

CURRICULUM VITAE
Samuel B. Trickey
Current as of: 30 May 2006

Personal

- Born November 28, 1940; Detroit, Michigan
- Married (1962); divorced (1981), two children (custodial parent, 1985 to majority)
- Married (1983), Ms. Cynthia R. Karle.
- Attended Denton High School, Denton, Texas; graduated 1958.

Degrees

- B.A., Rice University (Physics) 1962.
- M.S., Texas A&M University, (Physics) 1966.
- Ph.D., Texas A&M University, (Theoretical Physics) 1968.

Professional Record

A. Academic and Industrial

- Professor of Physics and Chemistry, University of Florida, Jan. 1981 - June 2005, Emeritus July 2005 - present
- Professor of Physics, University of Florida, Aug. 1979 - Jan. 1981.
- Professor of Physics, Texas Tech University, Aug. 1977 - July 1979.
- Associate Professor of Physics, University of Florida, July 1973 - July 1977.
- Assistant Professor of Physics, University of Florida, Sept. 1968 - June 1973.
- NASA PreDoctoral trainee, Texas A&M University, Sept. 1965 - Aug. 1968.
- Research Physicist, Mason & Hanger-Silas Mason Corp, Amarillo, Texas, June 1962 - June 1964.

B. Administrative

- Director, Quantum Theory Project, Jan. 1999 - Dec. 2004
- Executive Director, Office of Information Technologies and Services [in Office of the Provost], University of Florida, Sept. 1991 - July 1996.
- Director, J. C. Slater Memorial Computing Laboratory, Quantum Theory Project, Depts. of Physics and Chemistry, University of Florida, 1982 - 1993
- Director for Information Resources and Technological Programs, College of Liberal Arts and Sciences, University of Florida, August 1986 - July 1990.

- Acting Director of Space Resources, College of Liberal Arts and Sciences, University of Florida, August 1986 - Nov. 1987.
- Chair, Department of Physics and Engineering Physics, Texas Tech University, August 1977 - July 1979.

C. Other

- Consultant, Theoretical Division, Los Alamos National Laboratory, 1984 - 1994; Research Collaborator 1994 - 2000 (T-Division); 2001 - present (X-Division)
- Foreign Collaborator, Institut für Physikalische und Theoretische Chemie, Technische Universität München; Dec. 1998 - present
- Visiting Professor, Lehrstuhl für Theoretische Chemie, Technische Universität München, Sept. 1995, Oct. 1996, May 1998
- Visiting Scientist, Max-Planck Institut für Astrophysik, München, May 1985, June and Oct. 1986, Nov. 1987, June and Nov. 1988, June and Nov. 1989, Sept-Nov. 1990 (sabbatical); July 1991, May-June 1992, July and Dec. 1993, Aug. 1994
- Consultant, Programa de Investigación de Media Plaza en Simulación Molecular, Instituto Mexicano del Petroleo; Mar. 1999 - June 2004
- Visiting Staff Member, Los Alamos National Laboratory, August 1971 (Group T-6); Jan-May 1991 (Center for Materials Science; sabbatical).
- Visiting Scholar Universidad Autónoma Metropolitana - Unidad Iztapalapa, México DF México, August 1996.
- Visiting Scholar (1982 - 1989, summers), College of Sciences and Arts , College of Engineering (1990 - 1992, summers), Consultant (July 1994), College of Sciences and Arts, Michigan Technological University, Houghton, MI.
- Visiting Scientist, IBM Research Laboratories (San Jose), July - September 1973; September 1975 - August 1976 (sabbatical).
- Consultant, Quantum Physics Group, Redstone Arsenal, Huntsville, Alabama, 1972 - 1976.

D. Languages

- Spanish - fluent at the level of public lecturing.
- German - reading fluency, limited speaking fluency.

Membership in Professional Societies

- American Physical Society (Fellow, 1980).
- American Association of Physics Teachers.
- National Society of Hispanic Physicists (life member).

Honor Societies

- Phi Kappa Phi, Sigma Xi, Sigma Pi Sigma.
- Listed in: American Men and Women of Science, Who's Who in Science and Engineering, Who's Who in South and Southwest, Who's Who in America.

Publications

A. REFEREED:

1. "Exact Density Functional Study for the Hooke's Atom in an External Magnetic Field", Wuming Zhu and S.B. Trickey, *J. Chem. Phys.* [submitted]
2. "PUPIL: A Systematic Approach to Software Integration in Multi-scale Simulations", by J. Torras, Y. He, C. Cao K. Muralidharan, E. Deumens, H-P. Cheng, and S.B. Trickey, *Computer Phys. Commun.* [submitted]
3. "Faster Approximate Force Calculations via Quasi-spin Density Exchange-correlation Functionals", V.V. Karasiev, S.B. Trickey, F.E. Harris, *J. Comput. Phys.* [submitted]
4. "Software Integration in Multi-scale Simulations: the PUPIL System", J. Torras, E. Deumens, and S.B. Trickey, *J. Comput. Aided Matl. Design* [special topical issue; accepted]
5. "Born-Oppenheimer Interatomic Forces from Simple, Local Kinetic Energy Density Functionals", V.V. Karasiev, S.B. Trickey, and F.E. Harris *J. Comput. Aided Matl. Design* [special topical issue; accepted]
6. "Potential Parameterization from Proxy Systems", Wuming Zhu, K. Runge, and S.B. Trickey, *J. Comput. Aided Matl. Design* [special topical issue; accepted]
7. "Encoding Electronic Structure Information in Potentials for Multi-scale Simulations: SiO₂", Wuming Zhu, D.E. Taylor, A.R. Al-Derzi, K. Runge, S.B. Trickey, Ting Zhu, Ju Li, and S. Yip, *Computational Materials Science* [accepted]
8. "Analytical Solutions for Two Electrons in an Oscillator Potential and a Magnetic Field", Wuming Zhu and S.B. Trickey, *Phys. Rev. A* **72**, 022501 [1-5] (2005)
9. "Density Functional Energetics of α -Quartz for Calibration of SiO₂ Interatomic Potentials", N. Flocke, Wuming Zhu, and S.B. Trickey, *J. Phys. Chem. B* **109**, 4168-71 (2005)
10. "Basis Set Limitations on the Ab Initio Calculation of Stopping Cross Sections via Generalized Oscillator Strengths", J.A. Nobel, S.B. Trickey, J.R. Sabin, and J. Oddershede, *Chem. Phys.* **309**, 89-94 (2005)
11. "Molecular Prototypes for Simple SiO₂ Potentials", A.R. Al-Derzi, M.G. Cory, K. Runge, and S.B. Trickey, *J. Phys. Chem. A* **108**, 11679-683 (2004)
12. "Methods and Implementation of Robust, High-precision Gaussian Basis DFT Calculations for Periodic Systems: the GTOFF Code", S.B. Trickey, J.A. Alford, and J.C. Boettger, in "Computational Materials Science", vol. 15 of *Theoretical and Computational Chemistry*, J. Leszczynski ed. (Elsevier, Amsterdam, 2004)) 171-228
13. "Electronic Stopping and Momentum Density of Diamond from First-principles Treatment of the Microscopic Dielectric Function", R.J. Mathar, S.B. Trickey, and J.R. Sabin, in *Advances in Quantum Chemistry*, J.R. Sabin and E.J. Brändas, eds. (Academic Press) vol. 45, 277-288 (2004)
14. "Tests of Perturbative DFT Total Energy Estimates Implemented in a Gaussian Basis", Wuming Zhu and S.B. Trickey, *Internat. J. Quantum Chem.* **100**, 245-53 (2004)

15. "Deformation and Fracture of SiO₂ Nanorod", Ting Zhu, Ju Li, Sidney Yip, R.J. Bartlett, S.B. Trickey and, N.H. de Leeuw, *Molecular Simulations* **29**, 671-76 (2003).
16. "Shape-dependent Molecular Polarizabilities", S. Peter Apell, J.R. Sabin, S.B. Trickey, and J. Oddershede, *Internat. J. Quantum Chem.* **86**, 35 - 39 (2002).
17. "Challenges and State of the Art in Simulation of Chemo-Mechanical Processes," S.B. Trickey and P.A. Deymier, in *Chemical Mechanical Planarization IV* R.L. Opila, C. Reidsema-Simpson, K.B. Sundaram, and S. Seal eds (The Electrochemical Society, Pennington N.J. 2001) 3 - 17.
18. "Effect of Shape on Molecular Directional Compton Profiles", S. Peter Apell, R. Cabrera-Trujillo, J. Oddershede, S.B. Trickey, and J.R. Sabin, , *J. Molec. Struct. (Theochem)* **527**, 157-63 (2000).
19. "State Energy Functionals and Variational Equations in Density Functional Theory", B. Weiner and S.B. Trickey, *J. Molec. Struct. (Theochem)* **501-02**, 65-83 (2000).
20. "Inclusion of Relativistic Effects in Gaussian-basis Density Functional Calculations for Extended Systems", J.C. Boettger and S.B. Trickey, *J. Molec. Struct. (Theochem)* **501-02**, 285-96 (2000).
21. "Stopping Anisotropy in Molecular Chains", S.P. Apell, J. Aizpurua, J.R. Sabin, and S.B. Trickey, *Nucl. Inst. Meth. B* **164-165**, 318-23 (2000).
22. "Molecular Shape, Capacitance, and Chemical Hardness", J.R. Sabin, S.B. Trickey, S.Peter Apell, and J. Oddershede, *Internat. J. Quantum Chem.* **77**, 358-66 (2000).
23. "Electronic Stopping of Protons for Lithium in the Dielectric Formulation Obtained from First-Principles Calculations", R.J. Mathar, S.B. Trickey, and J.R. Sabin, *Nucl. Inst. Meth. B* **155**, 249-71 (1999).
24. "A Critical Assessment of Density Functional Theory with Regard to Applications in Organometallic Chemistry", A. Görling, S.B. Trickey, P. Gisdakis, and N. Rösch, in *Topics in Organometallic Chemistry.*, vol. 4, P. Hofmann and J.M. Brown eds (Springer Verlag, Heidelberg, 1999) 109 - 63.
25. "Time Dependent Variational Principle in Density Functional Theory", B. Weiner and S.B. Trickey, in *Advances in Quantum Chemistry*, P.-O. Löwdin, J.R. Sabin, M.C. Zerner, and E.J. Brändas, eds. (Academic Press, San Diego, 1999) vol. 35, 217 - 48.
26. "Calculation and Interpretation of Electron Momentum Densities", S.B. Trickey, in *Applications of Accelerators in Research and Industry: Proc. 15th International Conference*, AIP CP-475, J.L. Duggan and L.L. Morgan eds. (Amer. Phys. Soc., NY, 1999) 85-87.
27. "Momentum Density Effects Upon the Electronic Stopping of Elemental Solids", J. Wang, R.J. Mathar, S.B. Trickey, and J.R. Sabin, *J. Physics: Cond. Matt.* **11**, 3973 - 85 (1999).
28. " Geometrical Basis for Molecular Stopping Anisotropy", S.P. Apell, S.B. Trickey, and J.R. Sabin, *Phys. Rev. A* **58**, 4616 - 21 (1998).
29. "Fukutome Symmetry Classification of the Kohn-Sham Auxiliary One-Matrix and its Associated State or Ensemble", B. Weiner and S.B. Trickey, *Internat. J. Quantum Chem. Proc. Symposium on Density Functional Theory and Applications* **69**, 451-460 (1998).

30. "Comments on 'Extracting Convergent Surface Formation Energies from Slab Calculations' by V. Fiorentini and M. Methfessel", *J. Phys.: Cond. Matt.* **8** (1996) 6525", J.C. Boettger, John R. Smith, U. Birkenheuer, N. Rösch, S.B. Trickey, J.R. Sabin, and S. Peter Apell, *J. Phys.: Cond. Matt.* **10**, 893-94 (1998).
31. "Simple DFT-LSDA Modelling of the Molecular-like Aspects of Ultra-thin Film Properties", S.B. Trickey, R.J. Mathar, and J.C. Boettger, *Computational Chemistry and Chemical Engineering: Proc. Third UNAM-Cray Supercomputing Conference* G. Cisneros, J.A. Cogordan, M. Castro, and C. Wang, eds. (World Scientific Press, Singapore and New Jersey, 1997) p. 239-254.
32. "Surface Stopping", S.P. Apell, J.R. Sabin, and S.B. Trickey, *Phys. Rev. A* **56**, 3769 - 76 (1997).
33. "Simple Physical Model for Layer-Number Dependences of Proton Stopping in Ultra-thin Films", S. Peter Apell, J.R. Sabin, and S.B. Trickey, in *Applications of Accelerators in Research and Industry: Proc. 14th International Conference*, J.L. Duggan and I.L. Morgan, eds.,(American Physical Society, NY, 1997) AIP Conf. Proc. 392, vol. 1, 1369-72.
34. "Negative Ions in Density Functional Theory - Comment on *J. Chem. Phys.* **105**, 862 (1996)", N. Rösch and S.B. Trickey, *J. Chem. Phys.* **106**, 8940-41 (1997).
35. "Benchmark Comparison of Gradient Dependent and Local Density Calculations for Bulk Si and Al", S.B. Trickey, *Internat. J. Quantum Chem.* **61**, 641-46 (1997).
36. "High Precision Calculation of the Equation of State and Crystallographic Phase Stability for Aluminum", J.C. Boettger and S.B. Trickey, *Phys. Rev. B* **53**, 3007-12 (1996).
37. "Density Functional Calculations for Prediction of Ultra-thin Film Structure and Properties", S.B. Trickey and J.C. Boettger, in *Condensed Matter Theories, 11*, E.V. Ludeña, P. Vashishta, and R.F. Bishop, eds. (Nova Science Publishers, Commack, NY, 1996) 63 - 76.
38. "Prediction of Crystalline Properties from Ultrathin Layered Systems: Energy Deposition", S. P. Apell, J.R. Sabin, and S.B. Trickey, *Internat. J. Quantum Chem.* **S-29**, 153-59 (1995).
39. "Simulation of Ion Implantation in Si for 0.25 KeV H⁺ under Channeling Conditions", J.A. Nobel, J.R. Sabin, and S.B. Trickey, *Nucl. Instrum. Meth. B* **99**, 632-36 (1995).
40. "Theoretical Investigation of Na Adsorption on the Al (111) Surface", J.C. Boettger, U. Birkenheuer, N. Rösch, and S.B. Trickey, *Phys. Rev. B* **52**, 2025-31 (1995).
41. "High Precision Calculation of Crystallographic Phase Transition Pressures for Al", J.C. Boettger and S.B. Trickey, *Phys. Rev. B* **51**, 15623-25 (1995) [Rapid Communication].
42. "Calculated Properties of a Prototypical Ionic Monolayer", Jin Zhong Wu, S.B. Trickey, J.R. Sabin, and J.C. Boettger, *Phys. Rev. B* **51**, 14576-86 (1995); errata *Phys. Rev. B* **58**, 4182 (1998).
43. "Reply to: Note on Stopping Power and Statistics of Particle Penetration", S. B. Trickey and J. R. Sabin, *Nucl. Instrum. Meth. B* **95**, 480 (1995).

44. "Theoretical Ion Implantation Profiles for Low Energy Protons under Channeling Conditions", J. A. Nobel, J. R. Sabin, S. B. Trickey, *Internat. J. Quantum Chem.* S-**28**, 283-97 (1994).
45. "Energy Deposition of Protons in Allotropic Carbon Ultra-Thin Films", Jin Zhong Wu, S.B. Trickey, J.R. Sabin, and J.A. Nobel, *Internat. J. Quantum Chem.* S-**28**, 299-308 (1994).
46. "Materials Specificity, Quantum Length Scales, and Stopping Powers", S.B. Trickey, Jin Zhong Wu, and J.R. Sabin, *Nucl. Instrum. Meth. B* **93**, 186-94 (1994).
47. "On the Metallization of the LiF Monolayer", J.I. Juaristi, Jin Zhong Wu, J.A. Nobel, S.B. Trickey, and J.R. Sabin, *Solid State Commun.* **91**, 957-60 (1994).
48. "Quantum Size Effects in Hexagonal Aluminum Films", J. C. Boettger, U. Birkenheuer, N. Rösch, and S. B. Trickey, *Internat. J. Quantum Chem.* S-**28**, 675-86 (1994).
49. "Electronic Stopping Power for Protons in an LiF Monolayer", Jin Zhong Wu, S. B. Trickey, and J. R. Sabin, *Internat. J. Quantum Chem.* S-**27**, 219-26 (1993).
50. "Density Decomposition Options in the Orbital Local Plasma Approximation", David E. Meltzer, J.R. Sabin, S.B. Trickey, and Jin Zhong Wu, *Nucl. Instrum. Meth. B* **82**, 493-502 (1993).
51. "The Status of Density Functional Theory for Chemical Physics", S.B. Trickey in *Conceptual Trends in Quantum Chemistry*, J.-L. Calais and E. S. Kryachako, eds. (Kluwer, Amsterdam, 1993) vol. 1, 87 - 100.
52. "Proton Stopping in Ultra-thin Lithium Films", Jin Zhong Wu, S.B. Trickey, and J.R. Sabin, *Nucl. Instrum. Meth. B* **79**, 206-08 (1993).
53. "Structure, Energetics, and Molecular-to-Atomic-Ordering Transitions in Hydrogen Thin Films", Jin Zhong Wu, S.B. Trickey, J.R. Sabin, and J.C. Boettger, *Phys. Rev. B* **45**, 8610-22 (1992).
54. "Comment on 'Total Energy Calculations of Solid H, Li, Na, K, Rb, and Cs' ", J.C. Boettger, S.B. Trickey, and J.A. Nobel, *Phys. Rev. B* **45**, 7503-06 (1992).
55. "Low-Pressure Crystalline Phases in Lithium", J.A. Nobel, S.B. Trickey, P. Blaha, and K. Schwarz, *Phys. Rev. B* **45**, 5012-14 (1992).
56. "Interplanar Binding and Lattice Relaxation in a Graphite Di-Layer", S.B. Trickey, F. Müller-Plathe, G.H.F. Dierksen, and J.C. Boettger, *Phys. Rev. B* **45**, 4460-68 (1992).
57. "Quantum Size Effects in Equilibrium Lithium Ultra-thin Layers", J.C. Boettger and S.B. Trickey, *Phys. Rev. B* **45**, 1363-72 (1992).
58. "Ordering of the Crystalline Phases of Atomic Hydrogen near Equilibrium", G.A. Wilson, J.A. Nobel, and S.B. Trickey, *Internat. J. Quantum Chem.* **42**, 1037-45 (1992).
59. "Structural Optimization and d-band Holes in Cu Monolayers", U. Birkenheuer, N. Rösch, S.B. Trickey, and J. Noffke, *Z. Physik B - Cond. Matt.* **83**, 267-71 (1991).
60. "Stopping of Swift Projectiles in Material Thin Films: Hydrogen", Jin Zhong Wu, S.B. Trickey, J.R. Sabin, and David E. Meltzer, *Nucl. Instrum. Meth. B* **56/7**, 340-44 (1991).

61. "Mono- and Di-Layer Analogues of Crystalline Atomic Hydrogen", Jin Zhong Wu, J.R. Sabin, S.B. Trickey, and J.C. Boettger, *Internat. J. Quantum Chem. S* **24**, 873-79 (1990).
62. "Mono- and Di-Layer Lattice Modifications in Lithium", J.C. Boettger, S.B. Trickey, F. Müller-Plathe, and G.H.F. Diercksen, *J. Phys.: Cond. Matt.* **2**, 9589-9601 (1990).
63. "Beryllium-Hydrogen Ultra-thin Films: II. Ground State Properties of the Beryllium-Hydrogen Dilayer", Jin Zhong Wu, S.B. Trickey, and J.C. Boettger, *Phys. Rev. B* **42**, 1668-73 (1990).
64. "Calculation of Mean Excitation Energy and Stopping Cross-Section in the Local Plasma Approximation", David E. Meltzer, J.R. Sabin, and S.B. Trickey, *Phys. Rev. A* **41**, 220-32 (1990); erratum *A* **42**, 666 (1990).
65. "Full-Potential, Linearized Augmented Plane Wave Programs for Crystalline Systems", P. Blaha, K. Schwarz, P. Sorantin, and S.B. Trickey, *Computer Phys. Commun.* **59**, 399-415 (1990).
66. "Beryllium-Hydrogen Ultra-thin Films: I. Metallic Behavior in a BeH₂ Monolayer", Jin Zhong Wu, S.B. Trickey, and J.C. Boettger, *Phys. Rev. B* **42**, 1663-67 (1990).
67. "Static Quantum Size Effects in Ultra-thin Be Films", J.L. Vicente, A. Paola, A. Razzitte, E.E. Mola and S.B. Trickey, *Phys. Stat. Solidi (b)* **155**, K 93-98 (1989).
68. "A Computationally Feasible Strategy for Partitioning Theory of the Molecule-Surface Interaction", S.B. Trickey, *J. Molec. Struc. (Theochem)* **199**, 215-24 (1989).
69. "First Principles Systematics of the Ground State of Metal Monolayers. I: Groups I and II through Sr", J.C. Boettger and S.B. Trickey, *J. Phys.: Cond. Matt.* **1**, 4323-38 (1989).
70. "Calculation of Stopping Powers in Ordered Ultra-Thin Films", D.E. Meltzer, S.B. Trickey, and J.R. Sabin, *Nucl. Instrum. Meth. B* **40/41**, 321-23 (1989).
71. "Graphite Di-Layers and the Interstellar PAH Hypothesis", S.B. Trickey, G.H.F. Diercksen, and F. Müller-Plathe, *Astrophys. J.* **336**, L37-39 (1989).
72. "Electronic Structure of Fibonacci Copolymers and Superlattices", M. Seel and S.B. Trickey, *Solid State Commun.* **66**, 537 - 41 (1988).
73. "The Exact Kohn-Sham Direct Gap at an Insulator-Metal Transition", R.S. Jones and S.B. Trickey, *Phys. Rev. B* **36**, 3095 - 98 (1987).
74. "Electronic Surface States in Beryllium", J.C. Boettger and S.B. Trickey, *Phys. Rev. B* **34**, 3604 - 09 (1986).
75. "Approximate Electron Removal Energies in Density Functional Theory from Post-hoc Correction of Local Spin Density Eigenvalues", S.B. Trickey, *Phys. Rev. Lett.* **56**, 881 - 84 (1986).
76. "Structural Optimization and Properties of First-Row Monolayers", J.C. Boettger and S.B. Trickey, *J. Phys. F: Met. Phys.* **16**, 693 - 706 (1986).
77. "Avoiding Orthogonality Problems in the Application of the Alternant Molecular Orbital Method to Solids", R.S. Jones, and S.B. Trickey, *Internat. J. Quantum Chem. S* **19**, 669 -73 (1986).

78. "Structure and Properties of a Beryllium Dilayer", J.C. Boettger and S.B. Trickey, Phys. Rev. B **32**, 1356 - 58 (1985) [Rapid Communication].
79. "Equation of State and Properties of Lithium", J.C. Boettger and S.B. Trickey, Phys. Rev. B **32**, 3391 - 98 (1985).
80. "Correlated Wavefunctions for Crystalline Solids II: Metal-Insulator Transition in the Cubic Electron Gas", R. S. Jones and S.B. Trickey, J. Phys. C: Sol. State Phys. **18**, 6355 - 68 (1985).
81. "Band Reordering Effects in the Ultra-high Pressure Equation of State of Lithium", W.G. Zittel, J. Meyer-ter-Vehn, J.C. Boettger, and S. B. Trickey, J. Phys. F: Met. Phys. **15**, L247 - L251 (1985).
82. "Ground State Properties of a Beryllium Monolayer", J.C. Boettger and S. B. Trickey, J. Phys. F: Met. Phys. **14**, L151 - L153 (1984).
83. "Correlated Wavefunctions for Crystalline Solids: Multi-Parameter AMO Treatment of the Cubic Electron Gas", R.S. Jones, and S.B. Trickey, J. Phys. C: Sol. State Phys. **17**, 4609 - 24 (1984).
84. "Multi-parameter Iterative Convergence Accelerator for Crystalline LCGTO Calculations", J.C. Boettger and S.B. Trickey, Computer Phys. Commun. **32**, 361 - 65 (1984).
85. "Total Energy and Pressure in the Gaussian Orbitals Technique, II. Pressure-Induced Crystallographic Phase Transition and Equilibrium Properties of Aluminum", J.C. Boettger and S.B. Trickey, Phys. Rev. B **29**, 6434 - 42 (1984).
86. "Total Energy and Pressure in the Gaussian Orbitals Technique, I. Methodology with Applications to the High Pressure Equation of State of Neon", J.C. Boettger and S.B. Trickey, Phys. Rev. B **29**, 6425 - 33 (1984).
87. "Comment on 'Electron Removal Energies in Kohn-Sham Density Functional Theory'", S.B. Trickey, Phys. Rev. B **30**, 3523 - 24 (1984).
88. "Optical Absorption of Solid Xenon at High Pressure", A.K. Ray, S.B. Trickey, and A.B. Kunz, Phys. Stat. Solidi (b) **121**, K47 - K50 (1984).
89. "On the Systematic Assessment of Correlation Effects in Local Density Models", J.R. Sabin and S.B. Trickey in *Local Density Approximations in Quantum Chemistry and Solid State Theory*, Jens Peder Dahl and John Avery eds., (Plenum N.Y. 1984) 333 - 52.
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91. "Augmented-Plane-Wave to Gaussian-Orbital Conversion Procedure: One-Electron States and Compton Profiles of fcc Neon", A.K. Ray and S.B. Trickey, Phys. Rev. B **24**, 1751 - 60 (1981); erratum Phys. Rev. B **28**, 7352 (1983).
92. "Local Density Functional Methods in Two-Dimensionally Periodic Systems: Hydrogen and Beryllium Monolayers", J.W. Mintmire, J.R. Sabin, and S.B. Trickey, Phys. Rev. B **26**, 1743 - 53 (1982).
93. "BCC-FCC Allotropy, F-Bands and Metallization in Xenon and Krypton", A.K. Ray, S.B. Trickey, and A.B. Kunz, Solid State Commun. **41**, 351 - 53 (1982).

94. "Adequacy of Local-Exchange Excitation Hamiltonians in Insulators", S.B. Trickey, A.K. Ray, and J.P. Worth, *Phys.Stat. Solidi (b)* **106**, 613 - 20 (1981).
95. "Lattice Constant at the Insulator-Metal Transition of Crystalline Xenon", A.K. Ray, S.B. Trickey, R.S. Weidman, and A.B. Kunz, *Phys. Rev. Lett.* **45**, 933 - 35 (1980).
96. "APW- $X\alpha$ Compton Profiles in Crystalline Rare Gases", J.P. Worth, Corinne Lee Merry, and S B. Trickey, *J. Phys. Chem. Solids* **41**, 623 - 30 (1980).
97. "Energy Band Theory and the Lattice Dynamics of Rare Gas Crystals", J.P. Worth and S.B. Trickey, *J. Low Temp. Phys.* **38**, 393 - 411 (1980).
98. "APW Calculation of the Zero Temperature Isotherm of Solid Xenon", J.P. Worth and S.B. Trickey, *Phys. Rev. B* **19**, 3310 - 12 (1979).
99. "Non-Muffin-Tin Effects in the $X\text{-}\alpha$ Treatment of Ne_2 ", J.P. Worth, B.I. Dunlap, and S.B. Trickey, *Chem. Phys. Lett.* **55**, 168 - 70 (1978).
100. "Debye-Waller Factor of Solid Heavy Methane", S.B. Trickey and T.R. Koehler, *Solid State Commun.* **25**, 779 - 80 (1978).
101. "Euler Vectors and Rotations About an Arbitrary Axis", T.R. Koehler and S.B. Trickey, *Am. J. Phys.* **46**, 650 - 51 (1978).
102. "Electrons and Phonons in Crystalline Rare Gases: Numerical Studies of Simple Local Exchange Models", S.B. Trickey and J.P. Worth, *Internat. J. Quantum Chem. S-II*, 529 - 38 (1977).
103. "A Systematic Treatment of Quantum Mechanical Reaction Coordinates", N.M. Witriol, J.D. Stettler, M.A. Ratner, J.R. Sabin, and S.B. Trickey, *J. Chem. Phys.* **66**, 1141 - 59 (1977).
104. "Application of Model Hamiltonians to the Electron Dynamics of Organic Charge Transfer Salts", M.A. Ratner, J. R. Sabin, and S. B. Trickey, in *The Uncertainty Principle and the Foundations of Quantum Mechanics*, W.C.Price and S.S. Chissick, eds., (John Wiley, NY, 1977) 461 - 83.
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122. "Convergence of the Nosanow Cluster Expansion Assuming the Wu-Krumhansl Correlation Function", Susan J.M. Kuebbing and S.B. Trickey, J. Low Temp. Phys. **8**, 499 - 509 (1972).
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B. PUBLISHED COMPUTER CODE

1. "WIEN - Full-Potential Linearized APW Program for Crystalline Systems", P. Blaha, K. Schwarz, P. Sorantin and S. B. Trickey, Program ABRE of the Computer Physics Communications Program Library (Queen's Univ.-Belfast, 1990).

C. NON-REFEREED PUBLICATIONS AND POLICY REPORTS:

Non-refereed Articles:

1. "Dielectric Functions in LiF", S.B. Trickey, R.J. Mathar, and J.R. Sabin, Meeting Record, 20th Werner Brandt Workshop on Energy Deposition Phenomena, U. Florida, 10-11 Feb. 2000, J. Sabin, editor.
2. "Calculated Momentum Densities - Properties and Uses", S.B. Trickey, Meeting Record, 18th Werner Brandt Workshop on Energy Deposition Phenomena, U. Florida, 4-5 June 1998, J. Sabin, editor.
3. "Molecular Shape as the Determiner of Electronic Stopping Anisotropy", J.R. Sabin, S.B. Trickey, and S. Peter Apell, Meeting Record, 17th Werner Brandt Workshop on Energy Deposition Phenomena, U. Virginia, 8-9 May 1997, R. Baragiola, editor.
4. "First-Principles All-Electron Calculation of Proton Stopping in the Dielectric Formulation", R.J. Mathar, S.B. Trickey, and J.R. Sabin, Meeting Record, 17th Werner Brandt Workshop on Energy Deposition Phenomena, U. Virginia, 8-9 May 1997, R. Baragiola, editor.
5. "Layer-Number Scaling in Ultra-Thin Film Stopping and Energetics", S.B. Trickey, S. Peter Apell, and J.R. Sabin, Meeting Record, 16th Werner Brandt Workshop on Energy Deposition Phenomena, Oak Ridge, 7-9 Jan. 1996, ORNL Report CONF-960165, R. Ritchie, O. Crawford, and R. Hamm, editors.
6. "When the State of the Art Isn't Good Enough", J. Nobel, J. Oddershede, S.B. Trickey, and J.R. Sabin, Meeting Record, 15th Werner Brandt Workshop on Energy Deposition Phenomena, U. Florida, 10-11 Mar. 1994, J.R. Sabin editor.
7. "Laboratory Instrumentation Upgrade for Theoretical Chemistry", S.B. Trickey and G. D. Purvis III, Chemical Design and Automation News, Vol. 4, No. 3 (March 1989) [feature article].

Policy Reports:

1. "An Assessment of Opportunities for Vanderbilt Computing and Networking", 18 Jan. 1991 (visitor's report; 11 pages)

2. "Structural Stability Calculations for Films and Crystals", U.S. Dept. of Energy (Energy Conservation and Utilization Technology Program) Workshop on Theory and Modeling for Materials by Design (17-19 Sept. 1984); ORNL Report CONF-8409210, R. E. Allen, D. L. Cocke, J. J. Eberhardt, and A. Wilson editors; 393 - 428.
3. "Computational Resources for Forefront Studies of Real Crystalline Systems and their Defects", U.S. Dept. of Energy (Council on Material Science), in Report of Policy Panel on Theory and Computer Simulation of Materials Structure and Imperfections, A. B. Kunz, organizer, 6 - 10 Aug. 1984.
4. "Opportunities and Problems for Computation in the Quantum Theory of Molecules and Solids", S.B. Trickey and G.D. Purvis III (U.S. National Science Foundation, Chemical Physics Section, Division of Chemistry, June 1984).
5. "Eighteen Years Later - Report to National Science Foundation", S.B. Trickey, G. D. Purvis III, N. Y. Öhrn (U.S. National Science Foundation, Chemical Physics Section, Division of Chemistry, May 1983).
6. "Annual Information Resources Performance Report" U. Florida Fiscal Years 90 - 91 through 94 - 95 (required by state statute).
7. "Information Resources Strategic Plan for University of Florida": "1993-97" (Oct. 1991) "1995-99" (Nov. 1993); "1997-2000" (Nov. 1995) (required biennially by state statute).
8. "Information Resources Strategic Plan for 1988-90", (25 Jan. 1988.) and "Information Resources Strategic Plan for 1991-95", (16 Jan. 1990) College of Liberal Arts and Sciences (required by state statute).
9. "External Review of Institute of Food and Agricultural Sciences Computing and Networking Upgrade Plans", 22 Feb. 1989; with Mark P. Hale.
10. "Information Resources Operating Plan", U. Florida, College of Liberal Arts and Sciences, Sept. 1988, Aug. 1989 (required by state statute).
11. "Proposed Acquisition of Forefront Instrumentation for Computationally Intensive Collaborative Research", 21 May 1987 (justification documentation, 119 pages, for statutorily required review and approval process - Board of Regents, Information Resources Commission, Information Technology Resources Procurement Advisory Council); with G. D. Purvis III.
12. "Final Report of Ad Hoc Task Force on Advanced Computing", to Vice President for Academic Affairs, Univ. Florida, 8 Oct. 1984.
13. "Year-end Report of Ad Hoc Task Force on Advanced Computing", to Vice President for Academic Affairs, Univ. Florida, 15 May 1984.
14. "Five-Year Strategy for Computing - Report to Vice President for Academic Affairs", Texas Tech University, May 1978.

Reviews:

1. "Review of *Quantal Density Functional Theory* (V. Sahni, author)", S.B. Trickey, *Internat. J. Quantum Chem.* **100**, 60-1 (2004)

2. "Review of *Recent Advances in Density Functional Methods - Part I* (D.P. Chong, Editor) and *Recent Developments and Applications of Modern Density Functional Theory* (J. Seminario, Editor)", S.B. Trickey, *Internat. J. Quantum Chem.* **72** 155 - 56 (1999).
3. "Review of *Modern Density Functional Theory - A Tool for Chemistry* (J. Seminario, Editor)" S.B. Trickey, *Internat. J. Quantum Chem.* **59**, 259 - 60 (1996).
4. Book Review, *Physics of Solids Under High Pressures* (J.S. Schilling and R.N. Shelton, Editors) S.B. Trickey and J.R. Brookeman, *J. Magnet. Res.* **59**, 357 - 58 (1984).

Other:

1. "Preface" - Notker Rösch Festschrift issue of *Chemical Physics*, S.B. Trickey, S. Gemming, and E.J. Barends, *Chem. Phys.* **309**, 1-2 (2005)
2. "In Memoriam: Joseph Callaway, 1931-1994", S. B. Trickey, *Internat. J. Quantum Chem.* **S-29**, 29 (1995).
3. "In Memoriam: Michael Andreas Schlüter, 1945-1992", L. Fritsche, H. Monkhorst, and S.B. Trickey, *Internat. J. Quantum Chem.* **S-27**, 91 (1993).

D. EDITORSHIPS:

1. Specialist Editor for Condensed Matter Physics, *Computer Physics Communications* (1991–present)
2. Special Editor, *Chemical Physics*, Notker Rösch Festschrift issue (vol. 309, no. 1, 2005).
3. Special Editor with Julio Alonso (Universidad de Valladolid, España) *Proceedings of the Ninth International Conference on the Applications of Density Functional Theory in Chemistry and Physics*, San Lorenzo de El Escorial (Spain) 10-14 Sept. 2001; appeared as volume 91, issues 3 and 4 (2003), *Internat. Journal of Quantum Chemistry*; 67 papers
4. Special Editor (Mel Levy and Weitao Yang, Guest Editors), *Proceedings of the Symposium on Density Functional Theory and Applications*, Duke University, 3 - 7 June 1997, *Internat. J. Quantum Chem.* **69**, 227 - 628 (1998)
5. *Density Functional Theory of Many-Fermion Systems*, Vol. 21 *Adv. Quantum Chem.* (Academic, San Diego, 1990)
6. *Quantum Fluids and Solids - Proceedings of the 1977 Sanibel International Symposium on Quantum Statistics*, (Plenum Press, N.Y. 1977) with J. W. Dufty and E. D. Adams.
7. *Quantum Statistics and the Many-Body Problem - Proceedings of the 1975 Sanibel Symposium on Quantum Statistics and Many-Body Problems*, (Plenum Press, N.Y. 1975) with W. P. Kirk and J. W. Dufty.
8. Member, Advisory Editorial Board, *International J. Quantum Chemistry* (1988-93)

Invited Talks, Seminars, and Contributed Papers Presented (Physics)

1. "Overview of Some Multi-scale Materials Simulation Techniques and Issues", DoE (PNNL) Multi-scale Mathematics in Materials Science Workshop, Tacoma WA, 25-30 May 2006 (invited keynote).

2. "Quantum Mechanical Methods in Multi-scale Materials Simulations", DoE (PNNL) Multi-scale Mathematics in Materials Science Workshop, Tacoma, WA, 25-30 May 2006 (invited)
3. "Summary of PUPIL: A New Approach to Software Integration in Multi-scale Simulations", DoE (PNNL) Multi-scale Mathematics in Materials Science Workshop, Tacoma WA, 25-30 May 2006 (invited).
4. "Lessons from Experience about Competitive Realities at the University of Florida for Multi-disciplinary Funding in Computational Sciences", Flagship for Mathematical Sciences Workshop, 02 May 2006 Gainesville, FL (invited).
5. "Orbital-Free Density Functionals and Density Models for Driving Molecular Dynamics", DFTEM-2006 Conference, Vienna Austria, 20-22 April 2006 (invited)
6. "PUPIL: A New Concept of Software Integration in Multi-scale Simulations", Juan Torras-Costa, S.B. Trickey, and E. Deumens, Amer. Physical Society March Meeting 2006, contributed paper H27 7
7. "Prediction of Born-Oppenheimer Interatomic Forces Using Orbital-Free Density Functional Theory with Approximate Kinetic Energy Functionals", S.B. Trickey, V.V. Karasiev, and Frank E. Harris Amer. Physical Society March Meeting 2006, contributed paper P27 7
8. "Fitting of Molecular Densities by Compact, Atom-Centered Expansion", V.V. Karasiev, S.B. Trickey, and Frank E. Harris, Amer. Physical Society March Meeting 2006, contributed paper P27 8
9. "Magnetic Field Effects upon Exchange-Correlation in the Hooke's Atom", Wuming Zhu and S.B. Trickey Amer. Physical Society March Meeting 2006, contributed paper P27 9
10. "Simulation Studies of Mechanical Properties of Novel Silica Nano-structures", Krishna Muralidharan, Juan Torras Costa, and S.B. Trickey Amer. Physical Society March Meeting 2006, contributed paper R32 6
11. "Merging User Packages with PUPIL in Multi-scale Simulations", Juan Torras, E. Deumens, and S.B. Trickey, Poster, 46th Sanibel Symposium, Feb. 26 - Mar. 3, 2006.
12. "Fitting, Modeling, and Parameterization of Electron Density", V.V. Karasiev, S.B. Trickey, and F.E. Harris, Poster, 46th Sanibel Symposium, Feb. 26 - Mar. 3, 2006.
13. "Progress on Approximate Density Functionals for Materials Simulations", Seminario, Facultad de Química, Pontificia Universidad Católica de Chile, Santiago de Chile, Nov. 9, 2005 (invited; in Spanish).
14. "Progress on Approximate Density Functionals", Quantum Theory Project Seminar, Univ. Florida, 28 Sept. 2005 (invited).
15. "Approximate Density Functionals for Molecular Dynamics Simulations of Material Properties", Fifth Congress of Internat. Soc. for Theoretical Chemical Physics, New Orleans LA, 25 July 2005 (invited).

16. "Software for Integration of Quantum Mechanical and Classical Regions in Molecular Dynamics", Juan Torras, E. Deumens, K. Muralidharan, and S.B. Trickey, Fifth Congress of Internat. Soc. for Theoretical Chemical Physics, New Orleans LA, 22 July 2005 (poster).
17. "Kinetic Energy Density Functionals for Calculation of Interatomic Forces", V.V. Karsiev, S.B. Trickey, and F.E. Harris, Fifth Congress of Internat. Soc. for Theoretical Chemical Physics, New Orleans LA, 25 July 2005 (poster).
18. "Analytical Solutions for States of the 3D Hooke's Atom in an External B Field", S.B. Trickey and Wuming Zhu, Amer. Physical Society March Meeting 2005, paper U32.00004.
19. "Exact Current DFT Study of Hooke's Atom in Magnetic Fields", Wuming Zhu and S.B. Trickey, Amer. Physical Society March Meeting 2005, paper U32.00005.
20. "Object-oriented Development of an All-electron Gaussian Basis DFT Code for Periodic Systems", J. Ashley Alford and S.B. Trickey, Amer. Physical Society March Meeting 2005, paper H32.00009.
21. "Current Density Functional Theory from Analytical and Numerical Solutions for the 3D Hooke's Atom in an External B Field", Wuming Zhu and S.B. Trickey, 45th Sanibel Symposium, March 5-11, 2005.
22. "A New all-electron Gaussian-basis DFT Code for Systems Periodic in One-, Two- and Three Dimensions", J.A. Alford and S.B. Trickey, 45th Sanibel Symposium, March 5-11, 2005.
23. "Software for Integration of Quantum Mechanical and Classical Regions in Molecular Dynamics", J. Torras, E. Deumens, and S.B. Trickey, 45th Sanibel Symposium, March 5-11, 2005.
24. "Quasi-spin Density Exchange-correlation Functionals", V.V. Karasiev, S.B. Trickey, and F.E. Harris, 45th Sanibel Symposium, March 5-11, 2005.
25. "Prediction of Materials Properties Via Gaussian Orbital DFT Methods", 13th International Conference on Current Trends in Computational Chemistry, Jackson MS, 12 Nov. 2004 (invited).
26. "First Principles Electronic Structure Methods and the Prediction of Materials Properties", XXIV Congreso Anual, Sociedad Mexicana de Ciencia y Tecnologia de Superficies y Materiales, Rivera Maya, México, Sept. 29, 2004 (invited).
27. "Large-scale, Grid-enabled Gaussian Orbital Implementation of Current Density and Spin Density Functional Theory for Ordered Systems", NSF DMR Computational Materials Theory Review meeting, Univ. of Illinois, Urbana-Champaign, June 17, 2004 (invited)
28. "Object-oriented Development of a Gaussian Basis DFT Code", J. Ashley Alford and S.B. Trickey, NSF DMR Computational Materials Theory Review meeting, Univ. of Illinois, Urbana-Champaign, June 17, 2004

29. "Current DFT versus Ordinary DFT for Atomic Ground States in External Magnetic Fields", Wuming Zhu, S.B. Trickey, and J. Ashley Alford, poster, NSF DMR Computational Materials Theory Review meeting, Univ. of Illinois, Urbana-Champaign, June 17, 2004
30. "Current DFT versus Ordinary DFT for Atomic Ground States in External Magnetic Fields", W. Zhu, S.B. Trickey, and J.A. Alford, APS March meeting, Montreal, March 23, 2004.
31. "Comparison of Current and Ordinary DFT for Ground States of Atoms in External Magnetic Fields", W. Zhu, S.B. Trickey, and J.A. Alford, 44th Sanibel Symposium, Mar. 1, 2004.
32. "Tutorial on Plenary Sessions I - XI" 44th Sanibel Symposium graduate student tutorial session, Feb. 28, 2004
33. "Quantum Mechanics meets Classical Mechanics in Simulations", U. Florida Dept. of Physics Brown Bag Lunch talk, Nov. 5, 2003.
34. "Basics of the Art of Funding Research - Tutorial for Grad Students and Postdocs", Seminar, Quantum Theory Project, Univ. Florida, Oct. 15, 2003.
35. "Classical Potentials for Multi-scale Simulation of Fracture in Silica", Seminar, Institut für Physikalische und Theoretische Chemie, Technische Universität München, Germany, 20 May 2003.
36. "State of the Art for First Principles Calculation of Electronic Structure of Periodic Systems - Observations and Recommendations", CECAM Workshop on Rigorous Ab Initio Studies of Periodic Systems: Approaches to Electron Correlation, Lyon France, 14-16 May 2003 (invited).
37. "Tests of Perturbative DFT Total Energy Estimates Implemented in a Gaussian Basis", W. Zhu and S.B. Trickey, 43rd Sanibel Symposium, Feb. 22, 2003.
38. "MD Simulations of SiO₂ Nanorod Fracture as a Test of First-principles Potential Parameterization, W. Zhu, C. Taylor, A.R. Al-Derzi, K. Runge, R.J. Bartlett, S.B. Trickey, T. Zhu, J. Li, S. Yip, and N.H. deLeeuw, APS March meeting paper D27-7, Bull. Amer. Phys. Soc. **48**, 307 (2003)
39. "Tests of Gaussian Basis Implementation of Perturbative DFT Total Energy Estimates", S.B. Trickey and W. Zhu, APS March meeting paper W19-9, Bull. Amer. Phys. Soc. **48**, 1160 (2003)
40. "Method Development for Predictive Simulation of Chemo-Mechanical Processes in Materials," Sixth Pan American Workshop on Molecular and Materials Sciences, Cuernavaca México, Feb. 17, 2003.
41. "Multi-scale, Multi-pass Simulations from Molecules to Materials", NSF DMR Computational Materials Theory Review meeting, Univ. of Illinois Urbana-Champaign, June 19, 2002

42. "Encoding First-principles Electronic Structure Information in Classical Potentials:SiO₂" - S.B. Trickey, A.R. Al-Derzi, N. Flocke, Wuming Zhu, M. Cory, K. Runge, Ting Zhu, Ju Li, and S. Yip, APS March Meeting, Indianapolis, IN, 21 March 2002; Bull. Am. Phys. Soc. **47**, 1018 (2002).
43. "Encoding First-principles Cluster Information in Semi-Empirical Potentials: SiO₂" - A.R. Al-Derzi, K. Runge, M. Cory, W. Zhu, and S.B. Trickey, 42nd Sanibel Symposium, Feb. 23, 2002.
44. "Encoding First-principles Electronic Structure Information in Classical Potentials: α -Quartz" - W. Zhu, N. Flocke, and S.B. Trickey, 42nd Sanibel Symposium, Feb. 25, 2002.
45. "A Systematic Approach to Produce Approximate Time-dependent Density Functionals" - B. Weiner and S.B. Trickey, 41st Sanibel Symposium, March 1, 2001
46. "Constructive Approach to Density Functional Theory", Löwdin Memorial Symposium, Uppsala University (Sweden), invited talk, 25 Oct. 2000.
47. "Challenges and State of the Art in Simulation of Chemo-Mechanical Processes", 198th Meeting of Electrochemical Society, Phoenix AZ, invited talk, 23 Oct. 2000.
48. "Dielectric Functions in LiF", 20th Werner Brandt Workshop on Energy Deposition Phenomena, U. Florida, invited talk, 10-11 Feb. 2000.
49. "Jellium Blob Chemistry: Predicting and Understanding Trends in Molecular Response Anisotropy from Simple Models", III Congress, International Society for Theoretical Chemical Physics, Mexico City, invited talk, 8-13 Nov. 1999.
50. "Charged Particle Energy Deposition in Ordered Systems: Recent Progress on Approximate and Nearly Exact Methods", Group T1 Seminar, Los Alamos National Laboratory, 18 May 1999.
51. "Molecular Shape and Chemical Hardness", 39th International Sanibel Symposium, contrib. poster, 27 Feb. 05 Mar. 1999.
52. "Recent Developments in Formal Density Functional Theory", US-Latin American Workshop in Quantum Chemistry and Chemical Physics, Cuernavaca, México, invited talk, 24 -26 Feb. 1999.
53. "Calculation and Interpretation of Electron Momentum Densities", Invited paper, 15th International Conference on Application of Accelerators in Research and Industry, U. North Texas, Denton TX, 04-07 Nov. 1998.
54. "Calculated Momentum Densities - Properties and Uses", Invited lecture, 18th Werner Brandt Workshop on Energy Deposition Phenomena, U. Florida, 4-5 June 1998.
55. "Prediction of the Structure and Properties of Ordered Ultra-thin Films", Physics Department Colloquium, Iowa State University, Ames IA, 22 April 1998.

56. "Prediction of the Structure and Properties of Ordered Ultra-thin Films", Physics Department Colloquium, Texas Tech University, Lubbock TX, 26 Mar. 1998.
57. "First-Principles Systematics of Ordered Metallic Monolayers: 3D Transition Metals", Invited lecture, Fifth Chemical Congress of North American, Cancún, México, 11-15 Nov. 1997.
58. "Fukutome Symmetry Classification of the Kohn-Sham Auxiliary One-Matrix and its Associated State or Ensemble", Invited lecture, Symposium on Density Functional Theory and Applications, Duke University, 3-7 June 1997.
59. "First-Principles All-Electron Calculation of Proton Stopping in the Dielectric Formulation", Invited lecture, 17th Werner Brandt Workshop on Energy Deposition Phenomena, U. Virginia, 8-9 May 1997.
60. "Simple Physical Model for Layer-Number Dependences of Proton Stopping in Ultra-thin Films", Invited paper, 14th International Conference on Applications of Accelerators in Research and Industry, U. North Texas, Denton TX, 6-9 Nov. 1996.
61. "Simple DFT-LSDA Modelling of Molecular-like Aspects of Ultra-thin Films Properties", Invited lecture, 3rd UNAM-Cray Supercomputing Conference on Computational Chemistry, Universidad Nacional Autónoma de México, México DF, 15 Aug. 1996.
62. "Prediction of the Structure and Properties of Ultra-thin Films and Crystals", Seminario de Depto. de Química Física, Universidad de Valladolid, España, 16 Feb. 1996.
63. "A Partisan's View of Current Challenges in Density Functional Theory", Seminario de Depto. de Física Teórica, Atómica y Nuclear, Universidad de Valladolid, España. 15 Feb. 1996.
64. "Layer-Number Scaling in Ultra-Thin Film Stopping and Energetics", Invited lecture, 16th Werner Brandt Workshop on Energy Deposition Phenomena, Oak Ridge National Laboratory, 8-9 January 1996.
65. "First Principles Predictions of the Structure and Properties of Ultra-thin Films and Crystals", Departmental Seminar, Faculty of Chemistry, Division of Postgraduate Studies, Universidad Nacional Autónoma de México, Mexico DF, 17 Nov. 1995.
66. "Density Functional Calculations for Prediction of Ultra-thin Film Structure and Properties", Invited lecture, 19th International Workshop on Condensed Matter Theories, Caracas, Venezuela, 12-16 June 1995.
67. "Approach to Bulk Behavior from Ultrathin Layered Systems: Energy Deposition", S. P. Apell, J. R. Sabin, and SBT, 35th Internat. Sanibel Symposium, contributed poster, 28 Feb. 1995.
68. "High Precision First Principles Prediction of the Aluminum Equation of State", J. C. Boettger and SBT, 35th Internat. Sanibel Symposium, contributed poster, 28 Feb. 1995.
69. "Proton Stopping in Ultrathin Films: Chemical Effects", Invited paper, 13th International Conference on the Application of Accelerators in Research and Industry, Denton, Texas, 7-10 Nov. 1994.

70. "First-Principles Calculations of Ultrathin Film Structures and Properties: Challenges to Methods and Models", Invited paper, International Workshop on Electronic Structure Methods for Truly Large Systems, Braunlage Germany, 2-7 Aug. 1994.
71. "Novel Uses of the Local Density Approximation", Invited paper, Symposium on 30th Anniversary of Density Functional Theory, Cracow Poland, 13-16 June 1994.
72. "When the State of the Art Isn't Good Enough: Limits on the Rigorous Calculation of Stopping Cross Sections", Invited paper, 15th Werner Brandt Workshop on Energy Deposition Phenomena, 10-11 Mar. 1994.
73. "Energy Loss Properties of Swift Protons in Allotropic Carbon Ultra-thin Layers" Jin Zhong Wu, J. R. Sabin, SBT, and J. A. Nobel, 34th Internat. Sanibel Symposium, contributed poster, 17 Feb. 1994.
74. "Theoretical Ion Implantation Profiles for Low Energy Protons under Channeling Conditions", J.A. Nobel, J.R. Sabin, SBT, and P.M. Echenique, 34th Internat. Sanibel Symposium, contributed poster, 17 Feb. 1994.
75. "Quantum Size Effects in Hexagonal Aluminum Films", J.C. Boettger, U. Birkenheuer, N. Rösch, and SBT, 34th Internat. Sanibel Symposium, contributed poster, 17 Feb. 1994.
76. "First Principles Calculation of Stopping in Ultra-thin Films", Workshop on Electronic Energy Loss of Ions in Matter, Gmunden Austria, Invited paper, 14 July 1993.
77. "Recent Results for Ionic and Magnetic Monolayers", Workshop in Conjunction with Sonderforschungsbereich 338, Lehrstuhl für Theoretische Chemie, Technische Universität München, Garching Germany, invited lecture, 7 July 1993.
78. "Quasi-classical Simulation of Channeling in Extended Systems", J. A. Nobel, J. R. Sabin, SBT, A. Arnau, and P. Echenique, 33rd Internat. Sanibel Symposium, contributed poster, 19 Mar. 1993.
79. "Electronic Stopping Power for Protons in an LiF Monolayer and an Isolated LiF Molecule", J. Z. Wu, J. R. Sabin and SBT, 33rd Internat. Sanibel Symposium, contributed poster, 19 Mar. 1993.
80. "Density Functional Methods for Extended Systems", Host lecture, Q.T.P. Latin American Workshop, Gainesville, FL 12 Mar. 1993.
81. "Thickness-Dependent Properties of Ultra-thin Metallic Films: Predictive Calculations", Molecular Astrophysics Seminar, Max Planck Institut für Astrophysik, München, 25 May 1992.
82. "Calculation of the Electronic Properties of an Ionic Monolayer: LiF", J. Z. Wu, SBT, J. R. Sabin, and J. C. Boettger, 32nd Internat. Sanibel Symposium, contrib. paper, 20 Mar. 1992.
83. Physics Department Colloquium, Vanderbilt University, 10 Dec. 1990.

84. "Direct Kohn-Sham Theory for $n=1/2$?", Molecular Physics Seminar, Max-Planck Institut für Astrophysik, München, 16 Oct. 1990.
85. "Wave-Function versus Density-Functional Methods", Invited Panelist, South Eastern Theoretical Chemistry Assoc. Annual Meeting, 18–19 May 1990.
86. "Density Decomposition Options in the Orbital Local Plasma Approximation", D. E. Meltzer, J. R. Sabin, and SBT, 30th Internat. Sanibel Symposium, contrib. paper, 22 Mar. 1990.
87. "Structure of Hydrogen Thin Films", J. Z. Wu, J. R. Sabin, SBT, and J. C. Boettger, 30th Internat. Sanibel Symposium, contrib. paper, 22 Mar. 1990.
88. Physics Department Colloquium, Univ. of Alabama-Birmingham, 23 Feb. 1990.
89. "Orbital Local Plasma Calculation of Mean Excitation Energies and Stopping Numbers", SBT, D.E. Meltzer, and J.R. Sabin, 12th Werner Brandt Workshop on Energy Deposition and Charged Particle Penetration, 4-7 Sept. 1989, San Sebastian, Spain (invited).
90. "Central Concepts in Density Functional Theory - A Modern View", six lectures, Lehrstuhl für Theoretische Chemie, Technische Universität München, 13-22 June, 31 Oct., 7 Nov. 1989.
91. "Ground State Properties of Minimal Beryllium-Hydrogen Lamina", J. Z. Wu, S. B. Trickey, and J. C. Boettger, 29th Internat. Sanibel Symposium, contrib. paper, 7 April 1989.
92. "Calculation of Orbital Mean Excitation Energies and Stopping Cross Sections in the Local Plasma Approximation", D. E. Meltzer, J. R. Sabin, and SBT, 29th Internat. Sanibel Symposium, contrib. paper, 7 April 1989.
93. "Theoretical Properties of Hexagonal Monolayer and Dilayer Films of Lithium", J. C. Boettger and SBT, Bull Am. Phys. Soc. **34**, 720 (1989).
94. Physics Department Colloquium, Univ. of Akron, 8 Feb. 1989.
95. "Calculated Stopping Powers in Ultra-thin Films", Invited talk, Tenth Conference on Application of Accelerators in Research and Industry, Bull. Am. Phys. Soc. **33**, 1706 (1988).
96. "Pathological Behavior of the Kohn-Sham Direct Gap at a Metal-Insulator Transition", SBT and R. S. Jones, 27th Internat. Sanibel Symposium, contrib. paper, March 21, 1987.
97. "Static Quantum Size Effect in Ultra-thin Films", Molecular Physics Seminar, Max-Planck Institut für Astrophysik, München, 19 June 1986.
98. "Theoretical Confirmation of Highly Localized Electronic Surface States in Beryllium", SBT and J. C. Boettger, 26th Internat. Sanibel Symposium, contrib. paper, 14 March 1986.
99. "Density Functional Theory of the Band Gap of a Model Insulating System", R. S. Jones and SBT, Bull. Am. Phys. Soc. **31**, 302 (1986).
100. "Current Status of Density Functional Theory", Great Lakes Summer Workshop in Condensed Matter Research, 19 July 1985.

101. "Recent Research Problems in Density Functional Theory", T11/T4 Seminar, Los Alamos National Laboratory, 13 June 1985.
102. "Current Research Problems in Density Functional Theory", Seminar, Lehrstuhl für Theoretische Chemie, Technische Universität München, 14 May 1985.
103. "Correlated Wavefunctions for Crystalline Solids: Metal-Insulator Transitions in the Electron Gas", R. S. Jones and SBT, Bull. Am. Phys. Soc. **30**, 226 (1985).
104. "Avoiding Orthogonality Problems in the Application of the Alternant Molecular Orbital Method to Solids", R. S. Jones and SBT, contrib. paper 25th Internat. Sanibel Symposium, 19 March 1985.
105. "One-Electron Energies in Density Functional Theory", invited paper 25th Internat. Sanibel Symposium, 20 March 1985.
106. Physics Dept. Colloquium, Louisiana State Univ., 24 Jan. 1985.
107. Invited Speaker DOE (Energy Conversion and Utilization Technologies) Workshop on Theory and Modeling for Materials by Design, 17-19 Sept. 1984, Texas A&M Univ.
108. Invited Panelist, DOE (Council on Material Science) Policy Panel on Theory and Computer Simulation of Materials Structure and Imperfections, 6-10 August 1984, Michigan Technological Univ.
109. Materials Science and Technology (MST-5) Seminar (May 9, 1984) and Center for Materials Science Seminar (May 10, 1984), Los Alamos National Laboratory.
110. Physics Department Colloquium, Univ. of Cincinnati, Mar. 14, 1984.
111. "Electronic Properties of a Be Bilayer", J. C. Boettger, J. R. Sabin, and SBT, 24th Internat. Sanibel Symposium, contrib. paper, Mar. 8, 1984.
112. "Correlated Wavefunctions for Crystalline Solids", R. S. Jones and SBT, 24th Internat. Sanibel Symposium, contrib. paper, Mar. 6, 1984.
113. Physics Department Colloquium, Michigan Tech Univ., Jan. 12, 1984.
114. Physics Department Colloquium, Texas Tech Univ., Dec. 10, 1982.
115. Center for Materials Science Seminar, Los Alamos National Lab, Dec. 9, 1982.
116. Physics Department Colloquium, Univ. Texas at Arlington, Dec. 7. 1982.
117. "Generator Coordinate Treatment of Some Model Periodic Systems", Contributed Paper, IVth International Congress on Quantum Chemistry, Uppsala Sweden, 14-19 June 1982.
118. "Local Density Theories and Metallization in Crystalline Xenon", Contributed Paper, Conference on Local Density Approximations, Copenhagen, Denmark, 11-12 June 1982 .
119. Physics Dept. Colloquium, Michigan Technological University, 27 May 1981.

120. Physics Dept. Colloquium, Louisiana Tech Univ., 23 Oct. 1978.
121. Physics Dept. Colloquium, Univ. of Southwestern Louisiana, 13 Oct. 1978.
122. "Monte Carlo Calculations on Heavy Methane - Some Preliminary Results", Post-deadline Paper, Int'l. Conf. on Quantum Crystals, Colorado State Univ., Ft. Collins, Colo., 8-12 August 1977.
123. Physics Dept. Colloquium, Texas Tech Univ., 16 May 1977.
124. Physics Dept. Colloquium, Washington State Univ., 24 Feb. 1977.
125. Physics Dept. Colloquium, North Texas State Univ., 23 Apr. 1976.
126. Physics Dept. Colloquium, Texas A&M Univ., 22 April 1976.
127. Physics Dept. Colloquium, Rice Univ., 20 April 1976.
128. Joint Stanford-Berkeley Theoretical Chemistry Seminar, Stanford Univ. 3 March 1976.
129. Department Seminar (Dept. K32), IBM Research, San Jose, Calif., 5 Dec. 1975.
130. "Superfluid ^3He - Recent Progress in Theory and Experiment", Invited Review Lecture, International Symposium on Quantum Chemistry and Solid State Physics, Dalseter, Norway, August 30, 1975.
131. Physics Department Colloquium, Univ. of Georgia, 24 April 1975.
132. "Lattice Dynamics of Hard-Core Quantum Crystals via Point Transformation Theory", N. M. Witriol, SBT, and G. L. Morley, *Bull. Am. Phys. Soc.* **18**, 23 (1973).
133. "Energy Band Theory of the Cohesive Properties and Pair Potentials in Rare Gas Crystals", Invited Paper, Southeastern Section. Am. Phys. Soc., Birmingham. Ala., *Bull. Am. Phys. Soc.* **18**, 265 (1973).
134. "The Present Status of Computational Techniques for Molecular Structure. II. Unusual Methods", (Part I "Straightforward Methods" by J. R. Sabin). Invited Lecture, Quantum Physics Group Seminar, Redstone Arsenal, Alabama, September 20, 1972.
135. "Self-Consistent APW Calculation of the Cohesive Energy and Zero Temperature PV Relation for Solid Argon", SBT and Frank W. Averill, *Bull. Am. Phys. Soc.* **17**, 346 (1972).
136. "Lattice Dynamics of Hard-Core, Highly Anharmonic Crystals", SBT, N. M. Witriol, and G. L. Morley, Contribution to Conf. on Quantum Crystals, Banff, Canada, 6-10 Sept. 1971 (Invited Panelist).
137. "Difficulties in the $\mathbf{k} \cdot \mathbf{p}$ Method Induced by d Bands", SBT, T.J. Kuebbing, K. Schwarz, and J.B. Conklin, Jr., *Bull. Am. Phys. Soc.* **16**, 637 (1971).
138. "Temperature Dependence of Debye θ s for bcc ^3He and hcp ^4He ", E.D. Adams, P.N. Henriksen, SBT, and M.F. Panczyk, *Bull. Am. Phys. Soc.* **15**, 211 (1970).

139. "Transfer Integral Treatment of a Two-Dimensional Quantum Solid", Bull. Am. Phys. Soc. **14**, 528 (1969).
140. "Single Particle Functions in One-Dimensional Quantum Crystals", Bull. Am. Phys. Soc. **13**, 91 (1968).
141. "The Use of the Wave Functions of Double Minimum Potentials to Aid in the Determination of Structural Information", J. B. Coon, V. T. Jones, and SBT, Abstracts of the Symposium on Molecular Structure and Spectroscopy, Ohio State Univ. (Sept. 1966) , p. 67.
142. "Calculation of the Rotational Constants of Ammonia", J. B. Coon and SBT, Bull. Am. Phys. Soc. **11**, 711 (1966).

Invited Talks, Seminars, and Papers Presented (Information Technology)

1. "Emerging Roles for Information Technologies in the Contemporary, Land-Grant, State Research University", Information Technology Seminar, Univ. of Tennessee at Knoxville, Knoxville TN, 1 May 1996.
2. "Computation, Information, and Education: Interwoven but Distinct Categories", (in Spanish), Division de Estudios de Posgrado, Facultad de Química, Universidad Nacional Autónoma de México, México DF, 15 Nov. 1995.
3. "Challenges to Research Universities as Opportunities for High Performance Computing", Invited lecturer, IBM Higher Education North America, High Performance Computing Class, Cornell Theory Center, Ithaca NY, 29 Sept. 1995.
4. "Price-Performance is More Than a Number", Invited Lecture, SUPER! 1995 Annual Meeting, Univ. of Arizona, Tucson, 24 April 1995
5. "Connecting 'Them' - University Opportunities and Obligations", Invited Panelist, Southern Computer Center Directors Conference, U. Tenn.-Chattanooga, 6 April 1995.
6. "High Performance Computing in Public Universities: Trends and Implications for Policy", Utah Supercomputing Institute, Univ. of Utah, 31 Jan. 1994.

Conference and Symposium Organizing

1. Sanibel Symposium Organizer Committee (1970 - present). [Assoc. Director for Part IV in 1974 and 1977; Assoc. Director for Part III (1980-82); Assoc. Director Part II (1983); Assoc. Director Part I (1984).] See <http://www.qtp.ufl.edu/~sanibel/>
2. QTP Pam-American Workshop (with D.A. Micha); 2-day research workshop with approximately 35 Latin American participants at U. Florida March 10-11, 1993; February 8-9, 1994; February 27-28, 1997; at Universidad Nacional Autónoma de México (Cuernavaca branch), February 24-26, 1999, U. Florida Feb. 21-23, 2001; Cuernavaca MX, 17-19 Feb. 2003. See <http://www.fc.uaem.mx/CONGRESO/index.htm>

3. Group Leader, with Noam Bernstein (ONR), Jim Greer (University College, Cork Ireland), and Anatoli Korkin (Motorola) for Materials Research Society Fall 2003 meeting Symposium KK “Atomic Scale Materials Design: Modeling & Simulation” (7 oral sessions, 4 poster sessions, 142 papers).
4. Co-organizer, with John R. Sabin and chaired a Session of seven invited talks on “Atomic and Molecular Physics - Energy Loss” at the 17th International Conference on Application of Accelerators in Research and Industry, Univ. of North Texas, Denton TX, Nov. 14, 2002
5. Co-organizer, with J.R. Sabin and F.E. Dunnam, of two Sessions on Charged Particle Energy Deposition in Molecules and Materials, 16th International Conference on the Application of Accelerators in Research and Industry, Nov. 1 - 4, 2000, Univ. North Texas, Denton TX.
6. Co-Organizer (with R.J. Bartlett and J.L. Simmons), “Computational Materials Science Network Workshop On Scale-Parity, Multi-Scale Simulation of Chemo-Mechanical Processes”, St. Augustine Florida, Feb. 25-26, 2000.
7. Program Co-Chair, Southern Computer Center Directors Conference (1996 and 1997 meetings).
8. Member, Scientific Committee, Third UNAM-Cray Supercomputing Conference, August 1996, Mexico City.
9. Advisory Committee, Symposium on 30th Anniversary of Density Functional Theory, Cracow Poland, 13 - 16 June 1994.
10. Steering Committee, SUPER!, “Supercomputing for University Persons in Education and Research”, - national users group for numerically intensive computing on IBM systems 1988 - 1991; Chair 1989-90
11. Member, Organizing Committee, Great Lakes Summer Workshop in Condensed Matter Research, Michigan Technological Univ., 13 June - 29 July 1983, 9 July - 3 August 1984, 8 July - 2 August 1985, 14 July - 8 August 1986.
12. Member, Local Organizing Committee, Quantum Fluids and Solids 1983, 10-15 April 1983, Sanibel Island Florida.
13. Member, Local Organizing Committee, International Symposium on Super-heavy Elements, Texas Tech Univ., 9-11 March 1978.
14. Member of Advisory Committee, International Conference on Quantum Crystals, Colorado State University, 8-12 Aug. 1977.

Teaching

- Mini-curso, “Survey of Multi-scale Materials Simulation Techniques and Problems” Centro para la Investigación Interdisciplinaria Avanzada en Ciencias de los Materiales, Universidad de Chile and Grupo de Química Teórica Computacional, Pontificia Universidad Católica de Chile, Santiago de Chile, Nov. 7, 8, 10, 15, and 16, 2005 (in Spanish; 1:45 each session).

- “Teacher of the Year”, College of Arts and Sciences, University of Florida, 1973-1974.
- Courses Taught: General Physics (with, without Calculus), Physical Basis of Music (undergrad), Thermodynamics (undergrad), Solid State Physics (undergrad and grad), Classical Mechanics (undergrad); Quantum Mechanics of Molecules and Solids (grad); Density Functional Theory (grad). Details in separate tabulation

Supervision of Graduate and Undergraduate Students

University of Florida

Ph.D.: Wuming Zhu, August 2005.

Ph.D.: Joseph P. Worth, December 1976.

M.S. Guangyu Sun, Dec. 2001.

M.S.: Lonny Kauder, Aug. 1983.

M.S.: Glenn Bertiaux, June 1977.

M.S.: Corinne M. Lee, June 1974.

M.S.: Fred Green, May 1973.

M.S.: Edward W. Phillips, May 1973.

M.S.: Susan Magner Kuebbing (deceased), December 1971.

B.S: Greg R. Wilson (Undergraduate Research Asst. 1988–90; degree in Computer Science).

Other Current Graduate Committees

Rob Humkey (Chemistry)

Andrew Leathers (Chemistry)

Alex Pacheco (Chemistry)

Texas Tech University: None

Postdoctoral Associates

Valentin Karasiev (senior Postdoc, 2004 - 06), Krishna Muralidharan (2004 - 06), Juan Torras Costa (senior Postdoc, 2004 - 06); Wuming Zhu (2005 - 2006); J. Ashley Alford (2003 - 05); Andrew M. Kolchin (2002); Norbert Flocke (2000 - 02); Richard J. Mathar (1995 - 98); Jian Wang (1996 - 97); Steven A. Alexander (1995); Jan A. Nobel (1988 - 94); Jin Zhong Wu (1988 - 94); Gary R. Bamford (1988); David E. Meltzer (1987-90); Randall S. Jones (1982-85); Jonathan C. Boettger (1981-84); Asok K. Ray (1979-81); Joseph P. Worth (1976-77); Bernard C. Laskowski (1975-76).

University Service

1. Departmental

- Experimental Biological Physics Search, Physics Department (2003-04)
- Co-Chair, Chair Search Committee, Physics Department (Fall 2002)
- Strategy Committee, Physics Department (2000 - 2002)
- Experimental Particle-Astrophysics Search, Physics Department (Fall 2002)

- Preliminary Exam Committee, Physics Department (Fall 2000, Spring 2002, Fall 2003, Fall 2004)
- Physical Chemistry Theory Faculty Search, Chemistry Department (2000 - 2001)
- Comprehensive Exam Committee, Physics Department, [1999,1998, 1986-89 (chair 1987-88), 1980-84, 1972-75]
- Undergraduate Curriculum and Majors Committee, Physics Department (1997 - 99)
- Professorial Excellence Program Committee, Physics Department (1996 - 1997)
- Bylaws and Procedures Committee, Physics Department (1989 - 90)
- Astrophysics Faculty Search Committee, Physics Department (1988 - 90)
- Condensed Matter Theory Faculty Search Committee, Physics Department (1983 - 88)
- Hiring Planning Committee, Physics Department (1988 - 89)
- Shop Committee, Physics Department (1987 - 1989)
- Computer Committee, Physics Department (1983 - 87).
- Graduate Curriculum Committee, Physics Department (1979 - 83)
- Faculty Secretary, Physics Department (1973-75)
- Graduate Student Affairs Committee, Physics Department (1979 - 80)
- Computer Committee, Quantum Theory Project (1980 - 1982; 1993 - present)
- Library Committee, Quantum Theory Project (1979 - 1981)

2. College

- Mathematical Sciences Committee, College of Liberal Arts and Sciences (2004 - present)
- Committee on Computational Sciences Curriculum [Chair], College of Liberal Arts and Sciences (2004 - present)
- High-Performance Computing Committee, College of Liberal Arts and Sciences (2003 - present)
- Steering Committee for Networked Writing Environment, College of Liberal Arts and Sciences (1997 - 1999)
- Steering Committee, Imaging Systems Sciences and Technologies Center Development (1996 - 1999)
- Graduate Fellowship Committee, College of Liberal Arts and Sciences (1980-81).
- Nominating Committee, College of Arts and Sciences (1973-74).
- Minority Concerns Committee, College of Arts and Sciences (1972-73).

3. University

- High Performance Computing Committee (2001 - present)
- Faculty Senate Committee on Structure and Effectiveness (2003)
- Faculty Senate (2001-03, 1988 - 90, 1981 - 83, 1972 - 74)

- University Council on Information Technologies and Services, (1991 - 1996; first Chair, 1991 - 1994)
- Policy Board, Northeast Regional Data Center of the State Univ. System of Florida (Vice Chair, 1992 - 1996)
- Southeastern Universities Research Association ad hoc CIO's Committee on Future Networking (1995 - 96)
- University Research Computing Initiative Committee, Chair (1990 - 1991)
- University Advisory Council on Telecommunications and Computing (1988 - 1991; succeeded in 1991 by Council on Information Technologies and Services; see above)
- University Committee on Technical Issues in Computing and Telecommunications (1989 - 1990)
- Technical Executive Committee, MicrofabritechTM (1988 - 90)
- Instruction & Research Computer Users Committee for Northeast Regional Data Center, ex-officio (1986 - 1990)
- Southeastern Universities Research Association Networking Committee, Univ. Florida rep. (1985 - 1990)
- Florida State University Computer Center Allocations subcommittee, U. Florida representative (1985 - 1990)
- Academic Research Computing Committee (1985-1988; discontinued in 1988 in favor of University Advisory Council on Telecommunications and Computing, see above).
- Academic Affiliates, Pittsburgh Supercomputer Center, Univ. Florida alternate (1986 - 1990)
- University Ad-hoc Task Force on Advanced Computing, Chair (1983-1985).
- Chair, Program Coordinator Search Committee, Interdisciplinary Center for Biotechnology Research (1988)
- University Committee on Professional Relations and Standards (1974 - 75)
- University Ad Hoc Committee on Fixed Terms for Administrators (1974-75).

4. Board of Regents

- Committee on Distance Education (1995 - 96)

Grants and Contracts

University of Florida

Visiting Professor proposal to Agència de Gestió d'Adjuts Universitaris i de Recerca (Agency for Supervision of Aid to Universities and Research Centers, Province of Catalunya, Spain), "Sol·licitud Professors i investigadors vistant a Catalunya (PIV)", Joan ("Juan") Torras Costa and S.B. Trickey; travel and displacement expenses for 90 days for SBT to visit Universitat Politècnica de Catalunya in 2007 in support of new algorithm development for ν -GTOFF code (submitted 06 March 2006)

US National Science Foundation CNS-0421200, \$600,000 (plus \$254,000 Univ. Florida matching) (July 2004 -June 2006) “Acquisition of CASTOR: A High-performance Communications and Storage Backbone for Data-Intensive Scientific and Engineering Computing,” S. Ranka PI, P. Avery, A. George, Y. Sheng, and S.B. Trickey co-PIs

US Office of Naval Research N00014-04-1-0256, \$15,525 for 1 year, (Jan. - Dec. 2004); “Partial Support of 2004 Sanibel Symposium,” S.B. Trickey and J.L. Krause, co-PIs

US Army Research Office DAAD19-03-1-0365, \$28,000 for 2 years (Aug. 2003 - July 2005); “Partial Support of 2004 Sanibel Symposium: Participation by Younger Investigators in Nanoscience and Surface Sciences”, S.B. Trickey and J.L. Krause, co-PIs

US National Science Foundation DMR-0325553, \$2,500,000 for 4 years (Sept 2003 - Aug. 2007) “ITR: Science and Software for Predictive Simulation of Chemo-mechanical Phenomena in Real Materials ,” R.J. Bartlett PI, Hai-Ping Cheng and S.B. Trickey, co-PIs.

US National Science Foundation DMR-0218957 \$448,000 for 4 years (July 2002 - June 2006 + one year no-cost extension) “ITR: Large-scale, Grid-enabled Gaussian Orbital Implementation of Current Density and Spin Density Functional Theory for Ordered Systems,” S.B. Trickey PI.

US Dept. of Energy (via Oak Ridge National Lab) UPN 02032918 \$6,000 for 1 year; “Support of Sanibel Symposium,” N.Y. Öhrn and S.B. Trickey co-PIs.

NPACI Advanced Computing Resources UFL-206 (2001-02): 5000 units on U. Michigan SP system for support of KDI award below. S.B. Trickey PI.

US National Science Foundation DMR-0076329 (2000-01) \$80,000 (plus \$77,200 Univ. Florida match) “Acquisition of Semi-immersive Virtual Reality Instrumentation for Multi-scale Materials Research and Education”, S.B. Trickey PI, H-P. Cheng, J.L. Krause, C.J. Stanton, and M.C. Zerner co-PIs.

US NSF KDI(DMR)-9980015 (1999-2003) \$2,200,001 “Multi-scale Simulation Including Chemical Reactivity of Materials Behavior through Integrated Computational Hierarchy”, R.J. Bartlett, PI, H-P. Cheng, J.H. Simmons, S.B. Trickey, and M.C. Zerner, co-PIs

US Dept. of Energy AO-1247 (Ames Laboratory) (2000) \$12,000, “Travel Support for DOE Computational Materials Science Network Workshop On Scale-Parity, Multi-Scale Simulation of Chemo-Mechanical Processes”, S.B. Trickey.

US Army Research Office Renewal DAA H04-95-1-0326 [33605 PH] (1995–99), \$360,000 “Energy Deposition and Ion Implantation: Predictive Calculations of Channeling and Stopping for Technologically Important Materials Systems”, Co-Principal Investigators: J.R. Sabin and S.B. Trickey.

IBM Corporation Shared University Research Award (1995-96), \$732,800 (equipment at list value) “Visualization and Imaging Across the Disciplines”, Principal Investigator and coordinator (8 groups in 7 colleges): S.B. Trickey.

US Army Research Office, Travel award, \$600, invited lecture at 19th Internat. Workshop on Condensed Matter Theories, Caracas Venezuela, 12-16 June 1995.

IBM Corporation Shared University Research Award (1994-95), \$992,000 (equipment at list value) “Technology for Teaching of High Quality Writing”, Co-Principal Investigators: Michael Conlon and S. B. Trickey.

National Science Foundation CHE-900993, (June 1993) \$118,000 “Instrumentation Proposal - Quantum Chemical Visualization Systems”, Co-Principal Investigators: N.Y. Öhrn, S.B. Trickey, and E. Deumens. (Univ. Florida match: \$79,000)

Digital Equipment Corporation: “Loan of DEC Alpha-AXP System for Porting of QTP Codes”, 1992-93, S.B. Trickey and E. Deumens.

US Army Research Office DAA L03-91-G-0119 (1991-94), \$300,000, “Theoretical and Numerical Prediction of Stopping Properties of Counterpart Thin Films and Solids: A Renewal Proposal”, Co-Principal Investigators: J.R. Sabin and S.B. Trickey.

SUN Microsystems Inc. (August, 1990) \$278,000 (equipment at academic discount value) “Support of Meritorious Research in Quantum Theory Project”, S.B. Trickey and E. Deumens.

DARPA Defense Sciences Office (1988-90) \$120,104, “Computational Characterization of Prototype Interfacial Structures”, Co-Principal Investigators: S.B. Trickey and J.R. Sabin.

IBM Corp. (1988) \$331,252 (\$80,000 cash, \$251,252 equipment valued at academic discount) “Performance Enhancements of Numerically Intensive Codes on the IBM-3090 +VF”, S.B. Trickey P.I., R.L. Coldwell, E. Deumens, G.D. Purvis III, and M.C. Zerner co-PIs.

US Army Research Office, DAA L03-87-K-0046 (1986-1990) \$331,928 “Theoretical and Numerical Prediction of Stopping Properties of Counterpart Thin Films and Solids”, Co-Principal Investigators: J.R. Sabin and S.B. Trickey.

National Science Foundation CHE86-17036 (1987-8) \$230,000 “Purchase of a Mini Computer”, S.B. Trickey on behalf of members of Quantum Theory Project (University of Florida match: \$352,000).

National Science Foundation, NCR-8615061 (1986) \$20,000, “Connection to SURAnet”, Co-Principal Investigators: S.B. Trickey, G.W. Hemp and G.D. Purvis III.

Division of Sponsored Research, UF, Grant Prospect Support (1986) \$24,738 “A Theoretical Description of the Stopping of Swift Particles by Materials Foils”, Co-Principal Investigators: J.R. Sabin and S.B. Trickey.

NSF DMR8218498 (1983-86) \$197,400, “Quantum Theory of Solids and Molecules”, Co-Principal Investigators: S.B. Trickey and J.R. Sabin.

NSF CHE84-02203 \$11,255 “Symposium on Impact of Computers on Quantum Theory of Matter”, Sanibel Symposia 1984, S. B. Trickey and N. Y. Öhrn.

NSF CHE83-04837 \$5,470, “Symposium on Impact of Computers on Computational Quantum Chemistry”, Sanibel Symposia 1983, S.B. Trickey and N.Y. Öhrn.

“Microcomputer for Research in Chemical Physics”, Digital Equipment Corp. donation of PDP11/34A configuration, discounted value \$18,365 (1982), S.B. Trickey.

Division of Sponsored Research, U.Florida, Seed Money Grant (1980-81) \$1,600 “Rotational Ordering in Molecular Crystals”, S.B. Trickey.

NSF DMR79-09721 (1980-82) \$195,200 “Quantum Theory of Solids and Molecules”, Co-Principal Investigators: J.R. Sabin and S.B. Trickey.

NSF/AFOSR , \$8,700 “1977 Sanibel Symposium on Quantum Crystals and Quantum Fluids”, E.D. Adams, J.W. Dufty, and S.B. Trickey.

Research Corporation (1973-76) \$9,800 “One-Electron Theory of Phonon Dispersion in Rare Gas Crystals”, S.B. Trickey.

NSF DMR76-84577 (1977-78) \$139,000 “Quantum Theory of Solids and Molecules”, Co-Principal Investigators: S.B. Trickey and J.R. Sabin (Connolly on leave).

NSF DMR71-01775 A02 (Formerly GH 32006) “Quantum Theory of Molecules and Solids”, Initial Grant: (1972-73) \$107,100; Principal Investigator: J. C. Slater ; Co-Investigators: J.W.D. Connolly,

J.B. Conklin, S.B. Trickey. Amendment (1974-75) \$135,000; Added J.R. Sabin, dropped J.B. Conklin as Co-Investigators. Amendment (1976-77) \$108,000; Co-Principal Investigators: Connolly, Sabin, and Trickey.

Texas Tech University

NSF (1978) “International Symposium on Superheavy Elements”, M. A. K. Lodhi and S. B. Trickey, \$2,000.

Other Professional Service

- Scientific Oversight Committee for Computational Materials Science Network, U.S. Department of Energy, 2003-present
- Nominating Committee, Division of Computational Physics, American Physical Society (2003-06; Chair 2004-06)
- INCITE (“Innovative and Novel Computational Impact on Theory and Experiment”) Review Panel, U.S. Department of Energy, Sept. 13-14, 2005
- Site Reviewer, U.S. National Science Foundation [Div. Materials Research]: CalTech Center for Science and Engineering of Materials, Jan. 27-28, 2004; Materials Research Group Review Panel, Brookhaven National Laboratory (16 - 17 July 1992).
- Proposal reviewer (typically 4 to 6 per year):
 - U.S. National Science Foundation: Div. of Materials Research, Div. of Chemistry, Directorate for Computer and Information Science and Engineering
 - U.S. Army Research Office, Division of Physics
 - U.S. Department of Energy, Basic Energy Sciences Division
 - Petroleum Research Fund of American Chemical Society.
 - Research Corporation
 - Pittsburgh Supercomputer Center
 - National Science and Engineering Research Council (Canada)
- Reviewer for: *Physical Review Letters*, *Physical Review A* and *B*, *Journal of Chemical Physics*, *Computer Physics Communications*, *Surface Science*, *Modern Physics Letters B*, *Chemical Physics*, *Chemical Physics Letters*, *American Journal of Physics*, *Europhysics Letters*, *Journal of Physical Chemistry*, *International Journal of Quantum Chemistry*
- Coalition for Advanced Scientific Computing (formerly, Coalition for Academic Scientific Computing, Coalition of Academic Supercomputing Centers), Strategy Committee (1994 - 1996); wrote and/or edited twelve CASC one-page legislative hand-outs on role of high-performance computing in academe.
- IBM Higher Education Customer Advisory Council (1994 - 1996)

- Steering Committee, SUPER! (“Supercomputing for University Persons in Education and Research”, national users group for numerically intensive computing on IBM systems) 1988 - 1991; Chair 1989 - 1990.
- Site Reviewer, Minnesota Supercomputer Institute [team selected by U. Minn. Vice President for Research] (22 - 24 June 1993).
- Miembro de Tribunal de Juzgar Tesis Doctoral, Facultad de Ciencias, Universidad de Valladolid (Spain). Declared by the University as having the credentials of “Catedrático de Teoría Cuántica”; private and public exam of the student in Spanish, Jan. 1996.
- Gutachter Im Habilitationsverfahren, Technische Universität Wien (Austria), Technische Universität München (Germany); theses in German, reports in English.
- Tenure and Promotion Referee: Penn. State Univ., Rutgers Univ., Univ. of Missouri (Columbia), Tulane Univ., Mich. Tech. Univ., Montana State Univ., Univ. Texas at Arlington, Univ. N. Florida

Contributions to Life of the Wider Community

- Immediate Past President, Board of Directors, National Farm Worker Ministry (President, 2001 - 2004); previously Vice President and Treasurer, Board member for more than 20 years. present).
- Volunteer, Interfaith Hospital Network (current).
- Co-founder, Alachua County Organization for Rural Needs (ACORN Clinic).
- Principal donor (1999) and curator (current) of historic pipe organ (Johnson and Son, Opus 756, 1891) and sponsor (current) of annual organ recital series, Westminster Presbyterian Church, Gainesville.
- Commodore, Gulf Atlantic Yacht Club, Gainesville (2004 - 2006); previously Vice Commodore (2001 - 2004), Secretary (1999-2001), Race Committee Chair (1997-1999).