineo, S. D. Chao, K. Mishima, K. Nagaya, M. Hayashi, and S. H. Lin, *Phys. Rev. A*, **75**, 027402 (2007).
665. "Theoretical studies on sequential multiple ionizations of benzene and hexafluorobenzene in high-power lasers", K. Nagaya, H. Mineo, K. Mishima, A. A. Villaeys, M. Hayashi, and S. H. Lin, *Phys. Rev. A*, **75**, 013402 (2007).
666. "Calculation of the vibrationally non-relaxed photo-induced electron transfer rate constant in dye-sensitized solar cells", K. K. Liang, C. K. Lin, H. C. Chang, A. A. Villaeys, M. Hayashi, and S. H. Lin, *Phys. Chem. Chem. Phys.*, **9**, 853-861 (2007).
667. "Site specificity of alpha-H abstraction reaction among secondary structure motif - An ab initio study", H. F. Lu, F. Y. Li, and S. H. Lin, *J. Comput. Chem.*, **28**, 783-794 (2007).
668. "Excited-state dynamics of trans, trans-distyrylbenzene: Transient anisotropy and excitation energy dependence", F. C. Hsu, M. Hayashi, H. W. Wang, S. H. Lin, and J. K. Wang, *J. Phys. Chem. A*, **111**, 759-763 (2007).
669. "Theoretical studies on tunneling ionizations from the doubly degenerate highest occupied molecular orbitals of benzene in intense laser fields", K. Nagaya, H. F. Lu, H. Mineo, K. Mishima, M. Hayashi, and S. H. Lin, *J. Chem. Phys.*, **126**, 024304 (2007).

670. "Distal charge transport in peptides", Edward W. Schlag, Sheh-Yi Sheu, Dah-Yen Yang, Heinrich L. Selzle, and Sheng Hsien Lin, *Angew. Chem. Int. Ed.*, **46**, 3196-3210 (2007).
671. "Theoretical studies of high-harmonic generation based on the Keldysh-Faisal-Reiss theory", H. Mineo, K. Nagaya, M. Hayashi, and S. H. Lin, *J. Phys. B: At. Mol. Opt. Phys.* **40**, 2435-2451 (2007).
672. "A Molecular Theory of ZEKE Spectroscopy", S. D. Chao, H. L. Selzle, H. J. Neusser, E. W. Schlag, L. Yao, and S. H. Lin, *Z. Phys. Chem.* **221**, 633-646 (2007).
673. "Accuracy and convergence of the Wang-Landau sampling algorithm", Alexander N. Morozov, Sheng Hsien Lin, *Phys. Rev. E*, **76**, 026701(7) (2007).
674. "Theoretical investigations of spectroscopy and excited state dynamics of adenine", Chih-Hao Chin, Alexander M. Mebel, Gap-Sue Kim, K. Y. Baek, M. Hayashi, K. K. Liang, S. H. Lin, *Chemical Physics Letters*, **445**, 361-369 (2007).
675. "Autobiography of Sheng Hsien Lin", S. H. Lin, *J. Phys. Chem. A*, **111**, 9171-9176 (2007).
676. "Evidence of Rotational Isomerism in 1-Butyl-3-methylimidazolium Halides: A Combined High-Pressure Infrared and Raman Spectroscopic Study", Hai-Chou Chang, Jyh-Chiang Jiang, Jong-Chang Su, Chao-Yen Chang, and Sheng Hsien Lin, *J. Phys. Chem. A*, **111**, 9201-9206 (2007).
677. "Theoretical DFT Study of Fragmentation and Association of Heme and Hemin", O. P. Charkin, N. M. Kimenko, D. O. Charkin, H.-C. Chang and S. H. Lin, *J. Phys. Chem. A*, **111**, 9207-9217 (2007).
678. "A Solution Study on the Local and Global Structure Changes of Cytochrome c: An Unfolding Process Induced by Urea", I-Jui Hsu, Ying-Jen Shiu, U-Ser Jeng, Tung-Ho Chen, Yu-Shan Huang, Ying-Huang Lai, Ling-Na Tsai, Ling-Yun Jang, Jyh-Fu Lee, Li-Jiaun Lin, Sheng-Hsien Lin, Yu Wang, *J Phys. Chem. A*, **111**, 9286-9290 (2007).
679. "Symmetric double-well potential model and its application to vibronic spectra: Studies of inversion modes of ammonia and nitrogen-vacancy defect centers in diamond", Chih-Kai Lin, Huan-Cheng Chang, and S. H. Lin, *J Phys. Chem. A*, **111**, 9347-9354 (2007).
680. "Experimental and Theoretical Investigation of High-Power Laser Ionization and Dissociation of Methane", M. Sharifi, F. Kong, S. L. Chin, H. Mineo, Y. Dyakov, A. M. Mebel, S. D. Chao, M. Hayashi, and S. H. Lin, *J Phys. Chem. A*, **111**, 9405 -9416 (2007).

681. "Optical Properties of Oxygen Vacancies in Germanium Oxides: Quantum Chemical Modeling of Photoexcitation and Photoluminescence", A. S. Zyubin, A. M. Mebel, and S. H. Lin, *J Phys. Chem. A*, **111**, 9478–9485 (2007).
682. "Reciprocating Motion on the Nanoscale", Yu. A. Makhnovskii, V. M. Rozenbaum, D.-Y. Yang, and S. H. Lin, *J Phys. Chem. A*, **111**, 9486–9493 (2007).
683. "Photodissociation of 1,3,5-Triazine: An Ab Initio and RRKM Study", Y. A. Dyakov, A. M. Mebel, S. H. Lin, Y. T. Lee, and C.-K. Ni, *J Phys. Chem. A*, **111**, 9591–9599 (2007).
684. "Theory of Time-Resolved Sum-Frequency Generation and Its Applications to Vibrational Dynamics of Water", Michitoshi Hayashi, Ying-Jen Shiu, Kuo Kan Liang, Sheng Hsien Lin, and Yuan Ron Shen, *J Phys. Chem. A*, **111**, 9062–9069 (2007).
685. "Nonlinear responses of degenerate two-level systems to intense few-cycle pulses", Kuninobu Nagaya, Chaoyuan Zhu, Sheng Hsien Lin, *J. Chem. Phys.* **127**, 094304 (2007).
686. "Photodissociation of S atom containing amino acid chromophores", Ming-Fu Lin, Yuri A. Dyakov, Yuan T. Lee, S. H. Lin, Alexander M. Mebel, Chi-Kung Ni, *J. Chem. Phys.* **127**, 064308 (2007).
687. "Theoretical study of the structure and stability of the dimers of heme analogues (MC34H32N4O4)(2) and their ions (MC34H32N4O4)(2)(+) with 3d-metal atoms M", O. P. Charkin, N. M. Klimenko, D. O. Charkin, S. H. Lin, *Russ. J. Inorg Chem.* **52**, 1248–1261 (2007).
688. "The fragmentation of ethanol cation under an electric field: An ab initio/RRKM study", Hsiu-Feng Lu, F.-Y. Li, Chun-Chin Lin, K. Nagaya, Ito Chao and S.H. Lin, *Chem. Phys. Lett.* **443**, 178–182 (2007).
689. "Theoretical study of the structure and stability of the heme dimer (FeC34H32N4O4)(2) and its ion (FeC34H32N4O4)(2)(+) ", O. P. Charkin, N. M. Klimenko, D. O. Charkin, S. H. Lin, *Russ. J. Inorg. Chem.* **52**, 1088–1097 (2007).
690. "Anharmonic Effect on Unimolecular Reactions with Application to the Photodissociation of Ethylene", L. Yao, A. M. Mebel, H. F. Lu, H. J. Neusser, S. H. Lin, *J. Phys. Chem. A*, **111**, 6722–6729 (2007).
691. Reply to "Comment on 'Generalization of Keldysh's theory'", Mineo H, Chao SD, Mishima K, Nagaya K, Hayashi M, Lin SH, *Physical Review A*, **75**, 2, 027402 (2007) (TC:2)

692. Molecular theory of ZEKE spectroscopy, Chao SD, Selzle HL, Neusser HJ, Schlag EW, Lin SH, *Zeitschrift Fur Physikalische Chemie-International Journal of Research in Physical Chemistry & Chemical Physics*, **221**, 5, 633-646, (2007). (TC:4)(ISSN:0942-9352)
693. Photodissociation of Satom containing amino acid chromophores, Lin MF, Dyakov YA, Lee YT, Lin SH, Mebel AM, Ni CK, *Journal of Chemical Physics*, **127**, 6, 064308 (2007). (TC:2)
694. "Structural Organization in Aqueous Solutions of 1-Butyl-3-methylimidazolium Halides: A High-Pressure Infrared Spectroscopic Study on Ionic Liquids", H.-C. Chang, J.-C. Jiang, C.-Y. Chang, J.-C. Su, C.-H. Hung, Y.-C. Liou, S. H. Lin, *J. Phys. Chem. B*, **112** (14), 4351-4356 (2008).
695. "Chemical enhancement effects in SERS spectra: A quantum chemical study of pyridine interacting with copper, silver, gold and platinum metals", D.-Y. Wu, X.-M. Liu, S. Duan, X. Xu, B. Ren, S. H. Lin, Z. Q. Tian, *J. Phys. Chem. C*, **112**(11) 4195-4204 (2008).
696. "Theoretical study of binding interactions and vibrational Raman spectra of water in hydrogen-bonded anionic complexes:  $(\text{H}_2\text{O})(\text{n})(-)$  ( $\text{n}=2$  and  $3$ ),  $\text{H}_2\text{O}$  center dot center dot center dot  $\text{X}$  ( $\text{X} = \text{F}, \text{Cl}, \text{Br}, \text{and I}$ ), and  $\text{H}_2\text{O}$  center dot center dot center dot  $\text{M}$  ( $\text{M} = \text{Cu}, \text{Ag}, \text{and Au}$ )", D.-Y. Wu, S. Duani, X.-M. Liu, Y.-C. Xu, Y.-X. Jiang, B. X., S. H. Lin, Z.-Q. Tian, *J. Phys. Chem. A*, **112**(6), 1313-1321 (2008).
697. "Highly multiphoton molecular excitation by an intense laser pulse", Y. Teranishi, M. Hayashi, F Kong, S. L. Chin, S. D. Chao, H. Mineo, and S. H. Lin, *Molecular Physics*, **106**, 2-4, 333-339 (2008).
698. "Ultrafast Spectroscopy Studies on Thickness Dependence of Acoustic Phonon Modes in Silver Nanoprisms", P. Yu, Y. J. Shiu, Y.-T. Chen, S.-H. Lin, *JCCS*, **55**, 23-28 (2008).
699. "Nonadditive Interactions in Protein Folding: The Zipper Model of Cytochrome c", A. N. Morozov, Y. J. Shiu, C. T. Liang, M. Y. Tsai, S. H. Lin, *J. Biol. Phys.*, **33**(4), 255-270 (2008).
700. "Global and local structure changes of *cytochrome c* and *lysozyme* characterized by a multi-group unfolding process", Y. J. Shiu, U. S. Jeng, Y. S. Huang, Y. H. Lai, H. F. Lu, C. T. Liang, I. J. Hsu, C. H. Su, C. Su, I. Chao, A. C. Su, S. H. Lin, *Biophys. J.*, **94**, 4828-4836 (2008).
701. "Algorithmic decoherence time for decay-of-mixing non-Born-Oppenheimer dynamics", Shu Chun Cheng, Chaoyuan Zhu, Kuo Kan Liang, Sheng Hsien Lin, Donald G.

- Truhlar, *J. Chem. Phys.*, **129**, 024112 (2008).
702. "Defect Structure of highly-Zn-doped LiNbO<sub>3</sub> single crystal revealed by extended X-ray absorption spectra", P. C. Tsai, M. L. Sun, C. T. Chia, H. F. Lu, S. H. Lin, M. L. Hu, J. F. Lee, *Appl. Phys. Lett.* **92**(16), 161902 (2008).
703. "Theoretical study of multiphoton ionization of cyclohexadienes and unimolecular decomposition of their mono- and dications", T. S. Zyubin, A. M. Mebel, M. Hayashi, S. H. Lin, *Phys. Chem. Chem. Phys.* **10**(17), 2321-2331 (2008).
704. "The anharmonic effect study of coupled Morse oscillators for the unimolecular reaction", L. Yoa, S. H. Lin, *Science in China Series B: Chemistry*, 51:12, 1146-1152 (2008).
705. "Direct observation of super-excited states in methane created by a femtosecond intense laser field", A Azarm, H L Xu, Y Kamali, J Bernhardt, D Song, A Xia, Y Teranishi, S H Lin, F Kong and S L Chin, *J. Phys. B: At. Mol. Opt. Phys.* **41**, 225601 (2008).
706. "Triggering the proton transfer by H-bond network", M. Macerins, B. P. Kietis, J. Sulskus, S. H. Lin, M. Hayashi, L. Valkunas, *Chemical Physics Letters*. **466**, 223-226 (2008).
707. "Effects of water and methanol on the molecular organization of 1-butyl-3-methylimidazolium tetrafluoroborate as functions of pressure and concentration", H.-C. Chang, J.-C. Jiang, Y.-C. Liou, C.-H. Hung, T.-Y. Lai, S. H. Lin, *J. Chem. Phys.* **129**(4), 44506 (2008).
708. "Potential energy surfaces for the lowest excited states of the nitrogen-vacancy point defects in diamonds: A quantum chemical study", A.S. Zyubin, A.M. Mebel, H.C. Chang and S.H. Lin, *Chem. Phys. Lett.*, **462**(4-6), 251-255 (2008).
709. "One- and two-photon absorption properties of diamond nitrogen-vacancy defect centers: A theoretical study", C.-K. Lin, Y.-H. Wang, H.-C. Chang, M. Hayashi, S. H. Lin, *J. Chem. Phys.*, **129**, 124714 (2008).
710. "Photoinduced Structural Dynamics in Laser-Heated Nanomaterials of Various Shapes and Sizes", P. Yu, J. Tang, S. H. Lin, *J. Phys. Chem. C*, **112**(44), 17133-17137 (2008).
711. "Experimental and theoretical investigations of ionization/dissociation of cyclopentanone molecule in a femtosecond laser field", Qiaoqiao Wang, Di Wu, Mingxing Jin, Fuchun Liu, Feifei Hu, Xihui Cheng, Hang Liu, Zhan Hu, Dajun Ding, H. Mineo, Y. A. Dyakov, A. M. Mebel, S. D. Chao, and S. H. Lin, *J. Chem. Phys.*, **129**, 204302 (2008).

712. "Theoretical studies of Anharmonic effect in the Rice-Ramsperger-Kassel-Marcus theory", L. Yao, Y. L. Liu, S. H. Lin, *Modern Physics Letters B*, **22**, 31, 3043-3052 (2008).
713. "Theoretical study on S-1(B-1(3u)) state electronic structure and absorption spectrum of pyrazine", He RX, Zhu CY, Chin CH, Lin SH, *SCIENCE IN CHINA SERIES B-CHEMISTRY*, **51**(12), 1166-1173 (2008).
714. "Local Structures of Water in 1-Butyl-3-methylimidazolium Tetrafluoroborate Probed by High-Pressure Infrared Spectroscopy", Chang HC, Jiang JC, Liou YC, Hung CH, Lai TY, Lin SH, *ANALYTICAL SCIENCES*, **24**(10), 1305-1309 (2008).
715. "Proton-exchanged OH<sup>-</sup> absorption spectra of highly Zn-doped LiNbO<sub>3</sub> with and without polarization inversion", P. C. Tsai, C. T. Chia, S. T. Lin, Y. C. Huang, H. F. Lu, S. H. Lin, *Applied Physics Letters*, **94**, 081909 (2009).
716. "On the calculation of the dissociation rate constant of the water dimer by the *ab initio* anharmonic RRKM theory", L. Yao, R. X. He, A. M. Mebel, S. H. Lin, *Chemical Physics Letters*, **470**(4-6), 210-214 (2009).
717. "Theoretical treatment of anharmonic effect on molecular absorption, fluorescence spectra, and electron transfer", C. Zhu, K. K. Liang, M. Hayashi, S. H. Lin, *Chemical Physics*, **358**, 1-2, 137-146 (2009).
718. "Net transport due to noise-induced internal reciprocating motion", Y. A. Makhnovskii, V. M. Rozenbaum, D. Y. Yang, S. H. Lin, *The Journal of Chemical Physics*, **130**, 164101 (2009).
719. "Excitation properties of the H3 defect center in diamond: A theoretical study", C. K. Lin, H. C. Chang, M. Hayashi, S. H. Lin, *Chemical Physics Letters*, **475**, 68-72 (2009).
720. "Quantum Chemical Modeling of Photoabsorption Properties of Two- and Three-Nitrogen Vacancy Point Defects in Diamond", A. S. Zyubin, A. M. Mebel, M. Hayashi, H. C. Chang, S. H. Lin, *JOURNAL OF PHYSICAL CHEMISTRY C*, **113**(24), 10432-10440 (2009).
721. "Ab initio studies of excited electronic states S2 of pyrazine and Franck-Condon simulation of its absorption spectrum", Rongxing He, Chaoyuan Zhu, C. H. Chin, S. H. Lin, *Chemical Physics Letters*, **476**, 19-24 (2009).
722. "On the calculation of rate constants of the small cyclic water cluster by anharmonic RRKM theory", Y. Shao, L. Yao, and S. H. Lin, *Chemical Physics Letters*, **478**, 277-282 (2009).

723. "Quantum Chemical Modeling of Photoabsorption Properties of the Nitrogen-Vacancy Point Defect in Diamond", Zyubin AS, Mebel AM, Hayashi M, Chang HC, Lin SH, *JOURNAL OF COMPUTATIONAL CHEMISTRY*, **30**(1), 119-131 (2009).
724. "Thermodynamics of a conformational change using a random walk in energy-reaction coordinate space: Application to methane dimer hydrophobic interactions", Morozov AN, Lin SH, *JOURNAL OF CHEMICAL PHYSICS*, **130**(7), 074903 (2009).
725. "Structural change of ionic association in ionic liquid/water mixtures: A high-pressure infrared spectroscopic study", Umebayashi Y, Jiang JC, Shan YL, Lin KH, Fujii K, Seki S, Ishiguro SI, Lin SH, Chang HC, *JOURNAL OF CHEMICAL PHYSICS*, **130**(12), 124503 (2009).
726. "Photoinduced Structural Dynamics in Laser-Heated Nanomaterials of Various Shapes and Sizes (vol 112, pg 17135, 2008)", Yu P, Tang J, Lin SH, *JOURNAL OF PHYSICAL CHEMISTRY C*, **113**(17), 7480-7480 (2009).
727. "Matrix reorganization with intramolecular tunneling of H atom: Formic acid in Ar matrix", Trakhtenberg LI, Fokeyev AA, Zyubin AS, Mebel AM, Lin SH, *JOURNAL OF CHEMICAL PHYSICS*, **130**(14), 144502 (2009).
728. "Molecular Dynamics insight into the role of tertiary (foldon) interactions on unfolding in Cytochrome c", Tsai MY, Morozov AN, Chu KY, Lin SH, *CHEMICAL PHYSICS LETTERS*, **475**(1-3), 111-115 (2009).
729. "Influence of neighboring levels in three-pulse photon-echo processes", Villaeys AA, Dappe YJ, Liang KK, Lin SH, *PHYSICAL REVIEW A*, **79**(5), 053418 (2009).
730. "Rotationally resolved ultrahigh-resolution laser spectroscopy of the S-2 (1)A(1)<sup>-</sup> - S-0 (1)A(1) transition of azulene", Semba Y, Yoshida K, Kasahara S, Ni CK, Hsu YC, Lin SH, Ohshima Y, Baba M, *JOURNAL OF CHEMICAL PHYSICS*, **131**(2), 024303 (2009).
731. "Ionization and Dissociation Processes of Pyrrolidine in Intense Femtosecond Laser Field", Q. Wang, D. Wu, D. Zhang, M. Jin, F. Liu, H. Liu, Z. Hu, D. Ding, H. Mineo, Y. A. Dyakov, Y. Teranishi, S. D. Chao, A. M. Mebel, and S. H. Lin, *J. Phys. Chem. C*, **113**(27), 11805 (2009).
732. "Molecular Ionization of Cyclohexanone in Femtosecond Laser Fields: an Application of ADK Theory", Q. Wang, H. Mineo, D. Wu, M. Jin, C. H. Chin, Y. Teranishi, S. D. Chao, D. Ding, and S. H. Lin, *Laser Physics*, **19**(8), 1671 (2009).
733. "Theory of ZEKE spectroscopy and molecular Rydberg dynamics", S. D. Chao, S. H. Lin, H.

- L. Selzle, H. J. Neusser, and E. W. Schlag, *Trends in Applied Spectroscopy*, **7**, 1-18 (2009).
734. "Vibrational and rotational structure and excited-state dynamics of pyrene", Baba M, Saitoh M, Kowaka Y, Taguma K, Yoshida K, Semba Y, Kasahara S, Yamanaka T, Ohshima Y, Hsu YC, Lin SH, *JOURNAL OF CHEMICAL PHYSICS*, 131, 22, 224318 (2009).
735. "Highly Multiphoton Excitation of Molecule by Intense Laser Field", Teranishi Y, Hayashi M, Song D, Azarm A, Kong F, Chin SL, Mineo H, Lin SH, *2009 Lasers & Electro-Optics & The Pacific Rim Conference on Lasers and Electro-Optics*, VOLS **1 and 2**, 164-165 (2009).
736. "Theoretical and Experimental Investigations of Ionization-Dissociation of Polyatomic Molecules", *2009 Lasers & Electro-Optics & The Pacific Rim Conference on Lasers and Electro-Optics*, VOLS **1 and 2**, 14-14 (2009).
737. "Photoinduced Ultrafast Structural Dynamics of Nanomaterials", Tang J, Yu P, Tai PT, Lin SH, *Ultrafast Phenomena in Semiconductors and Nanostructure Materials XIII*, 7214, 72140F (2009).
738. "Dissociation Rate Constant of the Hydrogen Fluoride Dimer by the ab initio Anharmonic RRKM Theory, Yao L, Mebel AM, Lin SH", *Journal of Physical Chemistry A*, **113**, 52, 14664-14669 (2009). (TC:3)(ISSN:1089-5639)
739. "Blinking suppression of single quantum dots in agarose gel", H. C. Ko, C. T. Yuan, S. H. Lin, and Jau Tang, *Applied Physics Letters*, **96**, 012104 (2010).
740. "Reciprocating and Directed Motion on the Nanoscale: A Simple Kinetic Model", V. M. Rozenbaum, Yu. A. Makhnovskii, D. Y. Yang, S. Y. Sheu, and S. H. Lin, *J. Phys. Chem. B*, **114**(5), 1959-1966 (2010).
741. "Theoretical Studies of ZEKE Spectroscopy and Dynamics of High Rydberg States", Y. H. Wang, Y. Teranishi, H. Mineo, S. D. Chao, H. L. Selzle, H. J. Neusser, E. W. Schlag, and S. H. Lin, *Chemical Physics Letters*, **486**, 4-6 (2010).
742. "Neutral Dissociation of Superexcited Oxygen Molecules in Intense Laser Fields ", Song, D.; Azarm, A.; Kamali, Y.; Liu, K.; Xia, A. D.; Teranishi, Y.; Lin, S. H.; Kong, F. A.; Chin, S. L., *Journal of Physical Chemistry A* **114**, (9), 3087-3095 (2010).
743. "High pressure effect on the ultrafast energy relaxation rate of LDS698 (C<sub>19</sub>H<sub>23</sub>N<sub>2</sub>O<sub>4</sub>Cl) in a solution", Liu, B. G.; He, C. Y.; Jin, M. X.; Wang, Q. Q.; Lin, S. H.; Ding, D. J., *Optics Express* **18**(7), 6863-6870 (2010).
744. "Nonadiabatic Response Model of Laser-Induced Ultrafast pi-Electron Rotations in Chiral Aromatic Molecules", Kanno, M.; Kono, H.; Fujimura, Y.; Lin, S. H., *Physical Review*



*Letters* **104**(10), 108302 (2010).

745. "A theoretical study on the spectroscopy and the radiative and non-radiative relaxation rate constants of the S0 1A1 — S1 1A2 vibronic transitions of formaldehyde", Lin CK,\* Li MC, Yamaki M, Hayashi M, Lin SH, *Physical Chemistry Chemical Physics*, **12**, 37, 11432–11444, (2010).
746. "Symmetry Forbidden Vibronic Spectra and Internal Conversion in Benzene", Li J, Lin CK,\* Li XY,\* Zhu CY, Lin SH, *Physical Chemistry Chemical Physics*, **12**, 45, 14967–14976 (2010).
747. "Ultrafast Electronic Motion in Hydrogen Molecular ions induced by a high power intense laser", H. Mineo, Y. Teranishi, S. D. Chao, S. H. Lin., *Chemical Physics Letters*, **499**, 1–3, 45–50 (2010).
748. "Anharmonic RRKM Calculation for the Dissociation of (H2O)2H+ and Its Deuterated Species (D2O)2D+", Song D,\* Su H,\* Kong FA, Lin SH, *Journal of Physical Chemistry A*, **114**, 10217–10224 (2010).
749. "Blocked Electron Transfer and Suppressed Blinking of Single CdSe/ZnS Quantum Dots in Agarose Gel", Ko HC, Yuan CT, Lin SH, Tang J, *Journal of the Chinese Chemical Society*, **57**, 522–527 (2010).
750. "Spectroscopic Study of Organic Light-emitting Polymers: A Review", Chang RL, Hayashi M, Lin SH, *Journal of the Chinese Chemical Society*, **57**, 547–563 (2010).
751. "Clinical and Microbiological Characteristics of Nocardiosis Including Those Caused by Emerging Nocardia Species in Taiwan", Tan CK, Lai CC, Lin SH, Liao CH, Chou CH, Hsu HL, Huang YT, Hsueh PR, *Clinical Microbiology and Infection*, **16**, 7, 966–972 (2010).
752. "Investigation of Conformation-Dependent Properties of L-Phenylalanine in Neutral and Radical Cations by Using a Density Functional Taking into Account Noncovalent Interactions", Baek KY, Hayashi M, Fujimura Y, Lin SH, Kim SK, *Journal of Physical Chemistry A*, **114**, 28, 7583–7589 (2010).
753. "Special Issue Dedicated to the Nemory of Professor Wunshain Fann (1961–2008) Preface", Lin SH, Chen SA, Chang HC, *Journal of the Chinese Chemical Society*, **57**, 3B (2010).
754. "Population Trapping and Rotational Revival of N-2 Molecules During Filamentation of a Femtosecond Laser Pulse in Air", Azarm A, Ramakrishna S, Talebpour A, Hosseini S,

Teranishi Y, Xu HL, Kamali Y, Bernhardt J, Lin SH, Seideman T, Chin SL, *Journal of Physics B-Atomic Molecular and Optical Physics*, **43**, 23, 235602 (2010).

755. "Effect of the Medium on Intramolecular H-Atom Tunneling: Cis-Trans Conversion of Formic Acid in Solid Matrixes of Noble Gases", Trakhtenberg LI, Fokeyev AA, Zyubin AS, Mebel AM, Lin SH, *Journal of Physical Chemistry B*, **114**, 51, 17102-17112 (2010).

## 2011 – 1970

756. "A High-Pressure Infrared Spectroscopic Study on the Interaction of Ionic Liquids with PEO-PPO-PEO Block Copolymers and 1,4-Dioxane", Jiang JC, Li SC, Shih PM, Hung TC, Chang SC, Lin SH, Chang HC, *Journal of Physical Chemistry B*, **115**, 5, 883-888 (2011).
757. "A master equation approach to the dynamics of zero electron kinetic energy (ZEKE) states and ZEKE spectroscopy", Wang YH, Mineo H, Chao SD, Selzle HL, Neusser HJ, Schlag EW, Teranishi Y, Lin SH, *Journal of Chemical Physics*, **134**, 6, 064316 (2011).
758. "Association structures of ionic liquid/DMSO mixtures studied by high-pressure infrared spectroscopy", Jiang JC, Lin KH, Li SC, Shih PM, Hung KC, Lin SH, Chang HC, *Journal of Chemical Physics*, **134**, 4, 044506 (2011).
759. "Seebeck coefficients in nanoscale junctions: Effects of electron-vibration scattering and local heating", Hsu BC, Liu YS, Lin SH, Chen YC, *Physical Review B*, **83**, 4, 041404 (2011).
760. "Franck-Condon simulation of the  $A B-1(2) \rightarrow X(1)A(1)$  dispersed fluorescence spectrum of fluorobenzene and its rate of the internal conversion", He RX, Yang L, Zhu CY, Yamaki M, Lee YP, Lin SH, *Journal of Chemical Physics*, **134**, 9, 094313 (2011).
761. "Neutral dissociation of hydrogen molecules in a strong laser field through superexcited states", Azarm A, Song D, Liu K, Hosseini S, Teranishi Y, Lin SH, Xia A, Kong F, Chin SL, *Journal of Physics B- Atomic Molecular and Optical Physics*, **44**, 8, 085601 (2011).
762. "Theoretical and experimental study of fullerenol molecules and ions  $C-60(OH)(24-n)(OL)(n)$  and  $C-60(OH)(24-n)(OL)(n)L$  successively substituted by Alkali Metal atoms  $L(n=1-24)$ ", Charkin OP, Klimenko NM, Wang YS, Wang CC, Chen CH, Lin SH, *Russian Journal of Inorganic Chemistry*, **56**, 4, 580-590 (2011).

763. "Theoretical and experimental study of the structure and stability of multiply Na-substituted glucose and 2, 4, 6-trihydroxyacetophenone derivatives", Charkin OP, Klimenko NM, Chen BG, Lin SH, Chen CH, *Russian Journal of Inorganic Chemistry*, **56**, 1, 61-70 (2011).
764. "Density Functional Theory Study of Conformation-Dependent Properties of Neutral and Radical Cationic L-Tyrosine and L-Tryptophan", K. Y. Baek, Y. Fujimura, M. Hayashi, S. H. Lin and S. K. Kim", *Journal of Physical Chemistry A*, **115**, 34, 9658-9668 (2011).
765. "The visible spectrum of zirconium dioxide,  $ZrO_2$ ", A Le, TC Steimle, V Gupta, CA Rice, JP Maier and SH Lin, CK Lin, *Journal of Chemical Physics*, 135, 10, 104303(11) (2011).
766. "Two-state Brownian motor driven by synchronously fluctuating unbiased forces", V. M. Rozenbaum, Y. A. Makhnovskii, S. Y. Sheu, D. Y. Yang and S. H. Lin, *Physical Review E*, **84**, 2, 021104(8) (2011).
767. "Interactions of Silica Nanoparticles and Ionic Liquids Probed by High Pressure Vibrational Spectroscopy", H. C. Chang, T. C. Hung, S. C. Chang, J. C. Jiang and S. H. Lin, *Journal of Physical Chemistry C*, **115**, 24, 11962-11967 (2011).
768. Observation of Inverted Regime Electron Transfer in CdSe/ZnS QDs from pH-Sensitive Single-Particle and Ensemble Fluorescence Measurements", H. C. Ko, C. T. Yuan, S. H. Lin and J. Tang, *Journal of Physical Chemistry C*, **115**, 29, 13977-13984 (2011).
769. "Application of the Singular Perturbation Method to Reaction Kinetics", W. Richardson, L. Volk, K. H. Lau, S. H. Lin and H. Eyring, *Proceedings of the National Academy of Science of the United States of America*, **70**, 5, 1588-1592 (2011).
770. "A Theoretical Study of Spectroscopic Properties and Transition Moments of HBr", *Chemical Physics*, **118**, 3, 333-343 (2011).
771. "Monte Carlo Calculation of the Quantum Partition Function via Path Integral Formulations", *Journal of Chemical Physics*, **88**, 10, 6390-6398 (2011).
772. "Quenching of Phosphorescence by Paramagnetic Molecules in Rigid Media I", *International Journal of Quantum Chemistry*, **3**, 53a, 307-314 (2011).
773. "Solid-Phase Thermodynamic Interpretation of Ion Desorption in Matrix-Assisted Laser Desorption/Ionization", *Journal of Physical Chemistry B*, **114**, 43, 13847-13852 (2011).

774. "A theoretical search for stable bent and linear structures of low-lying electronic states of titanium dioxide (TiO<sub>2</sub>) molecule", Chih-Kai Lin, Jun Li, Zheyang Tu, Xiangyuan Li, Michitoshi Hayashi and Sheng Hsien Lin, *RSC Advances*, **1**, 1228 (2011).
775. "The role of the  $\pi\pi^* 1A_u$  state in the photoabsorption and relaxation of pyrazine", Chih-Kai Lin, Yingli Niu, Chaoyuan Zhu, Zhigang Shuai and Sheng Hsien Lin, *Chem. Asian J.* **6**, 2977 (2011).
776. "Ultrafast Coherent Dynamics of Nonadiabatically Coupled-degenerate Excited States in Molecules: Population and Vibrational Coherence Transfers", H. Mineo, M. Kanno, H. Kono, S. D. Chao, S. H. Lin and Y. Fujimura, *Chemical Physics*, **392**, 1, 136-142 (2012).
777. "Theoretical Design of Polythiénylenevinylene Derivatives for Improvements of Light-emitting and Photovoltaic Performances", Y. Jiang, Q. Peng, X. Gao, Z. Shuai, Y. L. Niu and S. H. Lin, *Journal of Materials Chemistry*, **22**, 4491-4501 (2012).
778. "Recent Developments in Theoretical Chemistry", Y. L. Niu, M. Yamaki, C. Y. Zhu, M. Hayashi, Y. Fujimura and S. H. Lin, *Association of Asia Pacific Physical Societies*, **22**, 12-16 (2012).
779. "Autoionization rate constants of zero electron kinetic energy Rydberg states", H. Mineo, Y. H. Wang, S. D. Chao, S. H. Lin, *Chemical Physics*, **397**, 74-81 (2012).
780. "Specific interactions between the quaternary ammonium oligoether-based ionic liquid and water as a function of pressure", Hai-Chou Chang, Jyh-Chiang Jiang, Tsai-Yi Chen, Hsing-Sheng Wang, Leo Yuxiu Li, Wei-Wen Huang and Sheng Hsien Lin, *Phys. Chem. Chem. Phys.*, **15**, 12734-12741 (2013).
781. "Frank-Condon Simulation of Vibrationally Resolved Optical Spectra for Zinc Complexes of Phthalocyanine and tetrabenzoporphyrin including the Duschinsky and Herzberg-Teller effects", Meiyuan Guo, Rongxing He, Yulan Dai, Wei Shen, Ming Li, Chaoyuan Zhu and Sheng Hsien Lin, *J. Chem. Phys.*, **136**(14), 144313(14) (2012).
782. "Electron-Deficient Pyrimidine Adopted in Porphyrin Sensitizers: A Theoretical Interpretation of  $\pi$ -Spacers Leading to Highly Efficient Conversion Performances in Dye-Sensitized Solar Cells", Guo Meiyuan, He Rongxing, Dai Yulan, Shen Wei, Li Ming, Zhu Chaoyuan and Lin Sheng Hsien, *Journal of Physical Chemistry C*, **116**(16), 9166-9179 (2012).

783. "New Implementation of Semi-classical Dynamic Simulation on the Photoisomerization of cis- and trans-Isomers of Free Stilbene", Lei Yibo, Zhu Chaoyuan, Wen Zhenyi and Lin Sheng Hsien, *Acta Chimica Sinica*, **70**(17), 1869–1876 (2012).
784. "Adiabatically Slow and Adiabatically Fast Driven Ratchets", V. M. Rozenbaum, Yu. A. Makhnovskii, I. V. Shapochkina, S. Y. Sheu, D. Y. Yang and S. H. Lin, *Phys. Rev. E*, **85**(4), 041116(5) (2012).
785. "Anharmonic Franck-Condon simulation of the absorption and fluorescence spectra for the low-lying S1 and S2 excited states of pyrimidine", Ling Yang, Chaoyuan Zhu, Jianguo Yuc, Sheng Hsien Lin, *Chemical Physics*, **400**, 126–136 (2012).
786. "Density matrix method and ultrafast processes", Yingli Niu, Chih-Kai Lin, Chaoyuan Zhu, Hirobumi Mineo, Shengder Chao, Yuichi Fujimura, Michitoshi Hayashi and Sheng Hsien Lin, *Sci. China Chem.*, **55**(4), 579 (2012).
787. "Recent Developments in Radiationless Transitions", Y Niu, CK Lin, L Yang, JG Yu, RX He, R Pang, CY Zhu, Michitoshi Hayashi, SH Lin, *Proccress in Chemistry*, **24**, 928–949 (2012).
788. "Absorption and fluorescence spectra of the neutral and anionic green fluorescent protein chromophore: Franck-Condon simulation", Tsung-Wei Huang, Ling Yang, Chaoyuan Zhu, Sheng Hsien Lin, *Chemical Physics Letters*, **541**, 110–116 (2012).
789. "Ultrafast coherent dynamics of nonadiabatically coupled quasi-degenerate excited states in molecules: Population and vibrational coherence transfers", H. Mineo, M. Kanno, H. Kono, S.D. Chao, S.H. Lin and Y. Fujimura, *Chemical Physics*, **392**(1), 136–142 (2012).
790. "Autoionization rate constants of zero electron kinetic energy Rydberg states", H. Mineo, Y.H. Wang, S.D. Chao and S.H. Lin, *Chemical Physics*, **397**(13), 74–81 (2012).
791. "Coherent pi-electron dynamics of (P)-2,2'-biphenol induced by ultrashort linearly polarized UV pulses: Angular momentum and ring current", H. Mineo, S.H. Lin, and Y. Fujimura, *J. Chem. Phys.*, **138**(7), 074304 (2013).
792. "Quantum chemical calculation of intramolecular vibrational redistribution and vibrational energy transfer of water clusters", Y.L. Niu, R. Pang, C.Y. Zhu, M. Hayahshi, Y. Fujimura, S.H. Lin and Y.R. Shen, *Chem. Phys. Lett.*, **586**, 153–158 (2013).
793. "Non-Markovian response of ultrafast coherent electronic ring currents in chiral aromatic molecules in a condensed phase", H. Mineo, S. H. Lin, Y. Fujimura, J. Xu, R.X. Xu, and Y. J. Yan, *J. Chem. Phys.*, **139**(21), 214306 (2013).

794. "Theory and Applications of Sum-Frequency Generations", C. K. Lin, L. Yang, M. Hayashi, C. Y. Zhu, Y. Fujimura, Y. R. Shen and S. H. Lin, *J. Chin. Chem. Soc.*, **61**(1), 77–92 (2014).
795. "Vibrational effects on UV/Vis laser-driven pi-electron ring currents in aromatic ring molecules", H. Mineo, S.H. Lin and Y. Fujimura, *Chemical Physics*, **442**(17), 103–110 (2014).
796. "Anharmonic effect of the unimolecular dissociation of CH<sub>3</sub>COOH", Liwei Zhang, Li Yao, Qian Li, Guiqiu Wang and S. H. Lin, *Mol. Phys.*, **112**(21), 2853–2871 (2014).
797. "Study on Anharmonic Effect of the Unimolecular Reaction of CH<sub>2</sub>(D<sub>2</sub>)FO", Jingjun Zhong, Qian Li, Ji Luo, Wenwen Xia, Li Yao, and S. H. Lin, *Bull. Korean Chem. Soc.*, **35**(12), 3559–3566 (2014).
798. "Theories and Quantum Chemical Calculations of Linear and Sum-Frequency Generation Spectroscopies, and Intramolecular Vibrational Redistribution and Density Matrix Treatment of Ultrafast Dynamics", L. Yang, Y.L. Niu, C.K. Lin, M. Hayashi, C.Y. Zhu and S.H. Lin, *Adv. Chem. Phys.*, 156, 295–391(2014).
799. "Constraint Trajectory Surface-Hopping Molecular Dynamics Simulation of the Photoisomerization of Stilbene", Yibo Lei, Shaomei Wu, Chaoyuan Zhu, Zhenyi Wen and Sheng-Hsien Lin, *Int. J. Photoenergy*, **2014**, 132149 (2014).
800. "Anharmonic Effect of the Unimolecular Isomerization/Decomposition of Benzyne", Qian Li, Li Yao and S. H. Lin, *J. Chin. Chem. Soc.*, **93**(6), 655–665 (2015).
801. "Calculation of anharmonic effects for the unimolecular dissociation of CH<sub>3</sub>OOH and its deuterated species CD<sub>3</sub>OOD using the Rice-Ramsperger-Kassel-Marcus theory", Qian Li, Li Yao and S.H. Lin, *Can. J. Chem.*, **93**(6), 655–665 (2015).
802. "Anharmonic Effect of the Unimolecular Dissociation of HFCO and DFCO", Jingjun Zhong, Weiwen Wang, Qian Li, Wenwen Xia, Ying Shao, Li Yao and S.H. Lin, *J. Chin. Chem. Soc.*, **62**(7), 582–891 (2015).
803. "Quantum-mechanical approach to predissociation of water dimers in the vibrational adiabatic representation: Importance of channel interactions", H. Mineo, Y. L. Niu, J. L. Kuo, S. H. Lin, and Y. Fujimura, *J. Chem. Phys.*, **143**(8), 084303 (2015).
804. "Calculation of anharmonic effects in the unimolecular dissociation of M<sup>2+</sup> (H<sub>2</sub>O)<sub>2</sub> (M = Be, Mg, and Ca)", Qian Li, Li Yao, Wenwen Xia and S.H. Lin, *Mol. Phys.*, **113**(22), 3480–3494 (2015).

805. "A Theoretical Investigation of Surface-enhanced Sum-frequency Generation", Y. L. Yeh, J. Lei, S. Y. Chen, A. H. H. Chang, C. K. Lin, R. Xe, S.H. Lin, *J. Chin. Chem. Soc.*, **63**(1), 136-144 (2016).
806. "Electronic sum-frequency generation (ESFG) spectroscopy: theoretical formulation of resonances with symmetry-allowed and symmetry-forbidden electronic excited states", Chih-Kai Lin, Jian Lei, Yu-De Lin and Sheng Hsien Lin, *Mol. Phys.*, **115**(15-16), 1803-1812 (2017).
807. "Laser manipulation of localised  $\pi$ -electron rotations in a molecule with two aromatic rings", Masahiro Yamaki, Yoshiaki Teranishi, Sheng Hsien Lin and Yuichi Fujimura, *Mol. Phys.*, **115**(15-16), 1880-1888 (2017).
808. "Franck-Condon simulation for unraveling vibronic origin in solvent enhanced absorption and fluorescence spectra of rubrene", Ying Hu, Chen-Wen Wang, Chaoyuan Zhu, Fenglong Gu and Sheng-Hsien Lin, *RSC Adv.*, **7**, 12407-12418 (2017).
809. "Exploration of hydrogen bond networks and potential energy surfaces of methanol clusters using a two-stage clustering algorithm", Po-Jen Hsu, Kun-Lin Ho, Sheng-Hsien Linab and Jer-Lai Kuo, *Phys. Chem. Chem. Phys.*, **19**, 544-556 (2017).
810. "The electronic structure, optical absorption and photocatalytic water splitting of (Fe + Ni)-codoped  $\text{TiO}_2$ : A DFT + U study", Yanming Lin, Zhenyi Jiang, Chaoyuan Zhu, Ruiqin Zhang, Xiaoyun Hu, Xiaodong Zhang, Haiyan Zhu, and Sheng Hsien Lin, *Int. J. Hydrog. Energy*, **42**(8), 4966-4976 (2017).
811. "Theory of slightly fluctuating ratchets", V.M. Rozenbaum, I.V. Shapochkina, S.H. Lin and L.I. Trakhtenberg, *Jetp Lett.*, **105**, 542-547 (2017).
812. "Directed motion from particle size oscillations inside an asymmetric channel", Yurii A. Makhnovskii, Sheh-Yi Sheu, Dah-Yen Yang, and Sheng Hsien Lin, *J. Chem. Phys.*, **146**, 154103 (2017).
813. "A TDDFT study on the excited-state double proton transfer reaction of 8-hydroxyquinoline along a hydrogen-bonded bridge", Yu-Hui Liu, Shi-Ming Wang, Chaoyuan Zhu and Sheng Hsien Lin, *New J. Chem.*, **41**, 8437-8442 (2017).
814. "Drift of particles caused by fluctuations of their sizes", V. Yu. Zitserman, Yu. A. Makhnovskii, L. I. Trakhtenberg, D.-Y. Yang and S.H. Lin, *Jetp Lett.*, **105**, 335-340 (2017).
815. "Calculation of anharmonic effect on the dissociation of ethylene glycol", Qiao Li, Li Yao and S.H. Lin, *J. Theor. Comput. Chem.*, **16**(8), 1750077 (2017).

816. "Magnetism-tuning strategies for graphene oxide based on magnetic oligoacene oxide patches model", Yanjie Wen, Chia-Liang Yen, Linyin Yan, Hirohiko Kono, Sheng-Hsien Lin and Yong-Chien Ling, *Phys. Chem. Chem. Phys.*, **20**, 3678–3686 (2018).
817. "Anharmonic effect of the unimolecular dissociation of Glycerol to Glycidol", Qian Li, Li Yao and S.H. Lin, *J. Comput. Biophys. Chem.*, **17**(6), 1850040 (2018).
818. "Quantum Design for Ultrafast Probing of Molecular Chirality through Enantiomer-Specific Coherent  $\pi$ -Electron Angular Momentum", Hirobumi Mineo, Gap-Sue Kim, Sheng Hsien Lin, and Yuichi Fujimura, *J. Phys. Chem. Lett.*, **9**, 18, 5521–5526 (2018).
819. "Relaxation high-temperature ratchets", I.V. Shapochkina, V.M. Rozenbaum, S.-Y. Sheu, D.-Y. Yang, S.H. Lin, and L. I. Trakhtenberg, *Physica A*, **514**, 71–78 (2019).
820. "First-principles study on sum-frequency generation spectroscopy of methanol adsorbed on  $\text{TiO}_2(110)$  surface: Effects of substrate and molecular coverages", Zhitao Shen, Chih-Kai Lin, Chaoyuan Zhu, and Sheng Hsien Lin, *J. Chem. Phys.*, **150**, 184112 (2019).
821. "Enhanced photovoltaic performance of dye-sensitized solar cells by the adsorption of Zn-porphyrin dye molecule on  $\text{TiO}_2$  surfaces", Yanming Lin, Chaoyuan Zhu, Zhenyi Jiang, Yali Zhao, QiWang, Ruiqin Zhang, and Sheng Hsien Lin, *J. Alloys Compd.*, **794**, 35–44 (2019).
822. "Dynamic Stark-Induced Coherent  $\pi$ -Electron Rotations in a Chiral Aromatic Ring Molecule: Application to Phenylalanine", Hirobumi Mineo, Gap-Sue Kim, Sheng Hsien Lin, and Yuichi Fujimura, *J. Phys. Chem. A*, **123**, 30, 6399–6410 (2019).
823. "On the validity of the independent interaction model for generation of dynamic Stark-induced degenerate states in chiral aromatic ring molecules", Hirobumi Mineo, Gap-Sue Kim, Sheng Hsien Lin, and Yuichi Fujimura, *Chem. Phys. Lett.*, **741**, 137124 (2020).
824. "Extremely solvent-enhanced absorbance and fluorescence of carbazole interpreted using a damped Franck-Condon simulation", Chen-Wen Wang, Chaoyuan Zhu, and Sheng Hsien Lin, *J. Chem. Phys.*, **152**, 104106 (2020).
825. "The absorption and fluorescence spectra of 4-(3-methoxybenzylidene)-2-methyl-oxazalone interpreted by Franck-Condon simulation in various pH solvent environments", Yu-Hui Liu, Ya-Jing Peng, Hang Su, Chaoyuan Zhu and Sheng-Hsien Lin, *Phys. Chem. Chem. Phys.*, **22**, 17559–17566 (2020).



826. "Excited-state intramolecular proton transfer with and without the assistance of vibronic-transition-induced skeletal deformation in phenol-quinoline", Yu-Hui Liu, Shi-Bo Yu, Ya-Jing Peng, Chen-Wen Wang, Chaoyuan Zhu and Sheng-Hsien Lin, *RSC Adv.*, **11**, 37299-37306 (2021).