

## CURRICULUM VITAE

### FRANK E. HARRIS

University of Utah  
Department of Physics  
115 S 1400 E Rm 201  
Salt Lake City, UT 84112-0830

and

University of Florida  
Quantum Theory Project  
P. O. Box 118435  
Gainesville, FL 32611-8435

**Born :** August 26, 1929, Boston MA

**Education:** **A. B.** (Chemistry), Harvard University, Cambridge, MA, 1951.  
**Ph.D.** (Physical Chemistry), University of California, Berkeley, CA, 1954.

**Positions:** **1969-** Professor of Physics and Chemistry, University of Utah.  
**1998-** Resident Adjunct Professor, Quantum Theory Project and Department of Chemistry, University of Florida.  
**1984-87** President, Golden Dawn Computer Systems, Inc.  
**1978-86** Director, College of Science Computer, University of Utah.  
**1977** Visiting Professor of Chemistry, University of Hawaii.  
**1973-75** Dean of the College of Science, University of Utah.  
**1968-69** Professor of Physics, University of Utah.  
**1959-68** Assistant, Associate Professor of Chemistry, Stanford University.  
**1967** Visiting Research Scientist, United Aircraft Research Laboratories.  
**1966-70** Consultant to Quantum Theory Group of the Center for Theoretical Biology, State University of New York at Buffalo.  
**1964-74** Staff Member, International Summer Institute for Quantum Chemistry, Solid State Physics, and Quantum Biology.  
**1957-59** Sloan Foundation Fellow.  
**1956-59** Assistant Professor of Chemistry, University of California, Berkeley.  
**1955** Summer Visitor, General Electric Research Laboratory.  
**1953-56** Instructor in Chemistry, Harvard University.  
**1952-53** National Science Foundation Predoctoral Fellow

**Fellow, American Institute of Chemists**

**Fellow, American Physical Society**

**Editorial Board:** International Journal of Quantum Chemistry, 2003-

**Cited:** American Men of Science, 11th Ed., p. 2125.  
Who's Who in Science, p. 575.  
Dictionary of International Biography.  
Leaders in American Science (Vol. 6).  
Outstanding Educators of America (1972).  
International Scholars Directory.  
Who's Who in America.

## PUBLICATIONS BY FRANK E. HARRIS

1. "Microeffusiometry of Gaseous Mixtures"  
F. E. Harris & L. K. Nash, *Anal. Chem.* **22**, 1552-1556 (1950).
2. "Determination of Traces of Water Vapor in Gases"  
F. E. Harris & L. K. Nash, *Anal. Chem.* **23**, 736-739 (1951).
3. "The Vapor Phase Association of Butyric and Heptanoic Acids"  
R. E. Lundin, F. E. Harris & L. K. Nash, *J. Am. Chem. Soc.* **74**, 743-745 (1952).
4. "The Vapor Phase Association of Trifluoroacetic Acid"  
R. E. Lundin, F. E. Harris & L. K. Nash, *J. Am. Chem. Soc.* **74**, 4654-4656 (1952).
5. "Dielectric Polarization in Polar Substances"  
F. E. Harris & B. J. Alder, *J. Chem. Phys.* **21**, 1031-1038 (1953).
6. "Dielectric Polarization and Self-Ionization in Carboxylic Acids"  
F. E. Harris & B. J. Alder, *J. Chem. Phys.* **21**, 1306-1307 (1953).
7. "Intermolecular Potentials from Dielectric Polarization in Polar Gases"  
F. E. Harris & B. J. Alder, *J. Chem. Phys.* **21**, 1351-1357 (1953).
8. "Restricted Rotation in Polar Gases Near the Critical Point"  
F. E. Harris & B. J. Alder, *Nature* **172**, 774-775 (1953).
9. "Pressure Dependence of the Dielectric Constant of Water and the Volume Contraction of Water and n-Butanol upon Addition of Electrolyte"  
F. E. Harris, E. W. Haycock & B. J. Alder, *J. Phys. Chem.* **57**, 978-979 (1953).
10. "Dielectric Polarization and Structure of Polar Liquids under Pressure"  
F. E. Harris, E. W. Haycock & B. J. Alder, *J. Phys. Chem.* **21**, 1943-1948 (1953).
11. "Thermodynamic Functions for Self-Ionization in Carboxylic Acids"  
F. E. Harris & B. J. Alder, *Trans. Faraday Soc.* **50**, 1-16 (1954).
12. "The Dielectric Constant of Liquid Trifluoroacetic Acid"  
F. E. Harris & C. T. O'Konski, *J. Am. Chem. Soc.* **76**, 4317-4317 (1954).
13. "A Chain Model for Polyelectrolytes. I"  
F. E. Harris & S. A. Rice, *J. Phys. Chem.* **58**, 725-732 (1954).
14. "A Chain Model for Polyelectrolytes. II"  
S. A. Rice & F. E. Harris, *J. Phys. Chem.* **58**, 733-739 (1954).
15. "Statistical Mechanical Derivation of Onsager's Equation for Dielectric Polarization"  
F. E. Harris & B. J. Alder, *J. Chem. Phys.* **22**, 1806-1808 (1954).
16. "Measurement of High Permittivity Dielectrics at Microwave Frequencies"  
F. E. Harris & C. T. O'Konski, *Rev. Sci. Inst.* **26**, 482-485 (1955).
17. "Ring Formation and Molecular Weight Distributions in Branched-Chain Polymers. I"  
F. E. Harris, *J. Chem. Phys.* **23**, 1518-1525 (1955).
18. "Contributions of Fluctuations and Anisotropy to Dielectric Polarization in Polar Substances"  
F. E. Harris, *J. Chem. Phys.* **23**, 1663-1672 (1955).

## Publications by Frank E. Harris (Continued)

19. "Note on Imperfect Gas Theory"  
F. E. Harris, J. Chem. Phys. **23**, 1965-1965 (1955).
20. "A Raoult's Law Experiment for the General Chemistry Course"  
F. E. Harris & L. K. Nash, J. Chem. Ed. **32**, 575-577 (1955).
21. "The Thermodynamics of Chelate Formation. I. Experimental Determination of Enthalpies and Entropies in Diamine-Metal Ion Systems"  
F.A. Cotton & F. E. Harris, J. Phys. Chem. **59**, 1203-1208 (1955).
22. "The Random Chain Model for Polyelectrolytes"  
F. E. Harris & S. A. Rice, J. Polymer Sci. **15**, 151-156 (1955).
23. Book Review: "Molecular Theory of Gases and Liquids" by J. O. Hirschfelder, C. F. Curtiss & R. B. Bird.  
F. E. Harris, J. Polymer Sci. **17**, 116-116 (1955).
24. "Equilibrium Distribution of Molecular Weights in Noncyclic Polymerizations"  
F. E. Harris, J. Polymer Sci. **18**, 351-357 (1955).
25. "Chain Model for Polyelectrolytes. III. Equimolar Polyampholytes of Regularly Alternating Structure"  
S. A. Rice & F. E. Harris, J. Chem. Phys. **24**, 326-335 (1956).
26. "A Chain Model for Polyelectrolytes. IV. Skeletal Distribution Effects in Equimolar Polyampholytes"  
F. E. Harris & S. A. Rice, J. Chem. Phys. **24**, 336-344 (1956).
27. "Model for Ion-Exchange Resins"  
F. E. Harris & S. A. Rice, J. Chem. Phys. **24**, 1258-1258 (1956).
28. "Electrostatic Contributions to Thermodynamic Functions of Systems Containing Polymeric Ions"  
F. E. Harris & S. A. Rice, J. Chem. Phys. **25**, 955-964 (1956).
29. "Dipole Moments and Dielectric Polarization in Solutions"  
F. E. Harris & S. G. Brush, J. Am. Chem. Soc. **78**, 1280-1287 (1956).
30. "Polyelectrolyte Gels and Ion Exchange Reactions"  
S. A. Rice & F. E. Harris, Z. Physik. Chem. **8**, 207-239 (1956).
31. "The Thermodynamics of Chelate Formation. II. A Monte Carlo Study of the Distribution of Configurations in Short Chains"  
F.A. Cotton & F. E. Harris, J. Phys. Chem. **60**, 1451-1454 (1956).
32. "Dielectric Properties of Aqueous Ionic Solutions at Microwave Frequencies"  
F. E. Harris & C. T. O'Konski, J. Phys. Chem. **61**, 310-319 (1957).
33. "Electric Free Energy and the Deformation of Droplets in Electrically Conducting Systems"  
C. T. O'Konski & F. E. Harris, J. Phys. Chem. **61**, 1172-1174 (1957).
34. "A Model for Ion Binding and Exchange in Polyelectrolyte Solutions and Gels"  
F. E. Harris & S. A. Rice, J. Phys. Chem. **61**, 1360-1364 (1957).

## Publications by Frank E. Harris (Continued)

35. "Tables of the Exponential Integral  $E_i(x)$ "  
F. E. Harris, *Mathematical Tables and Other Aids to Computation* **11**, 9-16 (1957).
36. "Molecular Orbitals for the Ground State of the  $H_2$  Molecule"  
F. E. Harris, *J. Chem. Phys.* **27**, 812-813 (1957).
37. "Comments on the 'Paper Potentiometric Titration, Association Phenomena, and Interaction of Neighboring Groups in Polyelectrolytes'"  
S.A. Rice & F. E. Harris, *J. Chem. Phys.* **28**, 988-989 (1958).
38. "Valence Bond Calculation of the Barrier to Internal Rotation in Molecules"  
G. M. Harris & F. E. Harris, *J. Chem. Phys.* **31**, 1450-1453 (1959).
39. "Molecular Orbital Studies of Diatomic Molecules. I. Method of Computation for Single Configurations of Heteronuclear Systems"  
F.E. Harris, *J. Chem. Phys.* **32**, 3-18 (1960).
40. Book Review: "Molecular Orbital Theory for Organic Chemists", by A. Streitwieser Jr.  
F. E. Harris & R. H. Eastman, *Science* **136**, 143-143 (1962).
41. "Molecular Orbital Studies of Diatomic Molecules II. Method of Computation for Multi-Configurations of Heteronuclear and Homonuclear Systems"  
H. S. Taylor & F. E. Harris, *Molecular Physics*, **6**, 183-192 (1963).
42. "Molecular Orbital Studies of Diatomic Molecules III. The Ground State of the Hydrogen Molecule"  
F. E. Harris & H. S. Taylor, *J. Chem. Phys.* **38**, 2591-2596 (1963).
43. "Gaussian Wave Functions for Polyatomic Molecules"  
F. E. Harris, *Rev. Mod. Phys.* **35**, 558-569 (1963).
44. "Discussion on Natural Expansions and Properties of the Chemical Bond"  
F. E. Harris (chairman), *Rev. Mod. Phys.* **35**, 629-630 (1963).
45. "Potential Curve for the  $^2\Sigma_u^+$  State of  $H_2^-$ "  
H. S. Taylor & F. E. Harris, *J. Chem. Phys.* **39**, 1012-1016 (1963).
46. "Molecular Orbital Studies of Excited States of HeH"  
H. H. Michels & F. E. Harris, *J. Chem. Phys.* **39**, 1464-1469 (1963).
47. "A Quantum-Mechanical Study of the LiH Molecule in the Ground State"  
F. E. Harris & H. S. Taylor, *Physica* **30**, 105-112 (1964).
48. "A Quantum-Mechanical Study of the He,  $H^-$ , He-He and He-H Systems"  
F. E. Harris & H. S. Taylor, *Molecular Physics* **7**, 287-294 (1964).
49. "Studies of Hydrogen-Bonded Systems. I. The Electronic Structure and the Double Well Potential of the N-H...N Hydrogen Bond of the Guanine-Cytosine Base Pair"  
R. Rein & F. E. Harris, *J. Chem. Phys.* **41**, 3393-3401 (1964).
50. "Proton Tunneling in Radiation-Induced Mutation"  
R. Rein & F. E. Harris, *Science* **146**, 649-650 (1964).

## Publications by Frank E. Harris (Continued)

51. "Studies of Hydrogen-Bonded Systems. II. Tunneling and Tautomeric Equilibria in the N-H... N Hydrogen Bond of the Guanine-Cytosine Base Pair"  
R. Rein & F. E. Harris, *J. Chem. Phys.* **42**, 2177-2180 (1965).
52. "Split-Shell Molecular Orbitals for Sigma-Bonded Systems: Hydrogen Halides"  
F.E. Harris & H. A. Pohl, *J. Chem. Phys.* **42**, 3648-3651 (1965).
53. "Evaluation of Multicenter Integrals Occurring in Molecular Quantum Mechanics"  
F. E. Harris & H. H. Michels, *J. Chem. Phys.* **42**, 3325-3326 (1965).
54. "Discussion Following Slater's Paper"  
F. E. Harris, *J. Chem. Phys.* **43**, S17-S17 (1965).
55. "Multicenter Integrals in Quantum Mechanics. I. Expansion of Slater-Type Orbitals about a New Origin"  
F.E. Harris & H. H. Michels, *J. Chem. Phys.* **43**, S165-S169 (1965).
56. "The Interaction Potential Surface for H<sub>3</sub>"  
F.E. Harris, D. A. Micha & H. A. Pohl, *Arkiv för Fysik* **30**, 259-266 (1965).
57. "Studies of Hydrogen Bonded Systems. III. Potential Energy Surface, Tunneling and Tautomeric Equilibria in the N-H...N and O...H-N Bonds of the Guanine-Cytosine Base Pair"  
F.E. Harris & R. Rein, *J. Chem. Phys.* **43**, 4415-4421 (1965).
58. "Potential Curve for HeH<sup>+</sup>"  
F. E. Harris, *J. Chem. Phys.* **44**, 3636-3637 (1966).
59. "Multicenter Integrals in Quantum Mechanics. II. Evaluation of Electron-Repulsion Integrals for Slater-Type Orbitals"  
F.E. Harris & H. H. Michels. *J. Chem. Phys.* **45**, 116-123 (1966).
60. "Studies of Hydrogen-Bonded Systems. IV. Radiation-induced Tunneling and Tautomeric Equilibria in the Guanine-Cytosine Base Pair"  
R. Rein & F. E. Harris, *J. Chem. Phys.* **45**, 1797-1799 (1966).
61. "On the Calculation of Spin Densities"  
F. E. Harris, *Molecular Physics* **11**, 243-256 (1966).
62. "Integral Approximations for Molecular Orbital Theory"  
F. E. Harris & R. Rein, *Theoret. Chim. Acta* **6**, 73-82 (1966).
63. "Iterative Extended Hückel Theory"  
R. Rein, N. Fukuda, H. Win, G. A. Clarke & F. E. Harris, *J. Chem. Phys.* **45**, 4743-4744 (1966).
64. "Approximation of Molecular Integrals"  
F. E. Harris & R. Rein, *Nature* **212**, 1232-1232 (1966).
65. "Molecular Orbital Theory"  
F. E. Harris, *Adv. Quant. Chem.* **3**, 61-127 (1967).
66. "The Evaluation of Molecular Integrals for Slater-Type Orbitals"  
F. E. Harris & H. H. Michels, *Adv. Chem. Phys.* **13**, 205-266 (1967).
67. "Open-Shell Orthogonal Molecular Orbital Theory"  
F. E. Harris, *J. Chem. Phys.* **46**, 2769-2776 (1967).

## Publications by Frank E. Harris (Continued)

68. "Matrix Elements of Spin-Interaction Operators"  
F. E. Harris, J. Chem. Phys. **47**, 1047-1061 (1967).
69. "Open-Shell Valence Configuration-Interaction Studies of Diatomic and Polyatomic Molecules"  
F. E. Harris & H. H. Michels, Int. J. Quantum Chem. **S1**, 329-338 (1967).
70. "Configuration Interaction Using Open-Shell Spin-Projected Functions"  
H. F. Schaefer III & F. E. Harris, Chem. Phys. Letters **1**, 407-408 (1967).
71. "Electronic Structure of Atomic Boron"  
F. E. Harris & H. F. Schaefer III, Phys. Rev. **167**, 67-73 (1968).
72. "Expansion Approach to Scattering"  
F. E. Harris, Phys. Rev. Letters **19**, 173-175 (1967).
73. "Expansion Approach to Low-Energy Electron-Hydrogen Atom Scattering"  
H. H. Michels & F. E. Harris, Phys. Rev. Letters **19**, 885-886 (1967).
74. "On Self-Consistent Methods in Hückel Theory"  
F. E. Harris, J. Chem. Phys. **48**, 4027-4028 (1968).
75. "Configuration-Interaction Study of the Linear H<sub>3</sub> System"  
H. H. Michels & F. E. Harris, J. Chem. Phys. **48**, 2371-2372 (1968).
76. "Electron Detachment in H<sup>-</sup> + F and H + F<sup>-</sup> Collisions"  
H. H. Michels, F. E. Harris, & J. C. Browne, J. Chem. Phys. **48**, 2821-2822 (1968).
77. "Ab initio Calculations on 62 Low-Lying States of the O<sub>2</sub> Molecule"  
F. E. Harris & H. F. Schaefer III, J. Chem. Phys. **48**, 4946-4955 (1968).
78. "Calculation of the Electron Affinity of Boron"  
H. F. Schaefer III & F. E. Harris, Phys. Rev. **170**, 108-115 (1968).
79. "Molecular Orbital Study of the Hydrogen Bonding of Water"  
R. Rein, G. A. Clarke & F. E. Harris, J. Molecular Structure, **2**, 103-109 (1968).
80. "Iterative Extended Hückel Study of Nucleic Acid Bases"  
R. Rein, N. Fukuda, G. A. Clarke, & F. E. Harris, J. Theor. Biol. **21**, 88-96 (1968).
81. "Spin-Extended and Configuration-Interaction Studies of First-Row Atoms"  
F. E. Harris, U. Kaldor & H. F. Schaefer III, Int. J. Quantum Chem. **S2**, 13-20 (1968).
82. "Construction and Use of Atomic L-S Eigenfunctions"  
H. F. Schaefer III & F. E. Harris, J. Computational Physics **3**, 217-225 (1968).
83. "Valence Configuration Interaction Calculations for Atomic Scattering"  
H. H. Michels & F. E. Harris, Int. J. Quantum Chem. **S2**, 21-27 (1968).
84. "Atomic Hyperfine Structure. I. Polarization Wavefunctions for the Ground States of B, C, N, O, and F"  
H. F. Schaefer III, R. A. Klemm & F. E. Harris, Phys. Rev. **176**, 49-58 (1968).
85. "Metastability of the <sup>1</sup>D State of the Nitrogen Negative Ion"  
H. F. Schaefer III & F. E. Harris, Phys. Rev. Letters **21**, 1561-1563 (1968).

### Publications by Frank E. Harris (Continued)

86. "Projection of Exact Spin Eigenfunctions"  
V. H. Smith, Jr. & F. E. Harris, *J. Math. Phys.* **10**, 771-778 (1969).
87. "Rapid Evaluation of Coulomb Integrals"  
F. E. Harris, *J. Chem. Phys.* **51**, 4770-4778 (1969).
88. "Comparison of Configuration-Interaction Methods for F<sub>2</sub>"  
F. E. Harris & H. H. Michels, *Int. J. Quantum Chem.* **S3**, 461-467 (1970).
89. "Atomic Hyperfine Structure. II. First-Order Wave Functions for the Ground States of B, C, N, O, and F"  
H.F. Schaefer III, R. A. Klemm & F. E. Harris, *Phys. Rev.* **181**, 137-143 (1969).
90. "Calculation of Cross-Sections for Electron-Helium Collisions"  
H. H. Michels, F. E. Harris & R. M. Scorsky, *Physics Letters* **28A**, 467-468 (1969).
91. "Spin-Optimized Self-Consistent Field Wave Functions"  
U. Kaldor & F. E. Harris, *Phys. Rev.* **183**, 1-7 (1969).
92. "Quantum Mechanics in Biochemistry"  
F. E. Harris & R. Rein, *Encyclopaedic Dictionary of Physics, Suppl. Vol. 4* (Pergamon, Oxford, 1971), pp. 351-354.
93. "Expansion Technique for Inelastic Scattering"  
F.E. Harris & H. H. Michels, *Phys. Rev. Letters* **22**, 1036-1039 (1969).
94. "Predissociation Effects in the A <sup>2</sup>Σ<sup>+</sup> State of the OH Radical"  
H. H. Michels & F. E. Harris, *Chem. Phys. Letters* **3**, 441-442 (1969).
95. "First-Order Wavefunctions, Orbital Correlation Energies, and Electron Affinities of First-Row Atoms"  
H. F. Schaefer III, R. A. Klemm & F. E. Harris, *J. Chem. Phys.* **51**, 4643-4650 (1969).
96. "Iterative Extended Hückel Studies of Electronic Structure with Application to Heterocyclic Compounds"  
R. Rein, G. A. Clarke & F. E. Harris, *The Jerusalem Symposia on Quantum Chemistry & Biochemistry, II.*, E. D. Bergmann & B. Pullman, Eds. (Israel Academy of Sciences and Humanities, Jerusalem, 1970), pp. 86-117.
97. "Integrals for Electron-Atom Scattering Calculations"  
F. E. Harris & H. H. Michels, *J. Comput. Phys.* **4**, 579-593 (1969).
98. "Multicenter Integrals via Gaussian Expansion of Slater-Orbital Products"  
H. J. Monkhorst & F. E. Harris, *Chem. Phys. Letters* **3**, 537-539 (1969).
99. "Molecular Orbital Studies of the Stability of CH<sub>5</sub><sup>+</sup> and BH<sub>5</sub>"  
H. H. Michels, F. E. Harris & J. B. Addison, *Int. J. Quantum Chem.* **4**, 149-151 (1971).
100. "Lattice Sums and Madelung Constants"  
F. E. Harris & H. J. Monkhorst, *Chem. Phys. Letters* **4**, 181-182 (1969).
101. "Complete Calculations of the Electronic Energies of Solids"  
F. E. Harris & H. J. Monkhorst, *Phys. Rev. Letters* **23**, 1026-1030 (1969).



### Publications by Frank E. Harris (Continued)

102. "Electronic-Structure Studies of Solids. I. Fourier Representation Method for Madelung Sums"  
F. E. Harris & H. J. Monkhorst, *Phys. Rev. B* **2**, 4400-4405 (1970) [erratum *B* **9**, 3946 (1974)].
103. "Application of New Madelung Summation Method to Close-Packed Alkali-Halide Structures"  
F. E. Harris & H. J. Monkhorst, *J. Chem. Phys.* **52**, 4310-4311 (1970).
104. "Pair Correlations and the Electronic Structure of Neon"  
J. W. Viers, F. E. Harris & H. F. Schaefer III, *Phys. Rev.* **A 1**, 24-27 (1970).
105. "Toward Hartree-Fock Calculations for Simple Crystals"  
F. E. Harris & H. J. Monkhorst, "Computational Methods in Band Theory", P. M. Marcus, J. F. Janak, and A. R. Williams, eds. (Plenum Press, 1971), pp. 517-541.
106. "Calculation of the Attractive He Pair Potential"  
H.F. Schaefer III, D. R. McLaughlin, F. E. Harris & B. J. Alder, *Phys. Rev. Letters* **25**, 988-990 (1970).
107. "Systematics of Atomic Correlation Energies"  
F.E. Harris, *J. Physique* **31**, C4 111-115 (1970).
108. "'Exact' Hartree-Fock Calculations for Atomic-Hydrogen Crystal"  
F. E. Harris & H. J. Monkhorst, *Solid State Comm.* **9**, 1449-1453 (1971).
109. "Balanced Zero-Differential-Overlap Approximations in Nonempirical Molecular Orbital Calculations"  
J. M. Herbelin & F. E. Harris, *J. Am. Chem. Soc.* **93**, 2565-2566 (1971).
110. "Exact Hartree-Fock Results for Atomic Hydrogen Crystals"  
F. E. Harris, L. Kumar & H. J. Monkhorst, *Int. J. Quantum Chem.* **S5**, 527-531 (1971).
111. "Accurate Calculation of Fourier Transform of Two-Center Slater Orbital Products"  
H.J. Monkhorst & F. E. Harris, *Int. J. Quantum Chem.* **6**, 601-607 (1972).
112. "Expansion Methods for Electron-Atom Scattering"  
F. E. Harris & H. H. Michels, in *Methods in Computational Physics*, Vol. 10, M. Rotenberg, S. Fernbach & B. J. Alder, Eds. (Academic Press, N.Y., 1971), pp. 143-210.
113. "Fourier Representation Methods for Electronic Structures of Linear Polymers"  
F.E. Harris, *J. Chem. Phys.* **56**, 4422-4425 (1972).
114. "The Hartree-Fock Problem for Lithium Crystals: A Preliminary Report"  
F.E. Harris, L. Kumar & H. J. Monkhorst, *J. Physique* **33**, C3 99-101 (1972).
115. "Reduction of Hybrid Electron-Repulsion Integrals to Overlap Integrals"  
M. Randic & F. E. Harris, *Croatica Chemica Acta* **52**, 347-352 (1979).
116. "Quantum Chemistry"  
F. E. Harris, in *Annual Review of Physical Chemistry*, Vol. 23 (Annual Reviews Inc., Palo Alto CA, 1972), pp. 415-438.
117. "Isomer Shift Calibration Using Multivalent States of Fe<sup>57</sup> in KMgF"  
A. Trautwein, J. R. Regnard, F. E. Harris & Y. Maeda, *Phys. Rev. B* **7**, 947-951 (1973).
118. "Molecular Orbital Structure, Mossbauer Isomer Shift and Quadrupole Splitting in Iron Complexes"  
A. Trautwein & F. E. Harris, *Theoretica Chimica Acta* **30**, 45-58 (1973).

## Publications by Frank E. Harris (Continued)

119. "Approximations for Large-Molecule Calculations"  
F. E. Harris in *Computational Methods for Large Molecules and Localized States in Solids*, F. Herman, A. D. McLean & R. K. Nesbet, Eds. (Plenum Pub. Corp., New York, 1973), p. 81-86.
120. "Electronic-Structure Studies of Solids. II. Exact Hartree-Fock Calculations for Cubic Atomic Hydrogen Crystals"  
F. E. Harris, L. Kumar & H. J. Monkhorst, *Phys. Rev. B* **7**, 2850-2866 (1973).
121. "Molecular Orbital Study of Mössbauer Results on Iron Dissolved in Solid Noble Gases"  
A. Trautwein & F. E. Harris, *Phys. Rev.* **B 7**, 4755-4757 (1973).
122. "Molecular Orbital and Mössbauer Study of Iron Oxygen Compounds"  
A. Trautwein, E. Kreber, U. Gonser & F. E. Harris, *J. Phys. Chem. Solids* **36**, 325-328 (1975).
123. "Mössbauer Measurements of the (bi-)Pyramidal Lattice Site in BaFe<sub>12</sub>O<sub>19</sub>"  
E. Kreber, U. Gonser, A. Trautwein & F. E. Harris, *J. Phys. Chem. Solids* **36**, 263-265 (1975).
124. "Electronic Structure Studies of Solids. III. Hartree-Fock Band Functions and Energies for Cubic Lithium Crystals"  
L. Kumar, H. J. Monkhorst & F. E. Harris, *Phys. Rev.* **B 9**, 4084-4095 (1974).
125. "Mössbauer and Molecular Orbital Study of the Myoglobin-CO Complex"  
A. Trautwein, Y. Maeda, F. E. Harris & H. Formanek, *Theoret. Chim. Acta* **36**, 67-76 (1974).
126. "Construction of Spin-Projected Matrix Elements"  
F. E. Harris, *Energy, Structure and Reactivity*, D. W. Smith & W. B. McRae, Eds. (John Wiley & Sons, N.Y., 1973), pp. 112-129.
127. "Peculiar Properties of the (bi-) Pyramidal Lattice Site in BaFe<sub>12</sub>O<sub>19</sub>"  
E. Kreber, U. Gonser, A. Trautwein & F. E. Harris, *Proceedings 5<sup>th</sup> International Conference on Mössbauer Spectroscopy, Bratislava/CSR Sept. 1973.*
128. "Interpretation of Experimental Mössbauer Quadrupole Splittings of Iron Pentacyanide Complexes Using Molecular Orbital Theory"  
A. Trautwein, F. E. Harris & I. Dezsi, *Theoret. Chim. Acta* **35**, 231-236 (1974).
129. "Relativistic Electron Densities and Isomer Shifts of Fe<sup>57</sup> in Iron-Oxygen and Iron-Fluorine Clusters and of Iron in Solid Noble Gases"  
A. Trautwein, F. E. Harris, A. J. Freeman & J. P. Desclaux, *Phys. Rev. B* **11**, 4101-4105 (1975).
130. "Interpretation of Experimental Quadrupole Splitting of Iron Containing Complexes Using Molecular Orbital Theory"  
A. Trautwein, R. Reschke, R. Zimmerman, I. Dezsi & F. E. Harris, *J. Physique* **35**, C6 235-239 (1974).
131. "Molecular Structure, Electric Quadrupole Splitting and Magnetic Susceptibility of Iron in Deoxygenated Myoglobin and Hemoglobin"  
A. Trautwein, R. Zimmerman & F. E. Harris, *Theoret. Chim. Acta* **37**, 89-104 (1975).
132. "Exact-Exchange Crystal and Hartree-Fock Calculations of Molecular and Metallic Hydrogen and Their Transitions"  
David E. Ramaker, Lalit Kumar & F. E. Harris, *Phys. Rev. Lett.* **34**, 812-814 (1975).

## Publications by Frank E. Harris (Continued)

133. "Electronic and Magnetic Structure of  $\alpha$ -FeSO<sub>4</sub>"  
R. Zimmerman, A. Trautwein & F. E. Harris, *Phys. Rev. B* **12**, 3902-3907 (1975).
134. "Calculated Electron Densities and Experimental Isomer Shifts of Fe<sup>57</sup> in the Deoxy and CO-compounds of Myoglobin and Hemoglobin"  
A. Trautwein & F. E. Harris, *Theoret. Chim. Acta* **38**, 65-69 (1975).
135. "Electronic Structure Calculations on Crystals and Polymers"  
F. E. Harris in *Electronic Structure of Polymers and Molecular Crystals*, J. Andre, J. Ladik and J. Delhalle, Eds. (Plenum Publishing Corp., N.Y., 1975), pp. 453-477.
136. "Hartree-Fock Studies of Electronic Structures of Crystalline Solids"  
F.E. Harris in *Advances in Theoretical Chemistry*, Vol. 1, D. Henderson and H. Eyring, Eds. (Academic Press, Inc., N.Y., 1975), pp. 147-218.
137. "*Ab Initio* Methods for Electronic Structures of Crystalline Solids"  
F. E. Harris in *Electrons in Finite and Infinite Structures*, P. Phariseau & L. Scheire, Eds. (Plenum Publishing Corp., N.Y., 1977), pp. 274-320.
138. "Spectroscopic Investigation of Ferrocene and Related Derivatives"  
A. Trautwein, R. Reschke, I. Dezsi & F. E. Harris, *J. Physique* **37**, C6 463-470 (1976).
139. "Electronic Structure, Pressure and Temperature Dependent Charge Densities and Electronic Field Gradients in FeF<sub>2</sub>"  
R. Reschke, A. Trautwein & F. E. Harris, *Phys. Rev. B* **15**, 2708-2717 (1977).
140. "Spectroscopic Investigation of Ferrocene and Related Compounds"  
A. Trautwein, R. Reschke, I. Dezsi & F. E. Harris, *Proceedings International Conference: "The Application of the Mössbauer Effect"*, Corfu, Greece, 1976.
141. "Coupled-Cluster Method for Excitation Energies"  
F.E. Harris, *Int. J. Quantum Chem.* **S11**, 403-411 (1977).
142. "Molecules"  
F. E. Harris, article for *Encyclopedia of Physics*, R. G. Lerner and G. L. Trigg, Eds. (Addison-Wesley, Reading, Mass. 1981), pp. 745-749.
143. "Hartree-Like Methods in Electronic Structure Theory"  
F.E. Harris, *Int. J. Quantum Chem.* **13**, 189-198 (1978).
144. "Convergence Acceleration Technique for Lattice Sums Arising in Electronic-Structure Studies of Crystalline Solids"  
F. E. Harris, *J. Math. Phys.* **18**, 2377-2381 (1977).
145. "Evaluation of Some Trigonometric Series Occurring in Infinite Chain Polymer Calculations"  
J. Delhalle, S. Delhalle & F. E. Harris, *Int. J. Quantum Chem.* **13**, 239-254 (1978).
146. "Fourier Representation Method for Electronic Structure of Linear Polymers. II. Linear Chain of Hydrogen Atoms"  
J. Delhalle & F. E. Harris. *Theoret. Chim. Acta* **48**, 127-141 (1978).
147. "Structure and Stability of Metallic Hydrogen"  
J. Delhalle & F. E. Harris, *Phys. Rev. Lett.* **39**, 1340-1342 (1977).

## Publications by Frank E. Harris (Continued)

148. "Fourier Representation Methods in Electronic Structure Studies of Crystals and Polymers"  
F. E. Harris, in *Electronic Structure and Properties of Polymers*, J.-M. André, J. Delhalle, & J. Ladik, Eds. (NATO Adv. Study Inst. C39, 1978), pp. 117-135.
149. "Electronic Structure, Electron Density, Electron Field Gradient, Magnetic Susceptibility and g-Tensor of  $K_3Fe(CN)_6$ "  
R. Reschke, A. Trautwein, F. E. Harris & S. K. Date, *J. Magnetism and Magnetic Materials* **12**, 176-186 (1979).
150. "Hartree-Fock Formalism for the Calculation of Total Energies and Charge Densities of Thin Films"  
F. E. Harris, H. J. Monkhorst, & W. A. Schwalm, *J. Vac. Sci. Technol.* **16**, 1318-1322 (1979).
151. "Electronic Structure and Electric Field Gradient Tensor in Potassium Ferricyanide"  
R. Reschke, A. Trautwein, F. E. Harris & S. K. Date, *J. Physique* **40**, C2 280-282 (1979).
152. "FAKE Molecular-Orbital Calculations"  
A. Trautwein, J. Delhalle, & F. E. Harris, *Chem. Phys. Lett.* **72**, 315-318 (1980).
153. "The FAKE Method of Molecular Orbital Calculations"  
F. E. Harris, A. Trautwein & J. Delhalle, *Int. J. Quantum Chem.* **S14**, 355-361 (1980).
154. "Coupled Cluster Method for Electron Correlation"  
F.E. Harris, Proceedings of Workshop on Effective Potentials for Real Materials, IBM, Poughkeepsie, NY, 1981.
155. "The Contraction Theorem for the Algebraic Reduction of (Anti-)Commutators Involving Operator Strings"  
F. E. Harris, B. Jeziorski & H. J. Monkhorst, *Phys. Rev. A* **23**, 1632-1638 (1981).
156. "Recursive Scheme for Order-by-Order Many-Body Perturbation Theory"  
H. J. Monkhorst, B. Jeziorski & F. E. Harris, *Phys. Rev. A* **23**, 1639-1644 (1981).
157. "Auxiliary Functions for STO Molecular Integrals: Si, Ci, and Ei"  
F. E. Harris, *ETO Multicenter Molecular Integrals*, C. A. Weatherford and H. W. Jones, eds. (D. Reidel Pub. Co. Dordrecht, Holland, 1982), pp. 135-140.
158. "Evaluation of GTO Molecular Integrals"  
F. E. Harris, *Int. J. Quantum Chem.* **23**, 1469-1478 (1983).
159. "Electronic-Structure Calculation, Photoelectron Spectra, Optical Spectra, and Mössbauer Parameters for the Pyrites  $MS_2$  (M: Fe, Co, Ni, Cu, Zn)"  
S. Lauer, A. Trautwein & F. E. Harris, *Phys. Rev. B* **29**, 6774-6783 (1984).
160. "Application of the FAKE Molecular-Orbital Method to Diatomic Molecules XY (X,Y = H, F, Cl, Br, I)"  
A. Trautwein, S. Lauer, J. Delhalle & F. E. Harris, *Theoretica Chimica Acta* **67**, 175-185 (1985).
161. "Fourier-Representation Method for Electronic Structure of Chainlike Systems: Restricted Hartree-Fock Equations and Applications to the Atomic Hydrogen  $(H)_x$  Chain in a Basis of Gaussian Functions"  
J. Delhalle & F. E. Harris, *Phys. Rev. B* **31**, 6755-6765 (1985).

## Publications by Frank E. Harris (Continued)

162. "An Alternative Computational Strategy for Direct-Space Hartree-Fock Calculations of Extended Model Chains"  
J. Delhalle & F. E. Harris, *Int. J. Quantum Chem.* **27**, 219-229 (1985).
163. "Evaluation of Computational Aspects of a Modified CS-LCAO-SCF-CO Strategy for Electronic Structure Calculations of Extended Model Chains"  
J. Delhalle, J. G. Fripiat & F. E. Harris, *Int. J. Quantum Chem.* **S18**, 141-152 (1984).
164. "New Method for Numerical Integration of the Radial Electronic Schrödinger Equation"  
A. G. Koures & F. E. Harris, *J. Chem. Phys.* **89**, 7344-7348 (1988).
165. "Coupled-Cluster Method for Quantum Lattices: Application to Square  $S=1/2$  Heisenberg Antiferromagnets"  
F. E. Harris, *Phys. Rev. B* **47**, 7903-7909 (1993).
166. "A Note on the Number of Spanning Trees in Buckminsterfullerene"  
N. Trinajstić, Z. Mihalić & F. E. Harris, *Int. J. Quantum Chem.* **S28**, 525-528 (1994).
167. "Critical Study of Plane-Wave Density Functional Methods for Extended Systems"  
F. E. Harris & A. G. Koures, *Int. J. Quantum Chem.* **S29**, 235-239 (1995).
168. "Light-Cone Hamiltonian in Quantum Chemistry: Gaussian Basis Representation for Quantum Electrodynamics"  
V. G. Koures & F. E. Harris, *Int. J. Quantum Chem.* **S29**, 277-282 (1995).
169. "Improved Correlation-Energy Functional"  
A. G. Koures & F. E. Harris, *Int. J. Quantum Chem.* **59**, 3-6 (1996).
170. "Sinc Collocation in Quantum Chemistry: Solving the Planar Coulomb Schrödinger Equation"  
V. G. Koures & F. E. Harris, *Int. J. Quantum Chem.* **S30**, 99-106 (1996).
171. "Analytic Evaluation of Three-Electron Integrals with Slater Wave Functions"  
F. E. Harris, *Phys. Rev. A* **55**, 1820-1831 (1997).
172. "New Approach to Calculation of the Leaky Aquifer Function"  
F. E. Harris, *Int. J. Quantum Chem.* **63**, 913-916 (1997).
173. "Graphs With the Same Detour Matrix"  
M. Randić, L. M. DeAlba & F. E. Harris, *Croatica Chemica Acta* **71**, 53-68 (1998).
174. "Ewald Summations in Systems with Two-Dimensional Periodicity"  
F. E. Harris, *Int. J. Quantum Chem.* **68**, 385-404 (1998).
175. "More About the Leaky Aquifer Function"  
F. E. Harris, *Int. J. Quantum Chem.* **70**, 623-626 (1998).
176. "Spherical Bessel Expansions of Sine, Cosine, and Exponential Integrals"  
F. E. Harris, *Applied Num. Math.* **34**, 95-98 (2000).
177. "Algebraic Reduction in Discrete Light-Cone Quantized Electrodynamics using Maple V"  
F. E. Harris, *Comput. Phys. Commun.* **132**, 21-29 (2000).

## Publications by Frank E. Harris (Continued)

178. "Computer Generation of Coupled-Cluster Equations"  
F. E. Harris, *Int. J. Quantum Chem.* **75**, 593-597 (1999).
179. "Analytic Quadratic Integration Over the Two-Dimensional Brillouin Zone"  
F. E. Harris, *J. Phys.: Condensed Matter* **14**, 621-630 (2002).
180. "Efficient Electronic Structure Calculations for Systems of One-Dimensional Periodicity with the RHF-LCAO Method Implemented in Fourier Space"  
I. Flamant, J.G. Fripiat, J. Delhalle & F.E. Harris, *Theoret. Chem. Accounts* **104**, 350-357 (2000).
181. "Computational Aspects of Polymer Band Structure Calculations by the Fourier Space Restricted Hartree-Fock Method"  
J.G. Fripiat, I. Flamant, F.E. Harris & J. Delhalle, *Int. J. Quantum Chem.* **80**, 856-862 (2000).
182. "On Kryachko's Formula for the Leaky Aquifer Function"  
F.E. Harris, *Int. J. Quantum Chem.* **81**, 332-334 (2001).
183. "Comments on 'Ewald Summation Technique for One-Dimensional Charge Distributions'"  
F. E. Harris, *Comput. Phys. Commun.* **146**, 271-273 (2002).
184. "Orientation Dependence in C<sub>60</sub> Surface-Impact Collisions"  
Q.-H. Tang, K. Runge, H.-P. Cheng & F. E. Harris, *J. Phys. Chem A* **106**, 893-896 (2002).
185. "Exchange Contributions in the Electronic Structure of Systems with 1D-Periodicity: Importance and Computation"  
J. Delhalle, J. G. Fripiat & F. E. Harris, *Int. J. Quantum Chem.* **90**, 587-593 (2002).
186. "Cumulant-Based Approximations to Reduced Density Matrices"  
F.E. Harris, *Int. J. Quantum Chem.* **90**, 105-113 (2002).
187. "Analytical Evaluation of Two-Center STO Electron Repulsion Integrals via Ellipsoidal Expansion"  
F. E. Harris, *Int. J. Quantum Chem.* **88**, 701-734 (2002).
188. "Numerical Integration of Exchange Energy in the Two-Dimensional Brillouin Zone"  
F. E. Harris, J. G. Fripiat & J. Delhalle, *J. Phys: Condensed Matter* **18**, 5493-5501 (2006).
189. "Expansions of the Exponential Integral in Incomplete Gamma Functions"  
W. Gautschi, F. E. Harris & N. M. Temme, *Appl. Math. Lett.* **16**, 1095-1099 (2003).
190. "Virtues and Potentialities of the Fourier Transform Method for Electronic Structure Calculations of 1D Periodic Systems at the Hartree-Fock Level and Beyond"  
J. Delhalle, J. G. Fripiat & F. E. Harris, *Int. J. Quantum Chem.* **90**, 1326-1333 (2002).
191. "Fragmentation of Fullerenes"  
R. T. Chancey, L. Oddershede, F. E. Harris & J. R. Sabin, *Phys. Rev. A* **67**, 043203 (1-7) (2003).
192. "Comment on 'Computation of Two-Center Coulomb Integrals over Slater-Type Orbitals Using Elliptical Coordinates'"  
F. E. Harris, *Int. J. Quantum Chem.* **93**, 332-334 (2003).
193. "Comment: On the Computation of Molecular Auxiliary Functions A<sub>n</sub> and B<sub>n</sub>"  
F. E. Harris, *Pramana* **61**, C779-C780 (2003).

## Publications by Frank E. Harris (Continued)

194. "Fragmentation of Fullerene"  
L. B. Oddershede, R. T. Chancey, F. E. Harris, and J. R. Sabin, *Kvant* **14** (2) 3-7 (2003).
195. "Efficient Evaluation of the Molecular Auxiliary Function  $B_n$  by Downward Recursion"  
F. E. Harris, *Int. J. Quantum Chem.* **100**, 142-145 (2004)..
196. "Exponential Variational Expansion in Relative Coordinates for Highly Accurate Bound State Calculations in Four-Body Systems"  
F. E. Harris, A. M. Frolov, and V. H. Smith, Jr., *J. Chem. Phys.* **119**, 8833-8841 (2003).
197. "Expansion(s) of  $r_{12}^{-2}$ "  
F. E. Harris, *Int. J. Quantum Chem.* **97**, 908-913 (2004).
198. "Gegenbauer Expansions for Three-Electron Integrals"  
F. E. Harris, *Int. J. Quantum Chem.* **102**, 940-947 (2005).
199. "Comment on: Analysis of Some Integrals Arising in the Atomic Four-Electron Problem"  
F. E. Harris, A. M. Frolov, and V. H. Smith, Jr., *J. Chem. Phys.* **120**, 3040-3041 (2004).
200. "Current Methods for Coulomb Few-Body Problems"  
F. E. Harris, *Adv. Quantum Chem.* **47**, 129-155 (2004).
201. "Rigorous Ab Initio Studies of Periodic Systems: Approaches to Electron Correlation"  
F. E. Harris and J. Delhalle, *CECAM Workshop Report* (36 pages) (2003).
202. "Comment on 'Analytic Value of the Atomic Three-Electron Correlation Integral with Slater Wave Functions'"  
F. E. Harris, A. M. Frolov, and V. H. Smith, Jr., *Phys. Rev. A* **69**, 056501 (1-2) (2004)..
203. "Integrals for Exponentially Correlated Four-Body Systems of General Angular Symmetry"  
F. E. Harris, in *Fundamental World of Quantum Chemistry: A Tribute Volume to the Memory of Per-Olov Löwdin*, vol. 3, E. J. Brändas and E. S. Kryachko, eds. (Kluwer, Dordrecht, 2004) , pp. 115-128.
204. "Highly Accurate Evaluation of Atomic Three-Electron Integrals of Lowest Orders"  
F. E. Harris, A. M. Frolov, and V. H. Smith, Jr., *J. Chem. Phys.* **120**, 9974-9983 (2004).
205. "New Methods for Old Coulomb Few-Body Problems"  
F. E. Harris, A. M. Frolov, and V. H. Smith, Jr., *Int. J. Quantum Chem.* **100**, 1086-1091 (2004).
206. "Singular and Non-singular Three-Body Atomic Integrals for Exponential Wavefunctions"  
F. E. Harris, A. M. Frolov, and V. H. Smith, Jr., *J. Chem. Phys.* **121**, 6323-6333 (2004).
207. "Angular Symmetry and Hylleraas Coordinates in Four-Body Problems"  
F. E. Harris, *Adv. Quantum Chem.* **50**, 61-75 (2005).
208. "Correlated Exponential-Basis Integrals with Logarithmic Integrand"  
F. E. Harris, V. H. Smith, Jr., and A. M. Frolov, *Mol. Phys.* **103**, 2047-2054 (2005).
209. "Singular Integrals and their Application to a Hypervirial Theorem"  
F. E. Harris, A. M. Frolov, and V. H. Smith, Jr., *Phys. Rev. A* **72**, 012511 (1-6) (2005).
210. "Fourier Representation Methods for Møller-Plesset Perturbation Theory in One-Dimensionally Periodic Systems"  
J. G. Fripiat, J. Delhalle, and F. E. Harris, *Chem. Phys. Lett.* **422**, 11-14 (2006).

### Publications by Frank E. Harris (Continued)

211. "Highly Compact Wavefunctions for He-like Systems"  
F. E. Harris and V. H. Smith, Jr. *J. Phys. Chem. A* **109**, 11413-11416 (2005).
212. "Highly Compact Wavefunctions for Two-Electron Systems"  
F. E. Harris and V. H. Smith, Jr., *Adv. Quantum Chem.* **48**, 407-419 (2005).
213. "Recurrence Relations for Matrix Elements of Few-Body Correlated Wavefunctions"  
F. E. Harris, *Int. J. Quantum Chem.* **105**, 857-865 (2005).
214. "Comment on 'Exponential Representation in the Coulomb Three-Body Problem'"  
F. E. Harris (submitted).
215. "Improving the Efficiency of Table-Driven CI"  
F. E. Harris, *Int. J. Quantum Chem.* **105**, 34-36 (2005).
216. "Quasi-Spin Density Exchange-Correlation Functionals"  
V. V. Karasiev, S. B. Trickey, and F. E. Harris, *Chem. Phys.* (in press).
217. "Re: Comment on 'New Methods for Old Coulomb Few-Body Problems' "  
F. E. Harris, A. M. Frolov, and V. H. Smith, Jr., *Int. J. Quantum Chem.* **106**, 552-553 (2006).
218. "Integrals for Fully Correlated Gaussians in Relative Coordinates"  
F. E. Harris and H. J. Monkhorst, *Int. J. Quantum Chem.* **106**, 54-64 (2006).
219. "Introduction" ( to special issue: "Mathematical Methods and Symbolic Calculation in Chemistry and Chemical Biology")  
F. E. Harris, *Int. J. Quantum Chem.* **106**, 1-2 (2006).
220. "Systematics of the Ground States of the He Isoelectronic Series"  
F. E. Harris and V. H. Smith, Jr., in *Symmetry, Spectroscopy and SCHUR* (proceedings of the Brian G. Wybourne Commemorative Meeting), R. C. King, M. Bylicki and J. Karwowski, eds. (Nicolaus Copernicus University Press, Torun, 2006), pp. 127-137.
221. "Born-Oppenheimer Interatomic Forces from Simple, Local Kinetic Energy Density Functionals"  
V. V. Karasiev, S. B. Trickey, and F. E. Harris, *J. Computer-Aided Materials Design* (in press).
222. "Density Fitting and Model Densities"  
V. V. Karasiev, S. B. Trickey, and F. E. Harris (submitted).
223. "The Representation of the Dirac Equation and the Variational Principle"  
J. Karwowski, G. Pestka, M. Stanke, and F. E. Harris, *Int. J. Quantum Chem.* (in press).
224. "Recurrence Relations for Fully Correlated Gaussians with Odd Powers of Interparticle Coordinates"  
F. E. Harris and H. J. Monkhorst, *Int. J. Quantum Chem.* (in press).
225. "Graded Methods for Rapid Generation of Quantum Mechanical Forces in Molecular Dynamics Simulations"  
D. E. Taylor, V. V. Karasiev, K. Runge, S. B. Trickey, and F. E. Harris (submitted).
226. "Comment on 'Numerical Treatment of Two-Center Overlap Integrals' "  
F. E. Harris, *J. Mol. Model.* (in press).



### **Publications by Frank E. Harris (Continued)**

227. "Current Studies of Few-Electron Systems"  
F. E. Harris, *Lecture Series on Computer and Computational Sciences* (in press).
228. "Graded Methods for Quantum Mechanical Force Generation in Molecular Dynamics Simulations"  
D. E. Taylor, V. V. Karasiev, K. Runge, S. B. Trickey, and F. E. Harris, *Lecture Series on Computer and Computational Sciences* (in press).

## BOOKS

*Principles of Chemistry*, a programmed textbook, F. E. Harris (Addison-Wesley, Boston, 1963-1965), 8 volumes.

*Software Standards in Chemistry*, F. E. Harris and N. H. F. Beebe, Eds., NRCC Proceedings No. 7 (Lawrence Berkeley Laboratory, University of California, 1980).

*Algebraic and Diagrammatic Methods in Many-Fermion Theory*, F. E. Harris, H. J. Monkhorst & D. L. Freeman (Oxford University Press, 1992).

## PRESENTATIONS

(Partial list; contains only those with archived abstracts)

1. "The Dielectric Constant of Trifluoroacetic Acid"  
F. E. Harris & C. T. O'Konski, Abstr. Pap. Am. Chem. Soc. **125**, 25Q (1954).
2. "A Chain Model fo Polyelectrolytes. Polyampholytes"  
F. E. Harris & S. A. Rice, Abstr. Pap. Am. Chem. Soc. **126**, 17S (1954).
3. "Polyelectrolyte Gels and Ion Exchange Reactions"  
S. A. Rice & F. E. Harris, Abstr. Pap. Am. Chem. Soc. **129**, 20Q (1956).
4. "Dipole Moments and Dielectric Polarization in Solutions"  
F. E. Harris & S. G. Brush, Abstr. Pap. Am. Chem. Soc. **129**, 21Q (1956).
5. "Energy Level Calculations for Small Diatomic Molecules"  
F. E. Harris, Spectrochim. Acta **10**, 232 (1957).
6. "Diatomic Molecule Studies Beyond the Hartree-Fock Approximation"  
F. E. Harris & H. H. Michels, Bull. Am. Phys. Soc. **13**, 191 (1968).
7. "Interaction Potentials for the Low-Lying States of HeNe<sup>+</sup>"  
H. H. Michels & F. E. Harris, Bull. Am. Phys. Soc. **13**, 192 (1968).
8. "Quantum Mechanics in the Chemistry Curriculum"  
F. E. Harris, Abstr. Pap. Am. Chem. Soc. **158**, CHED-21 (1969).
9. "Toward Hartree-Fock Calculations for Simple Crystals"  
F. E. Harris & H. J. Monkhorst, Bull. Am. Phys. Soc. **15**, 890 (1970).
10. "Expansion Calculations of Electron-Hydrogen Scattering"  
H. H. Michels, H. J. Kolker, J. W. Viers, & F. E. Harris, Bull. Am. Phys. Soc. **15**, 1523 (1970).
11. "Ab-Initio Quantum-Mechanical Calculations for Atomic and Molecular Processes"  
F. E. Harris, Bull. Am. Phys. Soc. **15**, 1525 (1970).
12. "Chemists Approach to Electronic-Structure Calculations on Crystalline Solids"  
F. E. Harris, Abstr. Pap. Am. Chem. Soc. **167**, PHYS-35 (1974).
13. "Meeting Computing Needs in Chemistry"  
F. E. Harris, Abstr. Pap. Am. Chem. Soc. **168**, COMP-3 (1974).
14. "Remote Access Programming System for Electronic Structure Calculations"  
F. E. Harris & R. H. Ault, Abstr. Pap. Am. Chem. Soc. **169**, COMP-30 (1975).
15. "A Closer Look at the Multiple Scattering-X $\alpha$  Method"  
F. E. Harris & A. G. Koures, Abstr. Pap. Am. Chem. Soc. **193**, PHYS-137 (1987).
16. "Simulated Surface-Impact Collisions of Fullerenes"  
F. E. Harris & R. Chancey, Bull. Am. Phys. Soc. **47**, 1196 (2002).
17. "Cumulant Approximations to Reduced Density Matrices"  
F. E. Harris, Bull. Am. Phys. Soc. **48**, 1160 (2003).

## PRESENTATIONS (cont)

18. "Methods for Coulomb Few-Body Problems"  
F. E. Harris, Bull. Am. Phys. Soc. **49**, 1282 (2004).
19. "Conventional and Unconventional Symbolic Computation in Chemistry"  
F. E. Harris, Abstr. Pap. Am. Chem. Soc. **228**, COMP-227 (2004).
20. "Highly Compact Wavefunctions for He-like Systems"  
F. E. Harris, Bull. Am. Phys. Soc. **50**, 1007 (2005).
21. "Approximate Density Functionals for Molecular Dynamics Simulations of Material Properties"  
S. B. Trickey, V. V. Karasiev, and F. E. Harris, ISTCP 2005
22. "Compact Wavefunctions for He-Like Systems"  
F. E. Harris, Bull. Am. Phys. Soc. (SESAPS Meeting), DB.0002 (2005).
23. "Molecular Properties from Compact Few-Electron Wavefunctions"  
F. E. Harris (Pacifichem 2005).
24. "Prediction of Born-Oppenheimer Interatomic Forces Using Orbital-Free Density Functional Theory with Approximate Kinetic Energy Functionals"  
S. B. Trickey, V. V. Karasiev, and F. E. Harris, Bull. Am. Phys. Soc. **51**, 1008 (2006).
25. "Fitting of Molecular Densities by Compact, Atom-Centered Expansion"  
V. V. Karasiev, S. B. Trickey, and F. E. Harris, Bull. Am. Phys. Soc. **51**, 1008 (2006).
26. "Explicitly Correlated Wavefunctions for Few-Body Problems"  
F. E. Harris, Bull. Am. Phys. Soc. **51**, 1380 (2006).
27. "Dilogarithms and Four-Body Atomic Coulomb Interaction Integrals for Fully Correlated Exponential Wavefunctions"  
F. E. Harris, American Mathematical Society, Abstract 1016-33-181 (2006).

## OTHER PAPERS FROM THE FEH RESEARCH GROUP

- X1. J. Michl and J. Kolc, "Photochemical Electrocyclic Reaction Requiring an Upper Triplet State", *J. Am Chem. Soc.* **92**, 4148 (1970).
- X2. J. Michl, "Energy Barriers in Photochemical Reactions. Case for the Relevance of Woodward-Hoffmann-type Correlations", *J. Am. Chem. Soc.* **93**, 523 (1971).
- X3. J. Michl and R. Jones, "Borazaro Analogues of Aromatic Hydrocarbons. I. Electronic Spectra", *Collect. Czech. Chem. Commun.* **36**, 1233 (1971).
- X4. J. Michl, "Borazaro Analogues of Aromatic Hydrocarbons. II. Semi-Empirical Calculations", *Collect. Czech. Chem. Commun.* **36**, 1248 (1971).
- X5. H. J. Monkhorst, "On Localized Orbitals in Infinite, Periodic Systems", *Chem. Phys. Lett.* **17**, 561 (1972).
- X6. M. Randic, "Certain Auxiliary Functions Occurring in the Study of Molecular Integrals", *J. Chem. Phys.* **56**, 5858 (1972).
- X7. M. Randic, "Tables of Hybrids Generated by the maximum Overlap Method. I. Highly Strained Small Ring Hydrocarbons", 1973.
- X8. Z. B. Maksic and M. Randic, "Comparative Study of Hybridization in Hydrocarbons", *J. Am. Chem. Soc.* **95**, 6522 (1973).
- X9. A. Graovac, H. J. Monkhorst, and T. Zivkovic, "Slater Orbital Molecular Integrals with Numerical Fourier Transform Methods. I. (Coplanar) Multicenter Exchange Integrals over 1s Orbitals", *Int. J. Quantum Chem.* **7**, 233 (1973).
- X10. M. Randic, "Hybridization by the Maximum Overlap Method", *Int. J. Quantum Chem.* **8**, 643 (1974).
- X11. L. Kumar and H. J. Monkhorst, "Electronic Structure Studies of Solids. IV. Physical Quantities from Rigorous Hartree-Fock Results for Lithium Crystals", *J. Phys. F* **4**, 1135 (1974).
- X12. M. Randic and L. Kumar, "Hybridization in Highly Strained Small Ring Hydrocarbons. V. Methylene and Isopropylene Substituted Spiropentanes", *J. Mol. Structure* **26**, 145 (1975).
- X13. A. Graovac, H. J. Monkhorst, and M. L. Glasser, "Computation of Fourier Transform Quantities in Hartree-Fock Calculations for Simple Crystals", *Int. J. Quantum Chem.* **9**, 243 (1975).
- X14. A. Graovac and H. J. Monkhorst, "Computation of the Fourier Transforms of Lattice Sums over Slater-Type Orbital Products", *Annales de la Societe Scientifique de Bruxelles* **89**, 252 (1975).
- X15. H. J. Monkhorst and J. D. Pack, "Special Points for Brillouin-Zone Integration", *Phys. Rev. B* **13**, 5188 (1976).
- X16. N. Trinajstic, "Recent Advances in the Application of Graph Theory to Organic Chemistry", 1976.
- X17. T. P. Zivkovic and H. J. Monkhorst, "Analytic Connection Between Configuration-Interaction and Coupled-Cluster Solutions", *J. Math. Phys.* **19**, 1007 (1978).
- X18. A. Graovac, I. Gutman, and N. Trinajstic, "Topological Approach to the Chemistry of Conjugated Molecules", *Lect. Notes Chem. No. 4* (1977).

## OTHER PAPERS FROM THE FEH RESEARCH GROUP (Continued)

- X19. I. Gutman and M. Trinajstic, "Factors Contributing to the Stability of Conjugated Heterocycles Containing a Single Heteroatom", *Chem. Phys. Lett.* **46**, 591 (1977).
- X20. T. P. Zivkovic, "Existence and Reality of Solutions of the Coupled-Cluster Equations", *Int. J. Quantum Chem.* **S11**, 413 (1977).
- X21. L. Kumar, H. J. Monkhorst, and J. Oddershede, "Electronic Structure Studies of Solids. V. Rigorous Hartree-Fock Treatment of Metallic Hydrogen Using a Plane-Wave Basis", *Int. J. Quantum Chem.* **12**, 256 (1977).
- X22. N. Trinajstic, "Computing the Characteristic Polynomial of a Conjugated System Using the Sachs Theorem", *Croatica Chimica Acta* **49**, 593 (1977).
- X23. H. J. Monkhorst, "Calculation of Properties with the Coupled-Cluster Method", *Int. J. Quantum Chem.* **S11**, 421 (1977).
- X24. D. L. Freeman, "Coupled-Cluster Expansion Applied to the Electron Gas: Inclusion of Ring and Exchange Effects", *Phys. Rev. B* **15**, 5512 (1977).
- X25. N. Trinajstic, "New Developments in Huckel Theory", *Int. J. Quantum Chem.* **S11**, 469 (1977).
- X26. J. D. Pack and H. J. Monkhorst, "Special Points for Brillouin-Zone Integrations – a Reply", *Phys. Rev. B* **16**, 1748 (1977).
- X27. D. Bonchev and N. Trinajstic, "Information Theory, Distance Matrix, and Molecular Branching", *J. Chem. Phys.* **67**, 4517 (1977).
- X28. D. Bonchev and N. Trinajstic, "On Topological Characterization of Molecular Branching", *Int. J. Quantum Chem.* **S12**, 293 (1978).
- X29. A. Graovac, I. Gutman, M. Randic, and N. Trinajstic, "Kekule Index for Valence Bond Structures of Conjugated Systems Containing Cyclobutane", *Collection Czech. Chem. Commun.* **43**, 1375 (1978).
- X30. K. Horvatic and N. Trinajstic, "Matemacka Kemija. Primjena Teorije Skupova u Kemiji", *Kemija U Industriji* br. **3**, 127 (1978).
- X31. H. J. Monkhorst, J. D. Pack, and D. L. Freeman, "On the X-ray Scattering Factors of Metallic and Molecular Hydrogen Crystals", *Solid State Comm.* **29**, 735 (1979).
- X32. J. D. Pack, H. J. Monkhorst, and D. L. Freeman, "Lithium Crystal Properties from High-Quality Hartree-Fock Wave Functions", *Solid State Comm.* **29**, 723 (1979).
- X33. H. J. Monkhorst and J. D. Pack, "The High-Temperature Resistivity of Beryllium", *Solid State Comm.* **29**, 675 (1979).
- X34. H. J. Monkhorst, "Hartree-Fock Density-of-States for Extended Systems", *Phys. Rev. B* **20**, 1504 (1979).
- X35. H. J. Monkhorst and B. Jeziorski, "No Linear Dependence or Many-Center Integral Problems in Momentum Space Quantum Chemistry", *J. Chem. Phys.* **71**, 5268 (1979).
- X36. H. J. Monkhorst, "Exact LCAO Method for Two-Dimensional Crystals Using Fourier Transforms", 1979.

## OTHER PAPERS FROM THE FEH RESEARCH GROUP (Continued)

- X37. H. J. Monkhorst and W. A. Schwalm, "Electrostatics for Periodic Films of Atoms", Phys. Rev. B **23**, 1729 (1981).
- X38. V. G. Koures, "Gaussian Basis Expansion of the QED Light Cone Hamiltonian", Phys. Lett. B **348**, 170 (1995).
- X39. V. G. Koures, "Gaussian Basis Representation of the QED Light Cone Hamiltonian", Proceedings DPF, p. 1426 (World Scientific, 1995).
- X40. V. G. Koures, "Solving the Coulomb Schrödinger Equation in  $d=2+1$  via Sinc Collocation", J. Comput. Phys. **128**, 1 (1996).
- X41. V. G. Koures, "Second Quantization with Sinc Kets and Sinc Bras", Report UTAH-IDR-CP-04(1996).