CURRICULUM VITAE

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Education:

B.S., Chemistry, Georgia Institute of Technology, 1972
Ph.D., Chemistry, University of Florida, 1977

Positions Held:

Professor, Department of Chemistry, University of Memphis, 9/93-present

Special Assistant to the Provost for Academic and Organizational Planning, 7/13-8/14

Dean, College of Arts & Sciences, University of Memphis, 7/02-7/13

Interim Dean, College of Arts & Sciences, University of Memphis, 5/00-6/02

Director, Computational Research on Materials Institute, University of Memphis, 6/98-6/02

Interim Chairman, Department of Microbiology & Molecular Cell Sciences, University of Memphis, 5/98-9/99

RDL/AFOSR Summer Research Fellow, Space Electronics Division, Phillips Laboratory, Kirtland AFB, 6/97-9/97

Chairman, Department of Chemistry, University of Memphis, 8/92-6/97

Interim Chair, Department of Chemistry, Memphis State University, 8/91-7/92

Associate Professor, Department of Chemistry, Memphis State University, 7/88-8/93

Assistant Professor, Department of Chemistry, Memphis State University, 8/83-8/88

USAF-UES Summer Research Fellow, F. J. Seiler Laboratory, USAF Academy, 5/87-7/87

Visiting Professor, Quantum Chemistry Group, Uppsala University, Sweden, 6/83-8/83

Instructor, Department of Chemistry, Duke University, 7/81-5/83

NORDITA Invited Professor, Research Institute of Physics, Stockholm & Quantum Chemistry Group, Uppsala University, Uppsala, Sweden, 6/82-8/82, 9/80-8/81

Research Assistant Professor, Department of Chemistry, University of Pittsburgh, 6/79-8/80

Postdoctoral Assistant, Department of Chemistry, University of Pittsburgh, 9/78-6/79

Lecturer in Chemistry, Department of Chemistry, Chatham College, Pittsburgh, 9/78-6/79

Postdoctoral Fellow, Yale University, 1/78-8/78

Society/Organization Memberships

American Chemical Society (ACS)
Sigma Xi
Phi Kappa Phi

Honors/Awards

College of Arts & Sciences Meritorious Faculty Award, University of Memphis, Fall 1998
Professional Development Assignment, University of Memphis, Fall 1997
Outstanding Environmental Health and Safety Award, University of Memphis, 1996
Superior Performance in University Research, Memphis State University, 1992
Superior Performance in University Research, Memphis State University, 1991

Courses Taught	**Institution**
Advanced Physical Chemistry (U/G)	University of Memphis
Solid State Theory (G)	University of Memphis
Electronic Structure and Symmetry (G)	University of Memphis
Principles of Chemistry I & II (U)	University of Memphis
Physical Chemistry I & II (U)	University of Memphis
Physical Chemistry Laboratory (U)	University of Memphis
Advanced Quantum Chemistry (G)	University of Memphis
Undergraduate Research (U)	University of Memphis
General Chemistry I & II (U)	Duke University
Physical Chemistry Laboratory (U)	Duke University
Physical Chemistry (U)	Chatham College

Full Publication List

1. "Calculation of the Amplitudes to the Electron Propagator from a Minimal Basis CI Calculation on N_2.", H. A. Kurtz, G. D. Purvis, and Y. Öhrn, *Intern. J. Quantum Chem. Symp.* **10**, 331-336 (1976).

2. "Elementary Finite Order Perturbation Theory for Vertical Ionization Energies.", G. Born, H. A. Kurtz, and Y. Öhrn, *J. Chem. Phys.* **68**, 74-85 (1978).

3. "On the Calculation of Electron Binding Energies." H. A. Kurtz and Y. Öhrn, *J. Chem. Phys.* **69**, 1162-1167 (1978).

4. "*Ab Initio* Study of the Positron Affinity of LiH", H. A. Kurtz and K. D. Jordan, *J. Phys. B: Atom. Molec. Phys.* **11**, L479-L482 (1978).

5. "Theoretical Study of $[F^-;e^+]$ and $[CN^-;e^+]$", H. A. Kurtz and K. D. Jordan, *Intern. J. Quantum Chem.* **14**, 747-755 (1978).

6. "Calculations of ^2P Shape Resonances in Be and Mg." H. A. Kurtz and Y. Öhrn, *Phys. Rev. A* **19**, 43-48 (1979).

7. "A Comparison of the Positron Energy Levels of $[F^-;e^+]$ and $[CN^-;e^+]$ with the Rydberg Levels of Na and NO.", H. A. Kurtz and K. D. Jordan, *J. Phys. B: Atom. Molec. Phys.* **12**, L473-L477 (1979).

8. "Theoretical Studies of Positron Complexes with Atomic Anions.", H. A. Kurtz and K. D. Jordan, *J. Chem. Phys.* **72**, 493-503 (1980).

9. "Comment on the Electronic Structure of HAlOH and H_2O-Al.", H. A. Kurtz and K. D. Jordan, J. *Amer. Chem. Soc.* **102**, 1177-1178 (1980).

10. "Theoretical Studies of Positron-Molecule Complexes.", H. A. Kurtz and K. D. Jordan, *J. Chem. Phys.* **75**, 1876-1887 (1981).

11. "Properties of the $X^1\Sigma$ State of BF.", H. A. Kurtz and K. D. Jordan, *Chem. Phys. Lett.* **81**, 104-109 (1981).

12. "Theoretical Study of Electron and Positron Scattering on Be, Mg, and Ca.", H. A. Kurtz and K. D. Jordan, *J. Phys. B: Atom. Molec. Phys.* **14**, 4361-4376 (1981).

13. "On Energy Optimization of the AGP Wavefunction: The Ground State of the Be Atom.", H. A. Kurtz, N. Elander, O. Goscinski, and E. Sangfelt, *Intern. J. Quantum Chem. Symp.* **15**, 143-149 (1981).

14. "An Analysis of the AGP and Projected AGP Wavefunctions." E. Sangfelt, O. Goscinski, N. Elander, and H. A. Kurtz, *Intern. J. Quantum Chem. Symp.* **15**, 133-141 (1981).

15. "Theory of Metal Atom-Water Interactions and Alkali Halide Dimers.", K. D. Jordan and H. A. Kurtz, ACS Symposium Series 179: *Metal Bonding and Interactions in High Temperature Systems*, 377-393 (1982).

16. "On the Calculation of Generalized Antisymmetrized Geminal Power (GAGP) Wavefunctions.", H. A. Kurtz and N. Elander, *Intern. J. Quantum Chem. Symp.* **16**, 605-614 (1982).

17. "Application of the AGP Wavefunction to the Ground States of Li_2 and CH^+.", N. Elander, E. Sangfelt, H. A. Kurtz, and O. Goscinski, *Intern. J. Quantum Chem.* **23**, 1047-1056 (1983).

18. "Treatment of Resonances with the Dilated Electron Propagator: The ^2P Shape Resonance in e-Mg Scattering.", M. Mishra, H. A. Kurtz, O. Goscinski, and Y. Öhrn, *J. Chem. Phys.* **79**, 1896-1902 (1983).

19. "The Polarization Propagator Based on an AGP State: Theory and Application to the Helium Atom.", H. A. Kurtz, B. Weiner, and H. J. Aa. Jensen, *Intern. J. Quantum Chem. Symp.* **17**, 415-423 (1983).

20. "LUMO Energies and Negative Electron Affinities.", H. A. Kurtz, *J. Chem. Ed.* **61**, 580-581 (1984).

21. "Excited States via the AGP Polarization Propagator I. Application to Li_2.", E. Sangfelt, H. A. Kurtz, N. Elander, and O. Goscinski, *J. Chem. Phys.* **81**, 3976-3986 (1984).

22. "The Antisymmetrized Geminal Power (AGP) Approximation to the Excitation Propagator.", B. Weiner and H. A. Kurtz, *Int. J. Quantum Chem.* **27**, 769-780 (1985).

23. "Theory and Calculations on Small Molecules Using Propagator Methods with an AGP Reference.", H. A. Kurtz, B. Weiner, and Y. Öhrn, in *Comparison of Ab Initio Calculations with Experiment: State of the Art* ed. R. J. Bartlett, Reidel, Dordrecht, Netherlands 1985.

24. "The Bridgehead Decalin Radicals. An MM2 and MNDO Study.", H. A. Kurtz, R. V. Lloyd, and R. V. Williams, *J. Org. Chem.* **52**, 302-304 (1987).

25. "Excited State Properties Utilizing Effective Core Potentials.", P. A. Kilzer and H. A. Kurtz, *Int. J. Quantum Chem. Symp.* **21**, 539-545 (1987).

26. "Experimental Evidence Establishing an Upper Limit to the Activation Barrier for the Butterfly Bending of the Double Bond in Anti-sesquinorbornene.", R. V. Williams, C-L. Sung, H. A. Kurtz, and T. M. Harris, *Tetrahedron Lett.* **29**, 19-20 (1988).

27. "The Quest for a Neutral Homoaromatic Hydrocarbon. The MNDO Study of Pentacyclo[$7.2.1.0^{4,11}.0^{6,9}.0^{6,10}$]dodeca-1,4-diene, an Annelated Semibullvalene Derivative.", R. V. Williams and H. A. Kurtz, *J. Org. Chem.* **53**, 3626-3628 (1988).

28. "The Use of Semiempirical Energy Partitioning Terms in the Study of Through Space (Homoaromatic) Interactions.", R. V. Williams, H. A. Kurtz, and B. Farley, *Tetrahedron* **44**, 7455-7460 (1988).

29. "An NMR and Computational Study of Diazepinediones.", P. K. Bridson, H. A. Kurtz, and F. Sayyarpour, *J. Mol. Struct. (THEOCHEM)* **199**, 175-181 (1989).

30. "Semiempirical Methods for the Calculation of Polarizabilities and Hyperpolarizabilities.", H. A. Kurtz, J. J. P. Stewart, and K. M. Dieter, *J. Comp. Chem.* **11**, 82-87 (1990).

31. "Semiempirical Calculation of the Hyperpolarizabilities of Polyenes.", H. A. Kurtz, *Intern. J. Quantum Chem. Sym.* **24**, 791-798 (1990).

32. "An MCSCF Study of the Electric Properties of the Be Atom.", T. Pluta and H. A. Kurtz, *Chem. Phys. Lett.* **189**, 255-258 (1992).

33. "Intermolecular Effects on Third-Order Nonlinear Optical Properties", D. S. Dudis, A. T. Yeates, and H. A. Kurtz, *Mat. Res. Soc. Symp. Proc*. **247**, 93-97 (1992).

34. "Calculation of Vibrational Dynamic Hyperpolarizabilities for H_2O, CO_2, and NH_3.", D. M. Bishop, B. Kirtman, H. A. Kurtz, and J. E. Rice, *J. Chem. Phys.* **98**, 8024-8030 (1993).

35. "A Theoretical Investigation of Through Space Interactions 3. The Semi-Empirical Study of the Cope Rearrangement in Singly Annelated Semibullvalenes.", R. V. Williams and H. A. Kurtz, *J. Chem. Soc. Perkins 2*, 147-150 (1994).

36. "Homoaromaticity", R. V. Williams and H. A. Kurtz, *Advances in Physical Organic Chemistry Vol. 29*, ed. D. Bethel, Academic Press, 1994, pp 273-331.

37. "Frequency Dependent Hyperpolarizabilities of Polyenes", P. Korambath and H. A. Kurtz, in *Theoretical and Computational Modeling of NLO and Electronic Materials*, ed. S. Karna and A. T. Yates, ACS Books, 1996.

38. "NLO Properties of Interacting Polyene Chains", S. Chen and H. A. Kurtz, *J. Molec. Struct. THEOCHEM*, **388**, 79-84, 1996.

39. "Annelated Semibullvalenes: A Theoretical Study of How They "Cope" with Strain", H. Jiao, R. Nagelkerke, H. A. Kurtz, R. V. Williams, W. T. Borden, P. v R. Schleyer, *J. Amer. Chem. Soc*, **119**, 5921-5929, 1997.

40. "Computation of Nonlinear Optical Properties", H. A. Kurtz, and D. S. Dudis, in *Reviews in Computational Chemistry*, Vol. 12, ed. K. B. Lipkowitz and D. B. Boyd, Wiley-VCH, New York, 1998, pp 241-279.

41. "Modeling Nonlinear Optical Properties of Transition Metal Complexes. Basis Set, Effective Core Potential and Geometry Effects", T. R. Cundari, H. A. Kurtz, and T. Zhou, *J. Phys. Chem A.* **102**, 2962-2966, (1998).

42. "Modeling Nonlinear Optical Properties of Inorganic Complexes. Counterion Effects", T. R. Cundari, H. A. Kurtz, and T. Zhou, *Chem. Phys.* **240**, 205-214 (1999).

43. "Quantum Mechanical Characterization of E'-Type Centers in *a*-SiO_2 Films", S. P. Karna and H. A. Kurtz, *Microelectronic Engineering* **48**, 109-112 (1999).

44. "Proton Mobility in *a*-SiO_2", H. A. Kurtz and S. P. Karna, *IEEE Trans. Nuc. Sci.*, **46**, 1574-1577 (1999).

45. "New Fundamental Defects in *a*-SiO_2", S. P. Karna, H. A. Kurtz, W. M. Shedd, R. D. Pugh, and "Babu" B. K. Singaraju, *IEEE Trans. Nuc. Sci.*, **46**, 1544-1552 (1999).

46. "The Effect of Near-Interface Network Strain on Proton Trapping in SiO_2", K. Vanheusden, P.P. Korambath, H. A. Kurtz, S. P. Karna, D. M. Fleetwood, W. M. Shedd, and R. D. Pugh, *IEEE Trans. Nuc. Sci.*, **46**, 1562-1567 (1999).

47. "Infrared Spectra, Photochemistry, and Ab Initio Calculations of Matrix Isolated Methanethiol/Sulfur Dioxide Complex", S. Li, H. Kurtz, P. Korambath, and Y.-S. Li, *J. Molec. Struct.*, **550/551**, 235-244 (2000).

48. "A Computational Study of Polarizabilities and Second Hyperpolarizabilities of Inorganic Transition Metal Thiometalates and Metalates in Solution", T. R. Cundari, H. A. Kurtz, and T. Zhou, *J. Phys. Chem. A* **104**, 4711-4717 (2000). **DOI:** 10.1021/jp993838l

49. "Hydrogen Cracking in SiO_2: Kinetics for H_2 Dissociation at Silicon Dangling Bonds", H. A. Kurtz and S. P. Karna, *J. Phys. Chem. A* **104**, 4780-4784 (2000). **DOI:** 10.1021/jp993804d

50. "Structural and Nonlinear Optical Properties of Cationic Defects in Amorphous Silicon Dioxide I. Cluster Studies", A. M. Ferreira, H. A. Kurtz, and S. P. Karna, *J. Phys. Chem. A* **104**, 4796-4800 (2000). **DOI:** 10.1021/jp993802t

51. "Point Defects in Si-SiO_2 Systems: Current Understanding", S. P. Karna, H. A. Kurtz, A. C. Pineda, W. M. Shedd, and R. D. Pugh, in *Defects in SiO_2 and Related Dielectrics: Science and Technology*, NATO Science Series II, eds. G. Pacchioni, L. Skuja, and D. L. Griscom, Kluwer Academic Publishers, Dordrecht, 2000, pp. 599-615.

52. "Microscopic Mechanisms of Electron Trapping by Self-Trapped Holes and Protons in Amorphous SiO_2", S. P. Karna, H. A. Kurtz, W. M. Shedd, and R. D. Pugh, *IEEE Trans. Nuc. Sci.* **47**, 2311-2315 (2000).

53. "Modeling Intermolecular Effects on Nonlinear Optical Properties of Transition Metal Complexes. An Effective Core Potential Study", T. R. Cundari, H. A. Kurtz, and T. Zhou, *J. Chem. Info. Comp. Sci.* special issue on "Effective Core Potentials in Hartree Fock and Density Functional Theory", 41, 38-42 (2001).

54. "The Role of Bond Coordination and Molecular Volume on the Dielectric Constant of Mixed Oxide Compounds", H. A. Kurtz and R. A. B. Devine, *J. Applied Physics*, **7**, 2342-2344 (2001).

55. "The Effect of Network Topology on Proton Trapping in Amorphous SiO_2", A. C. Pineda, S. P. Karna, H. A. Kurtz, W. M. Shedd, and R. D. Pugh, *IEEE Trans. Nuc. Sci.* **48**, 2081-2085 (2001).

56. "Mixed-Oxides as High-k Dielectrics", H. A. Kurtz and R. A. B. Devine, in *Alternative to SiO_2 as Gate Dielectrics for Future Si-Based Microelectronics*, Materials Research Society Workshop Series, Eds. J. Morais and I. J. R. Baumvol, 2001.

57. "An Augmented Effective Core Potential Basis Set for the Calculation of Molecular Polarizabilities", N. P. Labello, A. M. Ferreira, and H. A. Kurtz, *J. Comp. Chem.* **26**, 1464-1471 (2005).

58. "Silicon Radicals in Silicon Oxynitride: An ESR Study", L. D. Crosby and H. A. Kurtz, *J. Phys. Chem. A* **110**, 8637-8644 (2006).

59. "Utilizing Effective Core Potentials for Accurate Calculations of Molecular Polarizabilities in Molecules Containing Transition Metals", N. P. Labello, A. M. Ferreira, and H. A. Kurtz, *J. Phys. Chem. A* **110**, 13507-13513 (2006). **DOI:** 10.1021/jp0653611

60. “Correlated Molecular Polarizability Calculations with an Augmented Effective Core Potential Basis Set”, N. P. Labello, A. M. Ferreira, and H. A. Kurtz, *Int. J. Quantum Chemistry* **106**. 3140-3148 (2006).

61. “An Application of Electronic Structure and Transition State Theory: The Reaction of Hydrogen with Silicon Radicals”, L. D. Crosby and H. A. Kurtz, *Int. J. Quantum Chemistry* **106**, 3149-3159 (2006).

Books

“Propagating Insight: A Tribute to Yngve Öhrn”, Advances in Quantum Chemistry, Vol. 35, eds: H. A Kurtz, J. V. Ortiz, and J. R. Sabin, Academic Press, San Diego, 1999.