

# **John R. Sabin**

## **Curriculum Vitae**

current to 21.07.06

### **Position**

- Professor of Physics, University of Florida
- Adjungeret Professor, University of Southern Denmark
- Affiliate Faculty, National High Magnetic Field Laboratory
- Director of Information Technology, College of Liberal Arts and Sciences, University of Florida
- Interim Director, University Writing Program, University of Florida
- U.S. Director, University of Florida - University of Southern Denmark Exchange Program
- U.S. Director, University of Florida - Universidad Autonoma Metropolitana Unidad Iztapalapa Exchange Program

### **Personal Data**

- Birth: April 29, 1940 in Springfield, Massachusetts
- Marital Status: married to Birgit Horn

### **Education**

- Loomis School, Windsor, Connecticut; was graduated in 1958
- A.B., 1962, Williams College
- Ph.D., 1966, University of New Hampshire

### **Professional Record**

- NSF Cooperative Graduate Fellow, University of New Hampshire, 1964-1966
- N.I.H. Postdoctoral Fellow, Quantum Chemistry Group, Upsala University, 1966-67
- Postdoctoral Fellow, Northwestern University, 1967-68
- Assistant Professor of Chemistry, University of Missouri-Columbia, 1968-71
- Visiting Associate Professor of Chemistry, University of Florida, 1970-71
- Associate Professor of Physics and Chemistry, University of Florida, 1971-77
- Professor of Physics and Chemistry, University of Florida, 1977-present
- Interim Chairman, Department of Physics, University of Florida, 2002
- NORDITA Professor, 1982-83, Denmark
- Fulbright Research Scholar, Denmark, 1986, 1991
- Adjungeret Professor, University of Southern Denmark/Odense University, 1992-present

### **Membership in Professional and Honorary Societies**

- American Physical Society - Fellow
- American Chemical Society

- Dansk Fysisk Selskab (Danish Physical Society)
- Danish Spectroscopy Society
- Sigma Pi Sigma
- Sigma Xi
- Böhmsche Physical Society

### **Membership on Editorial Boards**

- Editor, *Advances in Quantum Chemistry*, 1985-pres.
- Editorial Board, *Croatia Chimica Acta*, 2001-pres.
- Editor, *International Journal of Quantum Chemistry*, 2006- pres.
- Associate Editor, *International Journal of Quantum Chemistry*, 1979-2005
- Assistant Editor, *International Journal of Quantum Chemistry*, 1973-79.

### **Visiting Appointments**

- University of Guelph, Visiting Professor, April, 1976.
- Århus University, Senior Lecturer, January, 1978.
- Lehrstuhl für Theoretische Chemie, der Technischen Universität München, Guest Professor, October-November 1982.
- Visiting Scientist, Max-Planck-Institut für Astrophysik, München, June, November, 1983; June, 1984; June, 1985; October, 1986; August, 1988; August, 1989; July, 1990; November-December, 1991.
- NAS/NRC Exchange Visitor, BAN, Sofia, Bulgaria, September, 1984.
- Chinese Academy of Science Guest Lecturer, October, 1988.
- Visiting Professor, University of the Basque Country, January-May, 1992.
- Guest Professor, Odense University, 1980-1992
- Visiting Scientist, UAM, Mexico City, November, 1993; January, 1996.

### **Administrative Positions**

- Director of Information Technology, College of Liberal Arts and Sciences, University of Florida, 1998-pres.
- Interim Chair, Department of Physics, 2002
- Associate Director, Quantum Theory Project, 1977-1982, 1995-2001.

### **Conferences Organized**

- Sanibel Symposia - organization committee, 1970-pres.
- Organizing Committee, Werner Brandt Workshops on Penetration Phenomena, 1993-pres.
- Session Organizer and Chair, International Conference on the Application of Accelerators in Research and Industry, Denton Texas, 1998, 2000, 2002, 2004.
- 1st Arrodondo Workshop on Energy Deposition, Gainesville, FL, November 12-13, 1992.
- Co-Chairman, Workshop on Electronic Energy Loss of Ions in Matter - Gmunden, Austria, July 12-16, 1993.

- Co-Chairman, Summer University, Johannes Kepler University of Linz, Gmunden, Austria, 1993.
- Werner Brandt Workshops:
  - 15th Werner Brandt Workshop, Gainesville, FL, March 9-11, 1994
  - 18th Werner Brandt Workshop, Gainesville, FL, June 4-5, 1998
  - 20th Werner Brandt Workshop, Gainesville, FL, February 9-11, 2000
  - 25<sup>th</sup> Ritchie-Brandt Workshop, Gainesville, FL, April 24-27, 2004
- Properties of Molecules in Strong Magnetic Fields: A Workshop, Gainesville, FL, October 23-26, 1996 (in cooperation with the National High Magnetic Field Laboratory).
- "We Can Do That!," An international symposium in honor of Mike Zerner, Gainesville, November 16-18, 2000.
- Invitational Symposium on Novel Computational Approaches to Low-Energy Atom-Atom and Atom-Ion Scattering, Gainesville, FL, February 3, 2001 (together with Frank Harris).

### Listed in

- American Men and Women of Science
- Who's Who in the World
- Who's Who in America
- Who's Who in the South and Southwest
- Who's Who in Science and Engineering
- Who's Who in American Education
- Men of Achievement
- Best Europe

### Publications

1. J.R. Sabin, "Hydrogen Bonding in Simple  $\pi$ -Electron Systems. I. Pyridinium-Pyridine," *Int. J. Quantum Chem.* **2**, 23 (1968).
2. J.R. Sabin, "Hydrogen Bonding in Simple  $\pi$ -Electron Systems. II. Pyridine-Pyrrol," *Int. J. Quantum Chem.* **2**, 31 (1968).
3. J.R. Sabin, S.F. Fischer and G.L. Hofacker, "Proton-Phonon Coupling in a Hydrogen Bonded System," *Phys. kondens. Materie* **8**, 268 (1969).
4. J.R. Sabin, S.F. Fischer and G.L. Hofacker, "S.C.F. Calculation for Proton-Phonon Coupling in a Linear Model of Ice," *Int. J. Quantum Chem.* **3S**, 257 (1969).
5. J.R. Sabin, R.E. Harris, T.W. Archibald, P.A. Kollman and L.C. Allen, "Ab Initio MO-SCF Calculations on a Model of Anomalous Water," *Theoret. Chem. Acta* **18**, 235 (1970).
6. J.R. Sabin, "Theoretical Study of the Bis(pyridine)iodine(I) Cation," *J. Mol. Struct.* **7**, 407 (1971).
7. J.R. Sabin, "Hydrogen Bonds Involving Sulfur. I. The Hydrogen Sulfide Dimer," *J. Am. Chem. Soc.* **93**, 3613 (1971).

8. J.R. Sabin, "Hydrogen Bonds Involving Sulfur. II. The Hydrogen Sulfide-Hydrosulfide Complex," *J. Chem. Phys.* **54**, 4675 (1971).
9. M.A. Ratner and J.R. Sabin, "Symmetry Considerations Concerning d-Orbital Participation in Chemical Bonding of Second Row Elements," *J. Am. Chem. Soc.* **93**, 3542 (1971).
10. T. Achibald and J.R. Sabin, "Theoretical Investigation of the Electronic Structure and Properties of  $N_3$ ,  $N_3^-$ ,  $N_3^+$ ," *J. Chem. Phys.* **55**, 1821(1971)
11. J.R. Sabin, "Some Calculations of the Lighter Bis(pyridine)Halogen(I) Cations," *J. Mol. Struct.* **11**, 33 (1972).
12. J.R. Sabin "A Comment Concerning S-H-S Type Hydrogen Bonds," *Int. J. Quantum Chem.* **5S**, 133 (1971).
13. J.R. Sabin, "CNDO Study of the Properties of Ionic Defect Structure in a Model One-Dimensional Hydrogen-Bonded Chain," *J. Chem. Phys.* **56**, **45** (1972).
14. J.R. Sabin and H. Kim, "A Theoretical Study of the Structure and Properties of Carbon Trioxide," *Chem. Phys. Letters* **11**, 593 (1971).
15. J.R. Sabin and H. Kim, "Ab Initio Calculation of the Electronic Structure of Carbon Suboxide," *J. Chem. Phys.* **56**, 2195 (1972).
16. J.W.D. Connolly and J.R. Sabin, "Total Energy in the Multiple Scattering Formalism: Application to the Water Molecule," *J. Chem Phys.* **56**, 5529 (1972).
17. M.A. Ratner and J.R. Sabin, "Fröhlich Polaron Model for Trapping of Compton Electrons in Hydrogen-Bonded Glasses," *Chem. Phys. Letters* **14**, 92 (1972).
18. J.R. Sabin, D.P. Santry and K. Weiss, "CNDO Molecular Orbital Calculations. On the Invariance of Methods for Second Row Elements," *J. Am. Chem. Soc.* **94**, 6651 (1972).
19. J.R. Sabin, "A Model Study of the Interaction of a Hydrogen Bond with a  $\pi$ -Electron System," *Theoret. Chem. Acta* **27**, 69 (1972).
20. P. Lindner and J.R. Sabin, "Electron Distribution in a Short A-Type Hydrogen Bond," *Int. J. Quantum Chem.* **6S**, 301 (1972).
21. W.R. Oegerle and J.R. Sabin, "On the CNDO Determination of the Molecular Conformation and Properties of Glycine and Its Zwitterion," *J. Mol. Struct.* **15**, 131 (1973).
22. J.R. Sabin and M.A. Ratner, "The Wave Mechanical Treatment of HydrogenBonded Systems," from *Wave Mechanics--The First Fifty Years*, S.S. Chissick, W.C. Price and T. Ravensdale, eds., Butterworths, pp. 72-87, 1973.
23. J.R. Sabin, "On the Barrier to Internal Rotation in Phosphineborane," *Chem. Phys. Letters* **20**, 212 (1973).
24. H. Kim and J.R. Sabin, "An Ab Initio Calculation of the Molecular Structure and Properties of Hypofluorous Acid," *Chem. Phys. Letters* **20**, **215** (1973).
25. M. Vucelič, Y. Öhrn and J.R. Sabin, "Ab Initio Calculation of the Vibrational and Electronic Properties of Carbon Dioxide," *J. Chem. Phys.* **59**, 3003 (1973).
26. M.A. Ratner, J.R. Sabin and E.E. Ball, "SCF Calculation of the Effective Parameters for the Hubbard Model of TCNQ Charge-Transfer Salts," *Mol. Phys.* **26**, 1177 (1973).
27. P. Lindner, Y. Öhrn and J.R. Sabin, "A Semi-Empirical Investigation of the Electronic Structure and Stability of the Oxycumulenes," *Int. J. Quantum Chem.* **7S**, 261 (1973).

28. N.H.F. Beebe and J.R. Sabin, "An Ab Initio Study of the Electronic Structure of  $C_2O_2$ ," Chem. Phys. Letters **24**, 389 (1974).
29. N. Rosch, G.L. Hofacker and J.R. Sabin, "Ion-Solvent Cluster in the Vicinity of an Electrode: Semiempirical SCF Model Including Image Forces," J. Chem. Phys. **60**, 4009 (1974).
30. R.L. Tyner, W.M. Jones, Y. Öhrn and J.R. Sabin, "Semiempirical Calculations on Phenylcarbene, Cycloheptatrienylidene, and Cycloheptatetraene and Their Benzo-Annulated Derivatives," J. Am. Chem. Soc. **96**, 3765 (1974).
31. T.C. Jao, N.H.F. Beebe, W.B. Person and J.R. Sabin, "Molecular Polarizability Estimates for Vibrational Spectral Interpretation," Chem. Phys. Letters **26**, 474 (1974).
32. P. Lindner and J.R. Sabin, "Localized Orbitals in Hydrogen Bonded Systems," Chem. Phys. Letters **27**, 214 (1974).
33. M.A. Ratner, J.R. Sabin and E.E. Ball, "SCF Calculations of Some Electronic Properties of Tetrathiofulvalene and of Some Methyl-Substituted Tetrathiofulvalenes," Chem. Phys. Letters **28**, 393 (1974).
34. N.M. Witriol, J.D. Stettler, J.R. Sabin and S.B. Trickey, "CNDO Calculations of Intermolecular V-T and V-V Potentials. The  $CO_2-N_2$  Systems," Chem. Phys. Letters **27**, 540 (1974).
35. J. Cornelius and J.R. Sabin, "A CNDO Estimate of the Relative Affinities of Taurine and Isethionic Acid for Alkali Metal Ions," Int. J. Quantum Chem. **QBS1**, 43 (1974).
36. J.R. Sabin, J.P. Worth and S.B. Trickey, "Cohesive Energy and the P-V Relation for fcc Neon in Two Variants of the  $X\alpha$  Model," Phys. Rev. B **11**, 3658 (1975).
37. N.M. Witriol, J.D. Stettler, J.R. Sabin and S.B. Trickey, "Investigation of the Computation of V-T and V-V Potentials," IEEE J. Quantum Elect. **QE-11**, 717 (1975).
38. N.M. Witriol, J.D. Stettler, J.R. Sabin and S.B. Trickey, " $CO_2-N_2$  Intermolecular V-T and V-V Potentials via CNDO," J. Chem. Phys. **63**, 3263 (1975).
39. J.R. Sabin and S.B. Trickey, "Comparison of Atomic Compton Profiles Obtained from Four Model Local Density Functionals," J. Chem. Phys. B **8**, 2593 (1975).
40. G. Born and J.R. Sabin, "Ab Initio Calculation of Some Electronically Excited States of a Hydrogen-Bonded System: A Preliminary Report," Int. J. Quantum Chem. **QBS2**, 259 (1975).
41. J. Rychlewski and J.R. Sabin, "Hydrogen Bonding in Linear  $(LiH)_2$ ," Chem. Phys. Letters **37**, **180** (1976).
42. J.R. Sabin, "A Semi-Empirical Study of the Structural Effects of Ionic Defect Formation in a Model -Helical System," from Quantitative Structure-Activity Relationships, M. Tichy, ed., Hungarian Acad. Science, Budapest, p.199 (1976)
43. M.A. Ratner and J.R. Sabin, "On Proton Mobilities in Individual Hydrogen Bonds," from Quantum Science, Methods and Structure, J.-L. Calais, *et al.*, eds., Plenum Press, p. 577 (1976).
44. J.W. Mintmire and J.R. Sabin, "Intermolecular Potential Studies of Hydrogen Molecule Interactions with Rare-Gas Atoms," Int. J. Quantum Chem. **10S**, 213 (1976).

45. M.A. Ratner, J.R. Sabin and S.B. Trickey, "Applications of Model Hamiltonians to the Electron Dynamics of Organic Charge Transfer Salts," from *The Uncertainty Principle and the Foundations of Quantum Mechanics*, W.C. Price and S.S. Chissick, eds., p. 461, Wiley (1977).
46. N.M. Witriol, J.D. Stettler, M.A. Ratner, J.R. Sabin and S.B. Trickey, "A Systematic Treatment of Quantum Mechanical Reaction Coordinates," *J. Chem. Phys.* **66**, 1141 (1977).
47. S.F. Abdulnur and J.R. Sabin, "Double Minimum Bending Potentials for AB<sub>2</sub>-Type Molecules in the CNDO Approximation," *Fla. Sci.* **40**, 73 (1977).
48. M.A. Ratner and J.R. Sabin, "Some Symmetry Considerations Concerning the Role of Atomic d-Orbitals in Chemical Bonds: Discussion and Some Computational Examples," *J. Am. Chem. Soc.* **99**, 3954 (1977).
49. B.I. Dunlap, J.W.D. Connolly and J.R. Sabin, "On the Applicability of LCAO-X $\alpha$  Methods to Molecules Containing Transition Metal Atoms: The Nickel Atom and Nickel Hydride," *Int. J. Quantum Chem.* **11S**, 81 (1977)
50. M.A. Ratner, A.A. Frost, S. Topiol and J.R. Sabin, "Comparison of FSGO, Hartree-Fock-Roothaan and Pseudopotential Calculations for Li<sub>2</sub>," *J. Chem. Soc. Faraday II* **74**, 324 (1978).
51. V.H. Smith and J.R. Sabin, "The Compton Profile as a Criterion for the Choice of the Local Exchange Parameter," *J. Phys. B: Atom. Molec. Phys.* **11**, 385 (1978).
52. W.J. Janis, P. Kaijser, J.R. Sabin and V.H. Smith, Jr., "The Influence of Polarization Functions on the Directional Compton Profiles of Water," *Mol. Phys.* **37**, 463 (1979).
53. E.E. Ball, M.A. Ratner and J.R. Sabin, "The Role of d-Orbital Basis Functions in the Electronic Structure Description of Molecules: Systems Containing Si, P, and Cl," *Chemica Scripta* **12**, 128 (1977); [Erratum, *Chemica Scripta* **13**, 203 (1978)].
54. M.J. Ondrechen, M.A. Ratner and J.R. Sabin, "Electron Transfer in Fixed-Nuclei Systems: A Comparison of Propagator Descriptions," *J. Chem. Phys.* **71**, 2244 (1979).
55. R. Lozes and J.R. Sabin, "Excited Electronic States of a Hydrogen Bond: Bifluoride Ion," *Int. J. Quantum Chem.* **16**, 273 (1979)
56. B.I. Dunlap, J.W.D. Connolly and J.R. Sabin, "On Some Approximations In Applications of X $\alpha$  Theory," *J. Chem. Phys.* **71**, 3396 (1979).
57. B. Crist, M.A. Ratner, A.L. Brower and J.R. Sabin, "Ab Initio Calculations of the Deformation of Polyethylene," *J. Appl. Phys.* **50**, 6047 (1979).
58. B.I. Dunlap, J.W.D. Connolly and J.R. Sabin, "On First Row Diatomic Molecules and Local Density Models," *J. Chem. Phys.* **71**, 4993 (1979).
59. J.W. Mintmire and J.R. Sabin, "A Comparison of the LCAO-X $\alpha$  Method with the Hartree-Fock and Multiple Scattering-X $\alpha$  Methods on Carbon Monoxide," *Chem. Phys.* **50**, 91 (1980).
60. A.L. Brower, J.R. Sabin, B. Crist and M.A. Ratner, "Ab Initio Molecular Orbital Studies of Polyethylene Deformation," *Int. J. Quantum Chem.* **18**, 651 (1980).

61. P. Kaijser and J.R. Sabin, "A Comparison Between LCAO- $X\alpha$  and Hartree-Fock Wavefunctions for Momentum Space Properties of Ammonia," *J. Chem. Phys.* **74**, 559 (1981).
62. J.W. Mintmire and J.R. Sabin, "Local Density Functional Methods in Two Dimensionally Periodic Systems. I. The Atomic Hydrogen Monolayer," *Int. J. Quantum Chem.* **S14**, 702 (1980).
63. R.L. Lozes, J.R. Sabin and J. Oddershede, "On the Carbon Suboxide Bending Potential ( $\nu_7$ )," *J. Mol. Spectrosc.* **86**, 357 (1981).
64. C.Th. Pedersen, J. Oddershede and J.R. Sabin, "Semiempirical Studies on 1,2- and 1,3-Tetrathiofulvalenes," *Int. J. Quantum Chem.* **20**, 369 (1981).
65. C.Th. Pedersen, J. Oddershede and J.R. Sabin, "The Stability of the Carbenes from 1,2-Dithiole and 1,3-Dithiole in Relation to the Synthesis of 1,1, 3,3- and 1,1, 2,2-Tetrathiafulvalenes," *J.C.S. Perkin II*, 1062 (1981).
66. J.W. Mintmire, J.R. Sabin and S.B. Trickey, "Local-Density-Functional Methods in Two-Dimensionally Periodic Systems. Hydrogen and Beryllium Monolayers," *Phys. Rev. B* **26**, 1743 (1982).
67. J. Oddershede and J.R. Sabin, "X-ray Scattering Factors, Compton Profiles, and Shell Corrections from Numerical Atomic Wavefunctions," *Chem. Phys.* **71**, 161 (1982).
68. J.R. Sabin and J. Oddershede, "Shell Corrections to Electronic Stopping Powers from Orbital Mean Excitation Energies," *Phys. Rev. A* **26**, 3209 (1982).
69. R.L. Lozes and J.R. Sabin, "Localized Electronic Excitation in a Hydrogen Bond," *Int. J. Quantum Chem.* **QBS9**, 289 (1982).
70. J. Oddershede and J.R. Sabin, "The Use of Modified Virtual Orbitals in Perturbative Polarization Propagator Calculations," *J. Chem. Phys.* **79**, 2295 (1983).
71. V.H. Smith, Jr., J.R. Sabin, E. Broclawik and J. Mrozek, "The Electronic Structure of the Trisulfur Trinitride Anion," *Inorg. Chem. Acta* **77**, L101 (1983).
72. J. Oddershede, J.R. Sabin and P. Sigmund, "Predicted  $Z_2$  Structure and Gas-Solid Differences in Low-Velocity Stopping Power of Light Ions," *Phys. Rev. Lett.* **51**, 1332 (1983).
73. J.R. Sabin and J. Oddershede, "Electronic Stopping Powers for Low Projectile Velocities," *Phys. Rev. A* **29**, 1757 (1984).
74. B. Crist, J. Oddershede, J.R. Sabin, J.W. Perram and M.A. Ratner, "Polymer Fracture - A Model for Chain Scission," *J. Poly. Sci. Poly.Phys.* **22**, 881 (1984).
75. J.R. Eyler, J. Oddershede, J.R. Sabin, G.H.F. Diercksen and N.E. Gruner, "Excitation Energy of Linear  $C_3H_3^+$ . Can This Ion Be Detected by Laser-Induced Fluorescence in Flames?" *J. Phys. Chem.* **88**, 3121 (1984).
76. J.R. Sabin and S.B. Trickey, "On the Systematic Assessment of Correlation Effects in Local Density Models," in *Local Density Approximations in Quantum Chemistry and Solid State Physics*, J.P. Dahl and J. Avery, eds., p. 333, (Plenum, 1984).
77. J. Oddershede and J.R. Sabin, "Orbital and Whole Atom Stopping Power and Shell Corrections for Atoms with  $Z < 36$ ," *At. Dat. Nuc. Dat. Tables* **31**, 275 (1984).

78. H. Jorg, N. Rosch, J.R. Sabin and B.I Dunlap, "Basis Sets in the LCAO- $X\alpha$  Method. On the Use of Bond-Centered Basis Functions in Second-Row Homonuclear Diatomics." *Chem. Phys. Lett.* **114**, 529 (1985).
79. G.H.F. Diercksen, N.E. Gruner, J. Oddershede and J.R. Sabin, "The Structure of  $Si_2C$  and  $Si_3$ ," *Chem. Phys. Lett.* **117**, 29 (1985).
80. J.R. Sabin, J. Oddershede and P. Sigmund, "On the Proton Stopping Power Maximum in Gasses and Vapours," *Nuc. Inst. Meth.* **B12**, 80 (1985).
81. J. Oddershede, J.R. Sabin, G.H.F. Diercksen and N.E. Gruner, "The Structure and Spectrum of  $SiC_2$ ," *J. Chem. Phys.* **83**, 1702 (1985).
82. J.R. Sabin, J. Oddershede, G.H.G. Diercksen and N.E. Gruner, "The Calculated Electronic Excitation Spectra of  $Si_2C$  and  $Si_3$ ," *J. Chem. Phys.* **84**, 354 (1986).
83. J.R. Sabin and J. Oddershede, "Theoretical Low Energy Stopping Powers: Effects of Sample Phase," *Int. J. Quantum Chem.* **S19**, 733 (1985).
84. G.H.F. Diercksen, N.E. Gruner, J.R. Sabin, and J. Oddershede, "Structures and Spectra of Triatomic Silicon-Carbon Compounds," *Int. J. Quantum Chem.* **S19**, 735 (1985).
85. J. Geertsen, J. Oddershede, and J.R. Sabin, "Calculation of Molecular Mean Excitation Energies via the Polarization Propagator Formalism:  $H_2$  and  $H_2O$ ," *Phys. Rev. A* **34**, 1104 (1986).
86. J. Oddershede and J.R. Sabin, "Stopping Powers from Velocity Distributions Derived from Compton Profiles," *Phys. Rev. A* **35**, 3283 (1987).
87. J.R. Sabin and J. Oddershede, "Calculated Stopping Cross Sections for Diamond and Solid Silicon and Germanium," *Nucl. Inst. Meth.* **B24/25**, 339 (1987).
88. J.R. Sabin and J. Oddershede, "Theoretical Stopping Cross Sections for C-H, C-C and C=C Bonds," *Nuc. Inst. Meth.* **B27**, 280 (1987).
89. J. Oddershede, J.R. Sabin and G.H.F. Diercksen, "Stability and Conformation of Silicon-Carbon Compounds. A Case study of  $SiC_2$ ,  $Si_2C$ , and  $Si_3$ ," in *Understanding Molecular Properties*, Aa. Hansen, J. Avery and J. P. Dahl, eds., p.465 (Plenum, 1987).
90. A. Sadlej, G.H.F. Diercksen, J. Oddershede and J.R. Sabin, "How Reliable is the Theoretical structure of  $SiC_2$ ?," *Chem. Phys.* **122**, 297 (1988).
91. J. Oddershede, J.R. Sabin, G.H.F. Diercksen and N.E. Gruner, "Calculation of the Radiative Lifetime of BH in the Polarization Propagator Formalism," *Chem. Phys.* **115**, 15 (1987).
92. J. Oddershede and J.R. Sabin, "Calculation of Rotational g-Factors and Magnetic Susceptibilities of  $H_3^+$ ," *Chem. Phys.* **122**, 291 (1988).
93. J.R. Sabin and J. Oddershede, "Stopping Powers and Mean Excitation Energies of the Transition Metals from Iron to Zinc," *Phys. Rev. A* **39**, 1033 (1989).
94. J. R. Sabin and J. Oddershede, "Predicted Phase Differences in Proton Stopping by Alkali Metal Targets," *Nucl. Inst. and Meth.* **B36**, 249 (1989).
95. J. Oddershede and J.R. Sabin, "Bragg Rule Additivity of Bond Stopping Cross Sections," *Nucl. Inst. and Meth.* **B42**, 7 (1989).
96. S.B. Trickey, D.E. Meltzer and J.R. Sabin, "Calculation of Stopping Powers in Ordered Ultra-Thin Films," *Nucl. Inst. and Meth.* **B40/41**, 321 (1989).
97. J. Oddershede and J.R. Sabin, "The Effect of Correlation on the Mean Excitation Energy of Beryllium," *Phys. Rev. A* **39**, 5565 (1989).



98. J. Oddershede and J.R. Sabin, "On the Orbital Implementation of the Kinetic Theory of Stopping," *Int. J. Quantum Chem.* **QC23**, 557 (1989).
99. J.R. Sabin and J. Oddershede, "A Comment on the Abstraction of Mean Excitation Energies from Experimental Reduced Stopping Powers," *Nucl. Inst. and Meth.* **B44**, 253 (1990).
100. D.E. Meltzer, J.R. Sabin and S.B. Trickey, "Calculation of Mean Excitation Energies and Stopping Cross Sections in the Orbital Local Plasma Approximation," *Phys. Rev. A* **41**, 220 (1990). [Erratum, **42**, 666 (1990)].
101. J. Oddershede and J.R. Sabin, "Mean Excitation Energy and Moments of the Dipole Oscillator Strength Distribution of Closed Shell Aluminum Ions," *Nucl. Inst. and Meth.* **B48**, 34 (1990)
102. J.R. Sabin, J. Oddershede and G.H.F. Diercksen, "Moments of the Dipole Oscillator Strength Distribution and Mean Excitation Energies of Helium," *Phys. Rev. A* **42**, 1302 (1990).
103. J.Z. Wu, J.R. Sabin, S.B. Trickey and J.C. Boettger, "Mono- and Dilayer Analogues of Crystalline Atomic Hydrogen," *Int. J. Quantum Chem.* **S24**, 873 (1990).
104. J. Oddershede and J.R. Sabin, "Polarization Propagator Calculations of Spectroscopic Properties of Molecules," *Int. J. Quantum Chem.* **39**, 371 (1991).
105. P. Jensen, J. Oddershede and J.R. Sabin, "Geometric Dependence of the Mean Excitation Energy and Spectral Moments of Water," *Phys. Rev. A* **43**, 4040 (1991).
106. G.H.F. Diercksen, J. Oddershede, I. Páidarova and J.R. Sabin, "Calculation of the Isotropic and Anisotropic Spectral Moments of the Dipole Oscillator Strength Distribution of N<sub>2</sub>," *Int. J. Quantum Chem.* **39**, 755 (1991).
107. J. Geertsen, J. Oddershede and J.R. Sabin, "Quadrupole Polarizability and Spectral Moments of the Quadrupole Oscillator Strength Distribution of N<sub>2</sub>," *Mol. Phys.* **72**, 1267 (1991).
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2. "The Theoretical Aspects of Hydrogen Bonding," University of Missouri, December 1967.
3. "Some Thoughts on Linear Water," University of Missouri, November, 1968.
4. "Proton-Phonon Coupling in a Linear Model of Ice," Eyring Symposium, Sanibel Island, Florida, January, 1969.
5. "Sulphur Participation in Hydrogen Bonds," International Symposium for Atomic, Molecular and Solid State Theory and Quantum Biology, Sanibel Island, Florida, January, 1971.
6. "Electron Distribution in a Short A-Type Hydrogen Bond," International Symposium for Atomic, Molecular and Solid State Theory and Quantum Biology, Sanibel Island, Florida, January, 1972.
7. "A Semi-Empirical Calculation of Defect Structure in  $(\text{HF})_6$ ," International Symposium on Hydrogen Bonding, Ottawa, Canada, August, 1972.
8. "The Present Status of Computational Techniques for Molecular Structure," with S.B. Trickey, Physical Sciences Directorate Seminar, Huntsville, Alabama, September 20, 1972.
9. "Molecular Structure and Constants of Hypofluorous Acid," with Hyunyong Kim, 1972 Midwest Regional ACS Meeting, Columbia, Missouri, November 8-10, 1972.
10. "A Semi-Empirical Investigation of the Electronic Structure and Stability of the Oxycumulenes," with P. Linder and Y. Öhrn, International Symposium for Atomic, Molecular and Solid State Theory in honor of Edward Condon, Sanibel Island, Florida, January, 1973.
11. "Surface Physics, Quantum Mechanics and Wishful Thinking," Chemistry Department, University of Florida, April 24, 1973.
12. "Theoretical Investigation of Ionic Defect Formation and Propagation in a Model Hydrogen Bonded  $\alpha$ -Helix," Conference on Chemical Structure and Biological Activity, Prague, Czechoslovakia, June, 1973.
13. "A Semi-Empirical Study of the Oxycumulenes," SETCA Conference, Tallahassee, Florida, May 26, 1973.

14. "The State-of-the-Art of Molecular Calculations Using the  $MSX\alpha$  Formalism," SETCA Conference, Tallahassee, Florida, May 25, 1973.
15. "A CNDO Calculation of the Relative Affinities of Taurine and Isethionic Acid for Alkali Metal Ions," International Symposium, Sanibel Island, Florida, January, 1974.
16. "Dicarbon Dioxide: A Challenge to Experimentalists," SETCA Meeting, Tuscaloosa, June, 1974.
17. "APW- $X\alpha$  Calculation of the Compton Profile of Solid Neon," Fifth Canadian Symposium, Ottawa, June, 1974.
18. "Compton Profiles of Atoms and Solids from  $X\alpha$  Wavefunctions," Physics Department, University of Florida, October 24, 1974.
19. "Investigation of the Computation of V-T and V-V Intermolecular Potentials," 4th Conference on Chemical and Molecular Lasers, St. Louis, Missouri, October 21-23, 1974, See IEEE J. Quantum Elect. **QE-11**, 717 (1975).
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22. "Atomic Compton Profiles from Local Exchange Wavefunctions," SETCA Meeting, Tallahassee, June 14, 1975.
23. "Ab Initio Studies of Rare Gas Molecules," with J.W. Mintmire, Sanibel Symposia, January, 1976.
24. "Concerning the Role of Atomic d-Orbitals in Chemical Bonds," University of Guelph, April 15, 1976.
25. "Intermolecular Potentials for the Interaction of  $H_2$  with Rare Gas Atoms," with J.W. Mintmire, SETCA Meeting, Tuscaloosa, May 21, 1976.
26. "Vibronic Model and Effective Temperatures in Reactive Collisions," with M. Ratner and S.F. Fischer, SETCA Meeting, Tuscaloosa, May 21, 1976.
27. "Semiempirical Calculation of Vibrational Modes and Their Coupling in BCl," Physical Sciences Directorate, U.S. Army Missile Command, Redstone Arsenal, July 22, 1976.
28. "Properties of Some Non-Normal Hydrogen Bonded Systems," Kemisk Institut, Århus Universitet, August 20, 1976.
29. "Ab Initio Studies of Electronically Excited Hydrogen Bonds," Symposium on the Future of Quantum Chemistry, Dalseter, Norway, September 2, 1976.
30. "A Semiempirical Study of the Interaction of a Hydrogen Molecule with Model Nickel and Copper Surfaces," Sanibel Symposia, January, 1977.
31. "Spin Polarized LCAO- $X\alpha$ -SCF Studies of the Interaction of a Hydrogen Atom and Molecule with Small Clusters of Nickel Atoms," with B.I. Dunlap and J.W.D. Connolly, APS Meeting, San Diego, California, March 21, 1977 [Bull. A.P.S. **22**, 314 (1977)].
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96. "Calculation of Rotational g-Factors and Magnetic Susceptibilities for
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108. "Energy Deposition in Molecules: The Bragg Rule", The University of Alabama, Birmingham, December 9, 1988.
109. "Calculation of Orbital Mean Excitation Energies and Stopping Cross Sections in the Local Plasma Approximation," with D.E. Meltzer and S.B. Trickey, 1989 Sanibel Symposia, St. Augustine, Florida, April 1--8, 1989.
110. "On the Orbital Implementation of the Kinetic Theory of Stopping," with J. Oddershede, 1989 Sanibel Symposia, St. Augustine, Florida, April 1-8, 1989.
111. "The Radiative Lifetime of the  $A^1\Pi$  State of  $BH$ ," with J. Oddershede, Dansk Kemisk Forenings Forarsmde, Odense, June 13, 1989.
112. "The Calculation of Molecular Mean Excitation Energies of Atoms, Molecules and Ions in the Polarization Propagator Formalism," with J. Oddershede, ICACS-13, Arhus, August 7-11, 1989
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117. "On the Implementation of an Orbital Local Plasma Approximation for Calculation of Stopping Powers in Ultra-Thin Films," Danish Physical Society Spring Meeting, Nyborg, Denmark, 17-18 May, 1990.
118. "On the Calculation of Oscillator Strength Moments in Atoms, Molecules and Ions in the Polarization Propagator Formalism," with J. Oddershede, Dansk Kemisk Forenings Forarsmde, Odense, June 7, 1990.
119. "Moments of the Oscillator Strength Distribution of N<sub>2</sub>," 8<sup>th</sup> Seminar on Computational Methods in Quantum Chemistry, Gl. Avern, September 1-8, 1990.
120. "Energy Deposition by Fast Protons in Molecules", H.C. Ørsted Institute, Copenhagen, September 24, 1990.
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123. "Status of the Calculation of Energy Loss of Swift Ions in Compounds," 10<sup>th</sup> Ion Beam Analysis Conference, Eindhoven, The Netherlands, July 1-5, 1991.
124. "Calculation of Stopping Cross Sections from Generalized Oscillator Strengths," STOP91, Middlefart, Denmark, August 6-9, 1991.
125. "Energy Deposition by Swift Ions in Matter: Bethe/Born Stopping without Bethe," Uppsala University, Sweden, October 8, 1991.
126. "Calculation of Generalized Oscillator Strengths and Stopping Cross Sections in the Polarization Propagator Approximation," Odense University, Denmark, October 30, 1991.
127. "Direct Calculation of Generalized Oscillator Strengths: Stopping Powers in the First Born Approximation," Aarhus University, Denmark, November 7, 1991.
128. "Stopping Powers for Atoms and Molecules from Generalized Oscillator Strength Distributions," Autonomous University of Madrid/Instituto Nicolas Cabrera, February 14, 1992.
129. "Stopping of Swift Ions in Ultra-Thin Films," University of Basque Country, May 7, 1992; at the award of the Doctor H.C. to Rufus Ritchie.
130. "Direct Calculation of the Stopping Power of Atoms and Molecules from the Generalized Oscillator Strength Distribution," University of Osnabruck, Germany, May 19, 1992.
131. "The Stopping Properties of Ultra-Thin Films," Odense University, June 1, 1992.

132. "Directional Dependence of Moments of the Dipole Oscillator Strength Distribution in Molecules," Dansk Kemisk Forenings Årsmøde, Odense, Denmark, June 19, 1992.
133. "Trajectory Dependant Ranges of Slow Ions under Channeling Conditions," Workshop on Problems in Low Energy Ion Implantation, Denton, Texas, November 1, 1992.
134. "Proton Stopping in Ultra-thin Lithium Films," 12<sup>th</sup> International Conference on the Application of Accelerators in Research & Industry, Denton, Texas, November 2-5, 1992.
135. "Trajectories of Low Energy Ions in the (1,1,0) Channel of Ge," Arredondo Workshop on Energy Deposition, Gainesville, Florida, November 12, 1992.
136. "Low Energy Channeling in Simple Crystals: a Simulation," Dansk Fysisk Selskabs Årsmøde, Rødby Havn, Denmark, May 16--28, 1993.
137. "Simulation of Channeling of Low Energy Ions in Simple Crystals," Spring Meeting of the Danish Chemical Society, Odense, Denmark, June 8, 1993.
138. "Simulation of Low Energy Channeling in Simple Systems," 11<sup>th</sup> Ion Beam Analysis Conference, Balatonfured, Hungary, July 5--9, 1993.
139. "Elementary Stopping Theory," Tutorial Lecture Series at the Summer University 1993 of Linz University, Gmunden, Austria, July 12--13, 1993.
140. "Stopping in Molecular Targets: The Fragment (Cores and Bonds) Approach," Workshop on Electronic Energy Loss of Ions in Matter, Gmunden, Austria, July 13-17, 1993.
141. "An Estimate of the Effect of Temperature on Molecular Stopping," Workshop on Electronic Energy Loss of Ions in Matter, Gmunden, Austria, July 13-17, 1993.
142. "Calculation of Stopping Powers of Atoms and Molecules from the Generalized Oscillator Strength Distribution," Department of Physics, Chalmers University, Göteborg, Sweden, August 16, 1993.
143. "Deposition of Energy by Swift Ions in Molecular Targets," Department of Chemistry, Odense University, Denmark, September 9, 1993.
144. "Stopping in Molecular Targets," Department of Physics, UNAM, Mexico City, November 9, 1993.
145. "Deposition of Energy by Swift Ions in Molecular Targets," Department of Chemistry, UAM, Mexico City, November 11, 1993.
146. "Stopping Powers from the Generalized Oscillator Strength Distribution," Physics Department, UAM, Mexico City, November 11, 1993.
147. "Calculation of Stopping Powers from the Generalized Oscillator Strength Distribution," US - Latin American Workshop in Molecular and Materials Sciences, Gainesville, 7-10 Feb., 1994.
148. "Simulation of the Stopping of Low Energy Protons in the  $\langle 1,0,0 \rangle$  and  $\langle 1,1,0 \rangle$  Channels of Si," 15<sup>th</sup> Werner Brandt Workshop on Charged Particle Penetration Phenomena, Gainesville, 10-11 March, 1994.
149. "Simulation of the Stopping of Channeled Low Energy Protons in Si," Spring Meeting of the Danish Physical Society, Odense, 2-3 June, 1994.

150. "On the Relative Importance of Temperature and Isotope Effects on the Dipole Oscillator Strength Distribution of H<sub>2</sub>" Annual Meeting of the Danish Chemical Society, Odense, 14 June, 1994.
151. "Simulation of the Stopping of Low Energy Protons in the <1,0,0> and <1,1,0> Channels of Si," Department of Physics, Chalmers University, Goteborg, Sweden, August 5, 1994.
152. "Calculation of the Dynamic Charge State of Swift Ions in Gaseous Targets: Some Preliminary Results," European Research Conference on Particle-Solid Interactions, Donostia, Spain, 1-6 October, 1994.
153. "Stopping Power in Finite Systems," European Research Conference on Particle-Solid Interactions, Donostia, Spain, 1-6 October, 1994 (with Peter Apell).
154. "A Bethe Theory for Directionally Dependent Stopping," Symposium on The Interaction of Swift Particles and Electromagnetic Fields with Matter, Oak Ridge, 23--25 October, 1994.
155. "A Simulation of Low Energy Channeling of Protons in Si," 13<sup>th</sup> International Conference on the Application of Accelerators in Research & Industry, Denton, Texas, 7-10 November, 1994.
156. "Approach to Bulk Behavior from Ultrathin Layered Systems: Energy Deposition," 35<sup>th</sup> Sanibel Symposium, Saint Augustine, Florida, 25 February - 4 March, 1995.
157. "Calculation of Non-linear Magneto-Optical Properties of Molecules at High Field Strength," 1000T Workshop, NHMFL, Tallahassee, Florida, 11-12 May, 1995.
158. "Orientational Dependence of Energy Deposition by Swift Ions in Molecular Targets," DAMOP, Toronto, 16-19 May, 1995 [Bull. APS **40**, 1301 (1995)].
159. "A Bethe Theory for Directionally Dependent Stopping," Spring Meeting of the Danish Physical Society, Odense, 1-2 June, 1995.
160. "Orientational Dependence of Energy Deposition by Swift Ions in Molecular Targets," Annual Meeting of the Danish Chemical Society, Odense, 13 June, 1995.
161. "Impact Parameter Dependence of Energy Loss and Charge Transfer," 16<sup>th</sup> Werner Brandt Workshop on Charged Particle Penetration Phenomena, Oak Ridge, 8-9 January, 1996.
162. "Properties of Molecules in High Magnetic Field: The Beginning," 36<sup>th</sup> Sanibel Symposium, Saint Augustine, Florida, 24 February - 2 March, 1996 (with Keith Runge).
163. "Energy Deposition of Swift Alpha Particles in Ne: An Electron Nuclear Dynamics Study," Recent Advances in Computational Quantum Chemistry ,Munich, 29-30 March, 1996.
164. "Calculation of Energy Deposition Cross Sections for He<sup>2+</sup> → Ne Using Electron Nuclear Dynamics," From Small to Large III, Computer Modeling of Microscopic Structures, Properties, and Reactions, Linkoping University, May 29-30, 1996.
165. "Conjugated Conducting Polymers," IFM, Linkoping University, May 31, 1996.
166. "Properties of Molecules in High Magnetic Fields," Annual Meeting of the Danish Chemical Society, Odense, 11 June, 1996.

167. "Generalized Oscillator Strengths (GOS's) for Calculation of Molecular Stopping Properties: CO," Swedish-American Symposium on the Foundations of Quantum Theory on Chemistry, Molecular Physics, and Biology, Sanibel Island, FL, 26-29 October, 1996.
168. "Generalized Oscillator Strengths for Calculation of Molecular Stopping Properties, Some Preliminary Results: CO," 14<sup>th</sup> International Conference on the Application of Accelerators in Research & Industry, Denton, Texas, 5-8 November, 1996.
169. "Study of Energy Deposition Characteristics of Swift Ions in Materials Using Electron-Nuclear Dynamics," Department of Physics, Universidad Autonoma Metropolitana -- Iztapalapa, Mexico City, 31 January, 1997.
170. "Electronic Properties in High Magnetic Fields," 1997 Latin American Workshop, Gainesville, FL, 27--28 February, 1997.
171. "Molecular Shape as a Determiner of Electronic Stopping Anisotropy," 37<sup>th</sup> Sanibel Symposium, Saint Augustine, FL, 1--7 March, 1997.
172. "Calculation of the Electronic and Geometric Properties of Some Small Molecules in High Magnetic Fields," 172--Heraeus Seminar on Atoms and Molecules in Strong External Fields, Bad Honnef, Germany, 7-11 April, 1997.
173. "Study of Energy Deposition Characteristics of Swift Ions in Materials Using Electron Nuclear Dynamics," Heidelberg University, 14 April, 1997.
174. "Calculation of Energy Deposition Cross Sections Using Electron Nuclear Dynamics," Florida ACS Sections Annual Meeting, Orlando, FL, 2-3 May, 1997.
175. "Molecular Stopping Anisotropy from Molecular Shape," 17<sup>th</sup> Werner Brandt Workshop, Charlottesville, VA, 8-9 May, 1997.
176. "Molecular Properties in High Applied Magnetic Fields ( $> 1000T$ )," Kemisk Forenings Årsmøde, Odense, 12 June, 1997.
177. "Geometrical Aspects of Swift Ion Energy Deposition," Department of Physics, Universidad Autonoma Metropolitana -- Iztapalapa, Mexico City, 30 April, 1998.
178. "Target Geometry and Swift Ion Energy Deposition," Department of Theoretical Chemistry, Århus University, 5 August, 1998.
179. "Geometrical Aspects of the Stopping Properties of Fullerenes for Swift Ions," 15<sup>th</sup> International Conference on the Application of Accelerators in Research & Industry, Denton, Texas, 2-6 November, 1998.
180. "Energy Deposition by Swift Ions in Materials," Physics, Astronomy and Chemistry Colloquium, Colgate University, 9 February, 1999.
181. "Stopping Powers of Swift Ions Calculated from Generalized Oscillator Strength Distributions," USLACC Workshop on Molecular and Material Sciences, Cuernavaca, Mexico, 24-26 February, 1999.
182. "Molecular Generalized Oscillator Strengths and Stopping Properties," 19<sup>th</sup> Werner Brandt Workshop, Bariloche, Argentina, 13--16 April, 1999.
183. "Direct Differential Cross Section Calculations for Ion-Atom and Atom-Atom Collisions in the keV Range," ICACS-18, Odense, Denmark, 3-8 August, 1999.
184. "Stopping in Molecular Chains," ICACS-18, Odense, Denmark, 3--8 August, 1999.

185. "Impact Parameter Dependence of Electronic and Nuclear Energy Loss of Swift Ions:  $H^+ \rightarrow He$  and  $H^+ \rightarrow H$ ," 20<sup>th</sup> Werner Brandt Workshop, Gainesville, 10-11 February, 2000.
186. "Calculation of Energy Loss and Charge Exchange Cross Sections for Ion/Atom and Ion/Molecule Collisions in the Kilovolt Energy Range," International Conference on Electronic Structure: Prediction and Applications, Donostia, Spain, October 4-6, 2000.
187. "Shape Dependent Molecular Properties," International Conference on Electronic Structure: Prediction and Applications, Donostia, Spain, October 4-6, 2000.
188. "POL, UF, & QTP," Löwdin Memorial Symposium, Uppsala, Sweden, 25 October, 2000.
189. "Calculation of Energy Loss Cross Sections:  $H^+ \rightarrow He$ ," Lowdin Memorial Symposium, Uppsala, Sweden, 25 October, 2000.
190. "Shape Dependent Molecular Properties: Energy Deposition," 16<sup>th</sup> International Conference on the Application of Accelerators in Research & Industry, Denton, Texas, 1-4 November, 2000.
191. "Collision Cross Sections Calculated with END," Invitational Symposium on Novel Computational Approaches to Low-Energy Atom-Atom and Atom-Ion Scattering, Gainesville, 3 February, 2001.
192. "Collision Cross Sections for Energy Deposition Studies," Pan-American Workshop on Molecular and Materials Science, Gainesville, 21-23 February, 2001.
193. "Shape Dependent Molecular Properties: Energy Deposition," Danish Chemical Society Annual Meeting, Odense, Denmark, 14 June, 2001.
194. "Collision Cross Sections for Energy Deposition Studies," INTERACTIONS, Odense, Denmark, 6 July 2001.
195. "Energy Deposition Studies  $N_4^+ \rightarrow H$ ," STOP01, Odense, Denmark, 6-8 August, 2001.
196. "Why is  $S_{max}$  for  $H^+$  around  $E_p = 100keV$  Most of the Time?" STOP01, Odense, Denmark, 6-8 August, 2001.
197. "Calculation of Molecular Collision Cross Sections for Energy Deposition Studies," 21<sup>st</sup> Werner Brandt Workshop, Donostia, Spain, 17-19 September 2001.
198. "Shape Dependent Energy Deposition," 21<sup>st</sup> Werner Brandt Workshop, Donostia, Spain, 17-19 September 2001.
199. "Calculation of Molecular Collision Cross Sections for Energy Deposition Studies," Quantum Theory Project Seminar, UF, 10 October, 2001.
200. "Breaking Bucky Balls," Danish Chemical Society Annual Meeting, Odense, Denmark, 12 June, 2002.
201. "Calculation of Stopping Properties of Molecules below the Bragg Peak," 22<sup>nd</sup> Werner Brandt Workshop, Namur, Belgium, 27-29 June, 2002.
202. "Calculation of Molecular Stopping Cross Sections," International Conference on the Application of Accelerators in Research & Industry, Denton, Texas, 12-16 November, 2002.

203. "Low Energy Stopping Properties of Molecules," 2003 Pan-American Workshop on Molecular and Materials Sciences, Cuernavaca, Mexico, 12-17 February, 2003.
204. "Swift Ion - Molecule Collisions: Energy Transfer," 23<sup>rd</sup> Werner Brandt Workshop, Playa del Carmen, Mexico, 3-6 June, 2003.
205. "Ion-Molecule Collisions: Cross Sections and Fragmentation Products," Seminar on Laboratory Astrophysics, Technical University of Dresden, 11 July, 2003.
206. "*Ab initio* Calculations of Molecular Fragmentation," ISAC XVIII, Stockholm/Helsinki, 30 July - 1 August, 2003.
207. "Breaking Bucky Balls," ISAC XVIII, Stockholm/Helsinki, 30 July - 1 August, 2003. (P)
208. "Ion Induced Molecular Fragmentation," 5<sup>th</sup> Donostia Encounter on Particle/Solid Interactions, Donostia, Spain, 8-13 September, 2003.
209. "Fragmentation of Fullerenes," 5<sup>th</sup> Donostia Encounter on Particle/Solid Interactions, Donostia, Spain, 8-13 September, 2003. (P)
210. "Study of Swift Ion-Molecule Collisions using Electron Nuclear Dynamics," Congreso Latinoamericano de Ciencias de Superficies y sus Aplicaciones XI, Puñón, Chile, 7-12 December, 2003.
211. "A Comparison of Shell Corrections in the Bohr and Bethe Formulations of Stopping Power," 24<sup>th</sup> Werner Brandt Workshop, Berlin, 12-14 July, 2004.
212. "Energy Deposition by Swift Ions in Molecular Targets: A Theoretical Approach," 18<sup>th</sup> International Conference on the Application of Accelerators in Research & Industry, Ft. Worth, Texas, 11-15 November, 2004.
213. "Ion-Biomolecule Collisions: Fragmentation Products and Cross-Sections," RADAM05 (Radiation Damage in Biomolecular Systems), Potsdam, Germany, 17 – 20 March, 2005.
214. "Quantum Treatment of Swift Ion – Molecule Collisions," Conference on Atomic Collisions and Spectroscopy, Berlin, Germany, 21 March, 2005.
215. "Negative Stopping Powers: A challenge to experimenters," 25<sup>th</sup> Brandt-Ritchie Workshop, Gainesville, Florida, 10 – 13 April, 2005.
217. "Ion-Biomolecule Collisions: Fragmentation Products and Cross Sections," SESAPS, Gainesville, Florida, 10 – 13 November, 2005.
218. "Grid computing at UF and QTP," Gridchem Workshop: Computational Chemistry on the Grid, Austin, Texas, 8 – 10 March, 2006.
220. "Directional Dependence of the Mean Excitation Energy of Glycine and its Zwitterion," Danish Physical Society Annual Meeting, Nyborg, Denmark, 1 – 2 June, 2006.
221. "Directional Dependence of the Mean Excitation Energy of Glycine and its Zwitterion," Danish Chemical Society Annual Meeting, Odense, Denmark, 8 June, 2006.
222. "Directional Dependence of the Mean Excitation Energy of Glycine and its Zwitterion," Radiation Damage in Biomolecular Systems, European Science Foundation COST Action P9, Groningen, The Netherlands, 6 - 9 June, 2006.
223. "Theoretical Investigation of Fragmentation and Energy Deposition Cross Sections for Swift Ion Impact on Prebiotic Molecules," Biomolecules –European

- Science Foundation Research Conference, Obergurgl, Austria, 24 – 29 June, 2006.
224. "Fragmentation and Energy Deposition Cross Sections for  $^3\text{He}^{2+}$  Impact on Formaldehyde," 26<sup>th</sup> Brandt-Ritchie Workshop, Paris, France, 16 – 19 July, 2006.

### **Schools, Workshops, and Conferences – No Presentation**

- Thirteenth Jerusalem Symposium, Jerusalem, Israel, April 28-May 2, 1980 (session chairman).
- Gordon Research Conference in Theoretical Chemistry, Tilton, New Hampshire, June, 1980.
- NATO Advanced Study Institute on Superionic Conductors, Odense, Denmark, August, 1980.
- NATO Advanced Study Institute on Methods in Computational Molecular Physics, Bad Windsheim, Germany, August, 1982.
- All Socialist Countries Conference in Theoretical Chemistry, Burgas, Bulgaria, September, 1984.
- Nils Bohr Centenary Symposium, Copenhagen, October 4-7, 1985.
- 7th Seminar on Computational Methods in Quantum Chemistry, University of York, September 1-4, 1987.
- DeepStar Workshop, Houston, December 5-6, 1995.
- Photochemical Energy Production, University of Southern Denmark, June 20-21, 2001.
- 1<sup>st</sup> Nanoworkshop at SDU, University of Southern Denmark, August 15, 2005.