Curriculum Vitae
Samuel B. Trickey
Current as of: 15 March 2025

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, Univ. of Florida, Jan. 1981 - June 2005
  Emeritus July 2005 - present
- Professor of Physics, Univ. of Florida, Aug. 1979 - Jan. 1981.
- Professor of Physics, Texas Tech Univ., Aug. 1977 - July 1979.
- Associate Professor of Physics, Univ. of Florida, July 1973 - July 1977.
- Assistant Professor of Physics, Univ. of Florida, Sept. 1968 - June 1973.
- NASA PreDoctoral trainee, Texas A&M Univ., Sept. 1965 - Aug. 1968.
- Scientist, Development Group, Mason & Hanger-Silas Mason Corp, Amarillo TX
  June 1962 - June 1964.

B. Administrative

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

- Acting Director of Space Resources, College of Liberal Arts and Sciences, Univ. of Florida, August 1986 - Nov. 1987.

- Chair, Dept. of Physics and Engineering Physics, Texas Tech Univ., August 1977 - July 1979.

C. Other

- Senior Fellow, Long Program in Computational Methods in High Energy Density Plasmas, Institute of Pure and Applied Mathematics, Univ. California Los Angeles, March - June 2012.

- Consultant, Theoretical Division, Los Alamos National Laboratory, 1984 - 1994; Research Collaborator 1994 - 2000 (T-Divsion) and 2001 - 2011 (X-Dvision)

- Foreign Collaborator, Institut für Physikalische und Theoretische Chemie, Technische Universität München; 1998 - 2013

- 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, and member, Comité Internacional de Evaluación, Programa de Investigación de Media Plaza en Simulación Molecular, Instituto Mexicano del Petróleo; 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.

- Profesor Catedrático de Teoría Cúantica (visiting), Universidad de Valladolid (Spain), Jan. 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 CA), 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.

Professional Society Memberships and Honors

- American Physical Society Fellow (1980).
- American Physical Society Outstanding Referee (2012).
- Miembro Correspondiente, Academia Mexicana de Ciencias (2016).
- National Society of Hispanic Physicists (life member).
- Materials Research Society.

Honor Societies

- Phi Kappa Phi, Sigma Xi, Sigma Pi Sigma.

Publications

A. Refereed:

1. "DFT-MD, KS, and OF", Mohan Chen, Aurora Pribram-Jones, François Soubiran, and S.B. Trickey, Chapter 2 of *Warm Dense Matter Roadmap*, Frank Graziani, David Riley, and Jan Vorberger, eds., in preparation for Plasma Physics and Controlled Fusion (invited).
2. "Uniform Electron Gas", Tobias Dornheim, Valentin Karasiev, Shigenori Tanaka, and S.B. Trickey, Chapter 14 of *Warm Dense Matter Roadmap*, Frank Graziani, David Riley, and Jan Vorberger, eds., in preparation for Plasma Physics and Controlled Fusion (invited).
3. "Performance Improvement of a De-orbitalized Exchange-Correlation Functional", Héctor Francisco R., Bishal Thapa, S.B. Trickey, and A.C. Cancio, in preparation for Comput. Mat. Sci.
4. "Fully thermal meta-GGA exchange-correlation free-energy density functional", K. Hilleke, V.V. Karasiev, S.B. Trickey, R.M.N. Gosshadze, and S. Hu, Phys. Rev. Mat. submitted 17 Jan. 2025.
5. "Discovery of Spin-crossover Candidates with Equivariant Graph Neural Networks and Relevance-based Classification", Angel Albavera-Mata, Pawan Prakash, Jason B. Gibson, Eric Fonseca, Sijin Ren, Xiaoguang Zhang, Hai-Ping Cheng, Michael Shatruk, S.B. Trickey, and Richard G. Hennig, J. Chem. Th. Comput. submitted 10 Dec. 2024, revised submitted 05 Feb. 2025.
6. "Free-energy OFDFT: Recent developments, perspective, and outlook", V.V. Karasiev, Katerina Hilleke and S.B. Trickey, (invited) Electr. Struct. **7**, 013001 (2025); doi:10.1088/2516-1075/adadd4
7. "Magnetic and Thermochemical Properties of Supramolecular Assemblies as Archetypes of Quantum Materials", Angel Albavera-Mata, Shuanglong Liu, Hai-Ping Cheng, Richard G. Hennig, and S.B. Trickey, J. Phys. Chem. A, **128**, 10929 (2024) doi: 10.1021/acs.jpca.4c06723
8. "Removing Orbital Dependence to Improve Exchange-Correlation Functional Accuracy", Héctor Francisco R., A.C. Cancio, and S.B. Trickey, J. Phys. Chem. A, submitted 17 June 2024.
9. "Effective Wang-Teter Kernels for Orbital-free DFT Simulations", Valeria Rios-Vargas, Xuecheng Shao, S.B. Trickey, and Michele Pavanello, Phys. Rev. B, **110**, 085129 (2024)
10. "Reworking the Tao-Mo Exchange-correlation Functional: III. Improved de-orbitalization strategy and faithful de-orbitalization", Héctor Francisco R., A.C. Cancio, and S.B. Trickey, J. Phys. Chem. A, **128**, 6010 (2024) doi:10.1021/acs.jcpa.4c02635
11. "Reworking the Tao-Mo exchange-correlation functional. I: Reconsideration and Simplification", Héctor Francisco R., A.C. Cancio, and S.B. Trickey, J. Chem. Phys. **159**, 214102 [9 pp] (2023).
12. "Reworking the Tao-Mo exchange-correlation functional. II: Deorbitalization", Héctor Francisco R., A.C. Cancio, and S.B. Trickey, J. Chem. Phys. **159**, 214103 [12 pp] (2023).

13. "Transition Temperature for Spin-crossover with the Mean Value Ensemble Hubbard-U Correction", Angel Albavera Mata, Richard G. Hennig, and S.B. Trickey, J. Phys. Chem. A, **127**, 7646-7654 (2023).
14. "Orbital-Free Density Functional Theory: An attractive electronic structure method for large-scale first-principles simulations", Wenhui Mi, Kai Luo, S.B. Trickey, and Michele Pavanello, Chemical Reviews **123**, 12039-12104 (2023) DOI: 10.1021/acs.chemrev.2c00758 (solicited review).
15. "Mean Value Ensemble Hubbard U Correction for Spin-Crossover Molecules", Angel Albavera Mata, S.B. Trickey, and Richard G. Hennig, J. Phys. Chem. Lett. **13**, 12049-12054 (2022).
16. "High-temperature Self-energy Correction to X-ray Aabsorption Spectra", Tun S. Tan, J. Kas, S.B. Trickey, and J.J. Rehr, Phys. Rev. B **117**, 115122 (2023); arXiv 2208.02930.
17. "Some Problems in Density Functional Theory", Jeffrey Wrighton, A. Albavera Mata, H. Francisco Rodríguez, Tun Sheng Tan, Antonio C. Cancio, James W. Dufty, and S.B. Trickey, Lett. Math. Phys. **113**, 41 [25 pp] (2023).
18. "All-electron APW+lo Calculations of Magnetic Molecules with the SIRIUS Domain-specific Package", Long Zhang, Anton Kozhevnikov, Thomas Schulthess, S.B. Trickey, and Hai-Ping Cheng, J. Chem. Phys. **158** 234801 [13 pp] (2023).
19. "Hardness of Molecules and Bandgap of Solids from a Generalized Gradient Approximation Exchange Energy Functional", J. Carmona-Espíndola, A. Flores, J.L. Gázquez, A. Vela, and S.B. Trickey., J. Chem. Phys. **157**, 114109 [8 pp] (2022).
20. "Dipole Switching by Intramolecular Electron Transfer in Single- Molecule Magnetic Complex [Mn12O12(O2CR)16(H2O)4]", Dmitry Skachkov, Shuang-Long Liu, Jia Chen, George Christou, Arthur Hebard, Xiao-Guang Zhang, S.B. Trickey, and Hai-Ping Cheng, J. Phys. Chem. A, **126**, 5265-5272 (2022) https://doi.org/10.1021/acs.jpca.2c02585.
21. "DFT Exchange: Sharing Perspectives on the Workhorse of Quantum Chemistry and Materials Science", Andrew M. Teale, Trygve Helgaker, Andreas Savin, Carlo Adamo, Ba´lint Aradi, Alexei V. Arbuznikov, Paul W. Ayers, Evert Jan Baerends, Vincenzo Barone, Patrizia Calaminici, Eric Cancés, Emily A. Carter, Pratim Kumar Chattaraj, Henry Chermette, Ilaria Ciofini, T. Daniel Crawford, Frank De Proft, John F. Dobson, Claudia Draxl, Thomas Frauenheim, Emmanuel Fromager, Patricio Fuentealba, Laura Gagliardi, Giulia Galli, Jiali Gao, Paul Geerlings, Nikitas Gidopoulos, Peter M. W. Gill, Paola Gori-Giorgi, Andreas Görling, Tim Gould, Stefan Grimme, Oleg Gritsenko, Hans Jørgen Aagaard Jensen, Erin R. Johnson, Robert O. Jones, Martin Kaupp, Andreas M. Kóster, Leeor Kronik, Anna I. Krylov, Simen Kvaal, Andre Laestadius, Mel Levy, Mathieu Lewin, Shubin Liu,apaq Pierre-François Loos, Neepa T. Maitra, Frank Neese, John P. Perdew, Katarzyna Pernal, Pascal Pernot, Piotr Piecuch, Elisa Rebolini, Lucia Reining, Pina Romaniello, Adrienn Ruzsinszky, Dennis R. Salahub, Matthias Scheffler, Peter Schwerdtfeger, Viktor N. Staroverov, Jianwei Sun, Erik Tellgren, David J. Tozer, Samuel B. Trickey, Carsten A. Ullrich, Alberto Vela, Giovanni Vignale, Tomasz A. Wesolowski, Xin Xu and Weitao Yang, Phys. Chem. Chem. Phys. published (online) 10 Aug. 2022, doi=10.1039/d2cp02827a .
22. "Matters arising: On the Liquid-liquid Phase Transition of Dense Hydrogen", Valentin V. Karasiev, Joshua Hinz, S. X. Hu, and S.B. Trickey, Nature **600**, E12-E14 (2021).

23. "Barriers to Predictive High-throughput Screening for Spin-crossover", Daniel Mejía-Rodríguez, Angel Albavera-Mata, Eric Fonseca, Dianteng Chen, H-P. Cheng, Richard G. Hennig and S.B. Trickey, Comput. Mat. Sci. **206**, 111161 [13 pp] (2022).
24. "Performance Enhancement of APW+*lo* calculations by Simplest Separation of Concerns", Long Zhang, Anton Kozhevnikov, Thomas Schulthess, Hai-Ping Cheng, and S.B. Trickey, Computation **10**, 43 [18 pp] (2022.).
25. "Variational Properties of Auxiliary Density Functionals", Daniel Mejía Rodríguez and S.B. Trickey, Theor. Chem. Acc. **140**, 37 [9 pp] (2021) (invited paper for deMon2k Topical volume).
26. "Spin-Crossover From a Well-Behaved, Low-Cost meta-GGA Density Functional", Daniel Mejía Rodríguez and S.B. Trickey, J. Phys. Chem. A **124**, 9889-9894 (2020); arXiv 2009.07808.
27. "Two-temperature warm dense hydrogen simulation with quantum protons driven by orbital-free density functional theory electrons", Dongdong Kang, Kai Luo, Keith Runge, and S.B. Trickey, Matter Rad. Extremes **5**, 064403 [12 pp] (2020).
28. "Meta-GGA Performance in Solids at Almost GGA Cost", Daniel Mejía Rodríguez and S.B. Trickey, Phys. Rev. B **102**, 121109(R) [4 pp] (2020).
29. "Fully Consistent DFT Determination of the Insulator-Metal Transition Boundary in Warm Dense Hydrogen", Joshua Hinz, Valentin V. Karasiev, S.X. Hu, Mohamed Zaghoo, Daniel Mejía-Rodríguez, S.B. Trickey, and L. Calderín, Phys. Rev. Research **2**, 032065(R) [7 pp] (2020).
30. "Generalized Gradient Approximations with Local Parameters", Angel Albavera-Mata, Karla Botello-Mancilla, S.B. Trickey, J.L. Gázquez, and Alberto Vela, Phys. Rev. B **102**, 035129 [11 pp] (2020).
31. "Towards accurate orbital-free simulations: a generalized gradient approximation for the non-interacting free-energy density functional", K. Luo, V.V. Karasiev, and S.B. Trickey, Phys. Rev. B **101**, 075116 [9 pp] (2020); arXiv 2001.10602 .
32. "Negative electron affinities and derivative discontinuity contribution from a generalized gradient approximation exchange functional", Javier Carmona-Espíndola, José L. Gázquez, Alberto Vela, and S.B. Trickey, J. Phys. Chem. A (invited paper),**124**, 1334-1342 (2020); DOI: 10.1021/acs.jpca.9b1095.
33. "Comment on 'Regularized SCAN functional' [J. Chem. Phys. **150**, 161101 (2019)]", Daniel Mejía-Rodríguez and S.B. Trickey,J. Chem. Phys. **151**, 207101 [2 pp] (2019).
34. "Analysis of Over-magnetization of Elemental Transition Metal Solids from the SCAN Density Functional", Daniel Mejía-Rodríguez and S.B. Trickey, Phys. Rev. B **100**, 041113(R) [5 pp] (2019).
35. "Status of Free-energy Representations for the Homogeneous Electron Gas", V.V. Karasiev, S.B. Trickey, and J.W. Dufty, Phys. Rev. B **99**, 195134 [8 pp] (2019).
36. "Generalized Gradient Approximation Exchange Functional with Near- best-meta-GGA Performance" Javier Carmona-Espíndola, José L. Gázquez, Alberto Vela, and S.B. Trickey, J. Chem. Theory Comput. **15**, 303-310 (2019)].
37. "A Simple Generalized Gradient Approximation for the Non-interacting Kinetic Energy Density Functional", K. Luo, V.V. Karasiev, and S.B.Trickey, Phys. Rev. B **98**, 041111(R) [5 pp] (2018); arXiv 1806.05205.

38. "Deorbitalized meta-GGA Exchange-Correlation Functionals in Solids", D. Mejía-Rodríguez and S.B. Trickey, Phys. Rev. B **98**, 115161 [9 p] (2018); arXiv 1807.09216.

39. "Density Response from Kinetic Theory and Time Dependent Density Functional Theory for Matter Under Extreme Conditions", James Dufty, Kai Luo, and S.B. Trickey, Phys. Rev. E **98**, 033203 (2018); arXiv 1805.06509.

40. "Nonempirical Semi-local Free-Energy Density Functional for Matter Under Extreme Conditions", Valentin V. Karasiev, James W. Dufty, and S.B. Trickey, Phys. Rev. Lett. **120**, 076401 (2018); arXiv 1612.06266v3.

41. "Trivial Constraints on Orbital-free Kinetic Energy Density Functionals", Kai Luo and S.B. Trickey, Chem. Phys. Lett. **695**, 190 (2018); arXiv 1711.04014v2.

42. "On the Kubo-Greenwood Model for Electron Conductivity", J. Dufty, J. Wrighton, K. Luo, and S.B. Trickey, Contrib. Plasma Phys. **58**, 150-154 (2018); arXiv 1709.04732.

43. "Long-Range Exchange Limit and Dispersion in Pure Silica Zeolites", Angel M. Albavera-Mata, Claudio M. Zicovich-Wilson, J.L. Gázquez, S.B. Trickey, and Alberto Vela, Theor. Chem. Acc. **137**, 26 (2018).

44. "Deorbitalization Strategies for meta-GGA Exchange-Correlation Functionals", D. Mejía-Rodríguez and S.B. Trickey, Phys. Rev. A **96**, 052512 [10 pp] (2017); arXiv 1710.06032.

45. "Accurate Anisotropic Gaussian Type Orbital Basis Sets for Atoms in Strong Magnetic Fields", Wuming Zhu and S.B. Trickey, J. Chem. Phys. **147**, 244108 [11 pp] (2017) [arXiv 1709.05553].

46. "Kubo-Greenwood Electrical Conductivity Formulation and Implementation for Projector Augmented Wave Datasets", L. Calderín, V.V. Karasiev, and S.B. Trickey, Comput. Phys. Commun. **221**, 118-142 (2017) [arXiv 1707.08437].

47. "Random Phase Approximation with Second-order Screened Exchange as a Practical Current Density Functional", Wuming Zhu, Liang Zhang, and S.B. Trickey, J. Chem. Phys. **145**, 224106 [9 pp] (2016).

48. "Temperature Effects in Static and Dynamic Polarizabilities from Distinct Generalized Gradient Approximation Exchange-correlation Energy Functionals", J. Carmona-Espíndola, J.L. Gázquez, A. Vela, and S.B. Trickey, Chem. Phys. Lett. **664**, 77–82 (2016).

49. "Importance of Finite-temperature Exchange-correlation for Warm Dense Matter Calculations" Valentin V. Karasiev, Lázaro Calderín, and S.B. Trickey, Phys. Rev. E **93**, 063207 [12 pp] (2016).

50. "A PW91-like Exchange with a Simple Analytical Form", J.C. Pacheco-Kato, J.M. del Campo, J.L. Gázquez, S.B. Trickey, and A. Vela, Chem. Phys. Lett. **651**, 268-273 (2016).

51. "Unexpected Cold Curve Sensitivity to GGA Exchange Form", S.B. Trickey, Theoret. Chem. Acc. (A. Vela Festschrift) **135**, 219 [7 pp] (2016).

52. "Revised Thomas-Fermi Functional for Singular Potentials", J.W. Dufty and S.B. Trickey, Phys. Rev. B. **94**, 075158 [9 pp] (2016).

53. "Global Hybrid Exchange Energy Functional with Correct Asymptotic Behavior of the Corresponding Potential", J. Carmona-Espíndola, J.L. Gázquez, A. Vela, and S.B. Trickey, Theoret. Chem. Acc. **135**, 120 [10 pp] (2016).

54. "Finite Temperature Scaling in Density Functional Theory", J.W. Dufty and S.B. Trickey, Mol. Phys. **114**, 988-996 (2016); DOI: 10.1080/00268976.2015.1122844.
55. "Comment on 'Single-point kinetic energy density functionals: a pointwise kinetic energy density analysis and numerical convergence investigation' ", S.B. Trickey, Valentin V. Karasiev and Debajit Chakraborty, Phys. Rev. B **92**, 117101 [3 pp](2015).
56. "Frank Discussion of the Status of Ground-state Orbital-free DFT", V.V. Karasiev and S.B. Trickey, Adv. Quantum Chem. (Frank Harris Workshop volume) **71**, 221-245 (2015).
57. "PUPIL: a Software Integration System for Multi-scale QM/MM-MD Simulation and its Application to Biomolecular Systems", J. Torras, B.P. Roberts, G.M. Seabra, and S.B. Trickey, invited review for Adv. Protein Chem. and Struct. Biology, Tatyana Karabencheva-Christova ed. Vol. 100 (Burlington: Academic Press, 2015), pp. 1-31.
58. "Generalized Gradient Approximation Exchange Energy Functional with Correct Asymptotic Behavior of the Corresponding Potential", J. Carmona-Espíndola, J.L. Gázquez, A. Vela, and S.B. Trickey, J. Chem. Phys. **142**, 054105 [13 pp] (2015).
59. "Improved Analytical Representation of Combinations of Fermi-Dirac integrals for Finite-temperature Density Functional Calculations", V.V. Karasiev, D. Chakraborty, and S.B. Trickey, Comput. Phys. Commun., **192**, 114-123 (2015).
60. "Finite-temperature Orbital-free DFT Molecular Dynamics: Coupling PROFESS and Quantum Espresso", V.V. Karasiev, T. Sjostrom, and S.B. Trickey, Computer Phys. Commun. **185**, 3240-3249 (2014).
61. "Accurate Homogeneous Electron Gas Exchange-correlation Free Energy for Local Spin-density Calculations", V.V. Karasiev, T. Sjostrom, J. Dufty, and S.B. Trickey, Phys. Rev. Lett. **112**, 076403 [5 pp] (2014).
62. "Comparative Studies of Density Functional Approximations for Light Atoms in Strong Magnetic Fields", W. Zhu, L. Zhang, and S.B. Trickey, Phys. Rev. A **90** 022504 [14 pp] (2014).
63. "Non-empirical Generalized Gradient Approximation Free Energy Functional for Orbital-free Simulations", V.V. Karasiev, D. Chakraborty, O.A. Shukruto, and S.B. Trickey, Phys. Rev. B **88**, 161108(R) [5 pp] (2013). Rapid Communication.
64. "Progress on New Approaches to Old Ideas: Orbital-free Density Functional Theory", V.V. Karasiev, D. Chakraborty, and S.B. Trickey, Chapter in *Many-electron Approaches in Physics, Chemistry, and Mathematics: A Multidisciplinary View*, L. Delle Site and V. Bach eds. (Springer, Heidelberg, 2014) 113-134.
65. "Innovations in Finite-Temperature Density Functionals", V.V. Karasiev, D. Chakraborty, J.W. Dufty, F.E. Harris, K. Runge, and S.B. Trickey, in *Frontiers and Challenges in Warm Dense Matter*, F. Graziani *et al.* eds. (Springer Verlag, Heidelberg, 2014) 61-85.
66. "Explicit Particle-number Dependence in Density Functional Theory" S.B. Trickey and A. Vela, J. Mex. Chem. Soc., **57**, 105-110 (2013).
67. "Analysis of the Generalized Gradient Approximation for the Exchange Energy", J. Martín del Campo, J.L. Gázquez, R.J. Alvarez-Mendez, S.B. Trickey, and A. Vela, for *Concepts and Methods in Modern Theoretical Chemistry, Volume 1*, in honor of in honor of Professor B.M. Deb,, S.K. Ghosh and P.K. Chattaraj, eds. (CRC Press, Boca Raton Florida USA, 2013) 295-311.

68. "Comparison of Density Functional Approximations and Finite-temperature Hartree-Fock Approxiation in Warm Dense Lithium", V.V. Karasiev, T. Sjostrom, and S.B. Trickey, Phys. Rev. E **86**, 056704 [12 pp] (2012)

69. "Generalized Gradient Approximation Non-interacting Free Energy Functionals for Orbital-free Density Functional Calculations", V.V. Karasiev, T. Sjostrom, and S.B. Trickey, Phys. Rev. B, **86**, 115101 [11 pp] (2012).

70. "A New meta-GGA Exchange Functional Based on an Improved Constraint-based GGA", J. Martín del Campo, A. Vela, J.L. Gázquez, and S.B. Trickey, Chem. Phys. Lett. **543**, 179-183 (2012).

71. "Comment on 'A Minimal Implementation of the AMBER-GAUSSIAN Interface for Ab Initio QM/MM-MD Simulation"', B.P. Roberts, G.M. Seabra, A.E. Roitberg, K.M. Merz, E. Deumens, J. Torras, and S.B. Trickey, J. Comput. Chem. **33**, 1643 - 1644, (2012).

72. "Non-empirical Improvement of PBE and Its Hybrid PBE0 for General Description of Molecular Properties", J.M. del Campo, J.L. Gázquez, S.B. Trickey, and A. Vela, J. Chem. Phys. **136**, 104108 [8 pp] (2012).

73. "Improved Constraint Satisfaction in a Simple GGA Exchange Functional", A. Vela, J.C. Pacheco-Kato, J.L. Gázquez, J.M. del Campo, and S.B. Trickey, J. Chem. Phys. **136**, 144115 [8 pp] (2012).

74. "Scalable Properties of Metal Clusters: A Comparative Study of Modern Exchange-Correlation Functionals", R. Koitz, T.M. Soini, A. Genest, S.B. Trickey, and N. Rösch; J. Chem. Phys. **137**, 034102 [9 pp] (2012).

75. "Issues and Challenges in Orbital-free Density Functional Calculations", V.V. Karasiev and S.B. Trickey, Comput. Phys. Commun. **183**, 2519-2527 (2012).

76. "Temperature-Dependent Behavior of Confined Many-electron Systems in the Hartree-Fock Approximation", T. Sjostrom, F.E. Harris, and S.B. Trickey, Phys. Rev. B **85**, 045125 [14 pp] (2012).

77. "Finite Temperature Scaling, Bounds, and Inequalities for the Non-interacting Density Functionals", J.W. Dufty and S.B. Trickey, Phys. Rev. B **84**, 125118 [11 pp] (2011); selected as "Editors Suggestion".

78. "Positivity Constraints and Information-theoretical Kinetic Energy Functionals", S.B. Trickey, V.V. Karasiev, and A. Vela, Phys. Rev. B **84**, 075146 [7 pp] (2011).

79. "Structure-dependence of the Magnetic Moment in Small Palladium Clusters: Surprising Results from the M06-L meta-GGA Functional", R. Koitz, T.M. Soini, A. Genest, S.B. Trickey, and N. Rösch, Internat. J. Quantum Chem. **112**, 113-120 (2012) DOI: 10.1002/qua.23168.

80. "Electronic Structure of Solids with WIEN2k", K. Schwarz, P. Blaha and S.B. Trickey, Mol. Phys. **108**, 3147-3166 (2010).

81. "Variational Fitting Methods for Electronic Structure Calculations", B.I. Dunlap, N. Rösch, and S.B. Trickey, Mol. Phys. **108**, 3167-3180 (2010).

82. "Of Science and Scientists in QTP" S.B. Trickey, Mol. Phys. **108**, 2841-2845 (2010).

83. "Incorporation of deMon2k as a New Parallel Quantum Mechanical Code for the PUPIL System", O. Bertran, S.B. Trickey, and J. Torras, J. Comput. Chem. **31**, 2669-2676 (2010).

84. "Constraint-based Single-point Approximate Kinetic Energy Functionals", V.V. Karasiev, R.S. Jones, S.B. Trickey, and F.E. Harris, Phys. Rev. B **80** 245120 [17 pp] (2009).

85. "Variable Lieb-Oxford Bound Satisfaction in a Generalized Gradient Exchange-Correlation Functional", A. Vela, V. Medel, and S.B. Trickey, J. Chem. Phys. **130** 244103 [6 pp] (2009).

86. "Conditions on the Kohn-Sham Kinetic Energy and Associated Density", S.B. Trickey, V.V. Karasiev, and R.S. Jones, Internat. J. Quantum Chem. **109**, 2943-52 (2009).

87. "Tightened Lieb-Oxford Bound for Systems of Fixed Particle Number", M.M. Odashima, K. Capelle, and S.B. Trickey, J. Chem. Theory and Comput. [special issue for the 65th birthday of John Perdew] **5**, 798-807 (2009).

88. "Predictive First-principles Simulations of Strain-induced Phenomena at Water-Silica-Nanotube Interfaces", Yao He, Chao Cao, S.B. Trickey, and H.-P. Cheng, J. Chem. Phys. **129**, 011101 [4 pp] (2008).

89. "Recent Advances in Developing Orbital-free Kinetic Energy Functionals", V.V. Karasiev, R.S. Jones, S.B. Trickey, and F.E. Harris, in "New Developments in Quantum Chemistry", J.L. Paz and A.J. Hernández, editors (Research Signpost, Kerala,2009) 25 - 54.

90. "A Versatile AMBER-Gaussian QM/MM Interface Through PUPIL", J. Torras, G. de M. Seabra, E. Deumens, S.B. Trickey, and A.E. Roitberg, J. Comput. Chem. **29**, 1564-1573 (2008)

91. "Energetics and Mechanical Properties of Silica Nano-tubes", K. Muralidharan, J. Torras Costa, and S.B. Trickey, J. Phys. Cond. Mat. **1**9, 386238 [25 pages] (2007).

92. "First Principles Calculation of Spin-orbit Splitting in Graphene", J.C. Boettger and S.B. Trickey, Phys. Rev. B **75**, 121402(R) [1-3] (2007); also Virtual Journal of Nanoscale Science & Technology, March 26, 2007, Volume 15, Issue 12 (Carbon Nanotubes, C60, and Related Studies); erratum Phys. Rev. B **75**, 199903 (2007).

93. "Fracture, Water Dissocation, and Proton Conduction in SiO_2 Nano-chains", C. Cao, Y. He, J. Torras, E. Deumens, S.B. Trickey, and H-P. Cheng, J. Chem. Phys. **126**, 211101 [1-3] (2007).

94. "PUPIL: A Systematic Approach to Software Integration in Multi-scale Simulations", J. Torras, Y. He, C. Cao, K. Muralidharan, E. Deumens, H-P. Cheng, and S.B. Trickey, Computer Phys. Commun. **177**, 265-79 (2007).

95. "Graded Methods for Rapid Generation of Quantum Mechanical Forces in Molecular Dynamics Simulations", D.E. Taylor, V.V. Karasiev, K. Runge, S.B. Trickey, and F.E. Harris, Computat. Mat. Sci. **39**, 705-08 (2007).

96. "Faster Approximate Force Calculations via Quasi-spin Density Exchange-correlation Functionals", V.V. Karasiev, S.B. Trickey, and F.E. Harris, Chem. Phys. **330**, 216-223 (2006).

97. "A Perspective on Multiscale Simulation: Toward Understanding Water Silica", S.B. Trickey, S. Yip, Hai-Ping Cheng, K. Runge, and P.A. Deymier, J. Computer-Aided Mat. Design, **13**, 1-12 (2006).

98. "Exact Density Functionals for Two-electron Systems in an External Magnetic Field", Wuming Zhu and S.B. Trickey, J. Chem. Phys. **125**, 094317 [1-12] (2006).

99. "Software Integration in Multi-scale Simulations: the PUPIL System", J. Torras, E. Deumens, and S.B. Trickey, J. Computer-Aided Mat. Design, **13**, 201-212 (2006).

100. "Graded Methods for Quantum Mechanical Force Generation in Molecular Dynamics Simulations", D.E. Taylor, V.V. Karasiev, K. Runge, S.B. Trickey, and F.E. Harris, in *Recent Progress in Computational Science and Engineering*, (ed. T. Simos and G. Maroulis), **7**, 532-535 (2006).

101. "Born-Oppenheimer Interatomic Forces from Simple, Local Kinetic Energy Density Functionals", V.V. Karasiev, S.B. Trickey, and F.E. Harris, J. Computer-Aided Mat. Design, **13**, 111-129 (2006).

102. "Potential Parameterization from Proxy Systems", Wuming Zhu, K. Runge, and S.B Trickey, J. Computer-Aided Mat. Design, **13**, 75-84 (2006).

103. "Encoding Electronic Structure Information in Potentials for Multi-scale Simulations: SiO_2", Wuming Zhu, D.E. Taylor, A.R. Al-Derzi, K. Runge, S.B. Trickey, Ting Zhu, Ju Li, and S. Yip, Computat. Mat. Sci. **38**, 340-49 (2006)

104. "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)

105. "Density Functional Energetics of α-Quartz for Calibration of SiO_2 Interatomic Potentials", N. Flocke, Wuming Zhu, and S.B. Trickey, J. Phys. Chem. B **109**, 4168-71 (2005)

106. "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)

107. "Molecular Prototypes for Simple SiO_2 Potentials", A.R. Al-Derzi, M.G. Cory, K. Runge, and S.B. Trickey, J. Phys. Chem. A **108**, 11679-683 (2004)

108. "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

109. "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)

110. "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)

111. "Deformation and Fracture of SiO_2 Nanorod", Ting Zhu, Ju Li, Sidney Yip, R.J. Bartlett, S.B. Trickey, and N.H. de Leeuw, Molecular Simulations **29**, 671-76 (2003).

112. "Shape-dependent Molecular Polarizabilities", S. Peter Apell, J.R. Sabin, S.B. Trickey, and J. Oddershede, Internat. J. Quantum Chem. **86**, 35 - 39 (2002).

113. "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.

114. "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).

115. "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).

116. "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).

117. "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).

118. "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).

119. "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).

120. "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.

121. "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.

122. "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.

123. "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).

124. "Geometrical Basis for Molecular Stopping Anisotropy", S.P. Apell, S.B. Trickey, and J.R. Sabin, Phys. Rev. A **58**, 4616 - 21 (1998).

125. "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).

126. "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).

127. "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) 239-254.

128. "Surface Stopping", S.P. Apell, J.R. Sabin, and S.B. Trickey, Phys. Rev. A **56**, 3769 - 76 (1997).

129. "Simple Physical Model for Layer-Number Dependences of Proton Stopping in Ultrathin 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. (Amer. Phys. Soc., NY, 1997) AIP Conf. Proc. 392, vol. 1, 1369-72.

130. "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).

131. "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).

132. "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).

133. "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.

134. "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).

135. "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).

136. "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).

137. "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].

138. "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).

139. "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).

140. "Theoretical Ion Implantation Profiles for Low Energy Protons under Channeling Conditions", J.A. Nobel, J.R. Sabin, and S.B. Trickey, Internat. J. Quantum Chem. S-**28**, 283-97 (1994).

141. "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).

142. "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).

143. "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).

144. "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).

145. "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).

146. "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).

147. "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.

148. "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).

149. "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).

150. "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).

151. "Low-Pressure Crystalline Phases in Lithium", J.A. Nobel, S.B. Trickey, P. Blaha, and K. Schwarz, Phys. Rev. B **45**, 5012-14 (1992).

152. "Interplanar Binding and Lattice Relaxation in a Graphite Di-Layer", S.B. Trickey, F. Müller-Plathe, G.H.F. Diercksen, and J.C. Boettger, Phys. Rev. B **45**, 4460-68 (1992).

153. "Quantum Size Effects in Equilibrium Lithium Ultra-thin Layers", J.C. Boettger and S.B. Trickey, Phys. Rev. B **45**, 1363-72 (1992).

154. "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).

155. "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).

156. "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).

157. "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).

158. "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).

159. "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).

160. "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).

161. "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).

162. "Beryllium-Hydrogen Ultra-thin Films: I. Metallic Behavior in a BeH_2 Monolayer", Jin Zhong Wu, S.B. Trickey, and J.C. Boettger, Phys. Rev. B **42**, 1663-67 (1990).

163. "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).

164. "A Computationally Feasible Strategy for Partitioning Theory of the Molecule-Surface Interaction", S.B. Trickey, J. Molec. Struc. (Theochem) **199**, 215-24 (1989).

165. "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).

166. "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).

167. "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).

168. "Electronic Structure of Fibonacci Copolymers and Superlattices", M. Seel and S.B. Trickey, Solid State Commun. **66**, 537 - 41 (1988).

169. "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).

170. "Electronic Surface States in Beryllium", J.C. Boettger and S.B. Trickey, Phys. Rev. B **34**, 3604 - 09 (1986).

171. "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).

172. "Structural Optimization and Properties of First-Row Monolayers", J.C. Boettger and S.B. Trickey, J. Phys. F: Met. Phys. **16**, 693 - 706 (1986).

173. "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).

174. "Structure and Properties of a Beryllium Dilayer", J.C. Boettger and S.B. Trickey, Phys. Rev. B **32**, 1356 - 58 (1985) [Rapid Communication].

175. "Equation of State and Properties of Lithium", J.C. Boettger and S.B. Trickey, Phys. Rev. B **32**, 3391 - 98 (1985).

176. "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); erratum J. Phys. C: Sol. State Phys. **21**, 3475 (1988).

177. "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).

178. "Ground State Properties of a Beryllium Monolayer", J.C. Boettger and S.B. Trickey, J. Phys. F: Met. Phys. **14**, L151 - L153 (1984).

179. "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).

180. "Multi-parameter Iterative Convergence Accelerator for Crystalline LCGTO Calculations", J.C. Boettger and S.B. Trickey, Computer Phys. Commun. **32**, 361 - 65 (1984).

181. "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 - 6442 (1984).

182. "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 - 6433 (1984).

183. "Comment on 'Electron Removal Energies in Kohn-Sham Density Functional Theory"', S.B. Trickey, Phys. Rev. B **30**, 3523 - 24 (1984).

184. "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).

185. "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 - 352.

186. "Generator Coordinate Treatment of Some Model Periodic Systems", L.R. Kauder, A.K. Ray, and S.B. Trickey, Internat. J. Quantum Chem. **23**, 1355 - 1361 (1983).

187. "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 - 1760 (1981); erratum Phys. Rev. B **28**, 7352 (1983).

188. "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 - 1753 (1982).

189. "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 - 353 (1982).

190. "Adequacy of Local-Exchange Excitation Hamiltonians in Insulators", S.B. Trickey, A.K. Ray, and J.P. Worth, Phys. Stat. Solidi (b) **106**, 613 - 620 (1981).

191. "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 - 935 (1980).

192. "APW-Xα Compton Profiles in Crystalline Rare Gases", J.P. Worth, Corinne Lee Merry, and S B. Trickey, J. Phys. Chem. Solids **41**, 623 - 630 (1980).

193. "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).

194. "APW Calculation of the Zero Temperature Isotherm of Solid Xenon", J.P. Worth and S.B. Trickey, Phys. Rev. B **19**, 3310 - 3312 (1979).

195. "Non-Muffin-Tin Effects in the X-α Treatment of Ne_2", J.P. Worth, B.I. Dunlap, and S.B. Trickey, Chem. Phys. Lett. **55**, 168 - 170 (1978).

196. "Debye-Waller Factor of Solid Heavy Methane", S.B. Trickey and T.R. Koehler, Solid State Commun. **25**, 779 - 780 (1978).

197. "Euler Vectors and Rotations About an Arbitrary Axis", T.R. Koehler and S.B. Trickey, Am. J. Phys. **46**, 650 - 651 (1978).

198. "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-**ll**, 529 - 538 (1977).

199. "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 - 1159 (1977).

200. "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 - 483.

201. "Ground State Properties of bcc ^{3}He - Test of the Point Transformation Method", S.B. Trickey, N.M. Witriol, and T.R. Koehler, in *Proc. Fourteenth Internat. Conf. Low Temp. Phys.*, M. Krusius and M. Vuorio, eds. (North Holland, Amsterdam, 1975) Vol. 1, 491 - 492.

202. "Comparison of Atomic Compton Profiles Obtained from Four Model Local Density Functionals", J.R. Sabin and S.B. Trickey, J. Phys. B **8**, 2593 - 2600 (1975).

203. "CO_2 - N_2 Intermolecular V-T and V-V Potentials via CNDO", N.M. Witriol, J.D. Stettler, J.R. Sabin, and S.B. Trickey, J. Chem. Phys. **63**, 3263 - 3271 (1975).

204. "Investigation of the Computation of V-T and V-V Intermolecular Potentials", N.M. Witriol, J.D. Stettler, J.R. Sabin, and S.B. Trickey, IEEE J. Quantum Electr. **QE-ll**, 717 (1975).

205. "Cohesive Energy and the PV Relation for fcc Neon in Two Variants of the X-α Model", J.R. Sabin, J.P. Worth, and S.B. Trickey, Phys. Rev. B **11**, 3658 - 3661 (1975).

206. "CNDO Calculation of Intermolecular V-T and V-V Potentials - the CO_2 - N_2 System", N.M. Witriol, J.D. Stettler, J.R. Sabin, and S.B. Trickey, Chem. Phys. Lett. **27**, 540 - 543 (1974).

207. "Pair Potentials for van der Waals Solids from a One-Electron Model", S.B. Trickey, F.W. Averill, and F.R. Green, Jr., in *Low Temperature Physics - LT13*, K.D. Timmerhaus, W.J. O'Sullivan, and E.F. Hammel, eds. (Plenum, N.Y., 1974) vol. 2, 251 - 254.

208. "Ensemble Representable Reduced Density Matrices Suggested by the X-α Transition State", S.B. Trickey, Chem. Phys. Lett. **21**, 581 - 585 (1973).

209. "One-Electron Theory of the Bulk Properties of Crystalline Ar, Kr, and Xe", S.B. Trickey, F.R. Green, Jr., and F.W. Averill, Phys. Rev. **B 8**, 4822 - 4832 (1973).

210. "Suitability of Jastrow Functions of WKB Type to Cluster Calculations of the Quantum Crystal Ground State", S.B. Trickey, J. Low Temp. Phys. **13**, 313 - 315 (1973).

211. "Point Transformation Theory and Quantum Crystals: Zero Temperature Self-Consistent Phonons Assuming Two-Body Additivity", S.B. Trickey, N.M. Witriol, and G.L. Morley, Phys. Rev. A **7**, 1662 - 1673 (1973).

212. "Calculation of the Magnetization and Total Energy of Vanadium as a Function of Lattice Parameter", T.M. Hattox, J.B. Conklin, Jr., J.C. Slater, and S.B. Trickey, J. Phys. Chem. Solids **34**, 1627 -1638 (1973).

213. "Comments on Analysis of Low-Temperature Heat Capacity Data", S.B. Trickey, Am. J. Phys. **41**, 296 (1973).

214. "MS-Xα Calculation of the Energy-Level Structure of XeF_6", E.W. Phillips, J.W.D. Connolly, and S.B. Trickey, Chem. Phys. Lett. **17**, 203 - 206 (1972).

215. "Self-Consistent One-Electron Calculation of the Zero-Temperature Cohesive Properties of Solid Argon", S.B. Trickey, F.W. Averill, and F.R. Green, Jr., Phys. Lett. **41A**, 385 - 386 (1972).

216. "Thermodynamic, Elastic, and Magnetic Properties of Solid Helium", S.B. Trickey, W.P. Kirk, and E.D. Adams, Rev. Mod. Phys. **44**, 668 - 715 (1972).

217. "Lattice Dynamics of Hard-Core, Highly Anharmonic Crystals", S.B. Trickey, N.M. Witriol, and G.L. Morley, Solid State Commun. **11**, 139-143 (1972).

218. "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).

219. "d-Band Difficulties in the $\mathbf{k}\cdot\mathbf{p}$ - APW Method", T. Kuebbing, K. Schwarz, S.B. Trickey, and J.B. Conklin, Jr., Phys. Rev. Lett. **26**, 1251-1253 (1971); erratum Phys. Rev. Lett. **26**, 1519 (1971).

220. "Interpretation of Elastic Debye Temperature in Solid ^{3}He", S.B. Trickey and E.D. Adams, Phys. Lett. **33A**, 483-484 (1970).

221. "Self-Consistent Non-Muffin-Tin $\mathbf{k}\cdot\mathbf{p}$ - APW Method", S.B. Trickey and J.B. Conklin, Jr., Phys. Lett. **32A**, 481-482 (1970).

222. "Realistic One-Dimensional Example of the Failure of Lattice Dynamics in the Harmonic Approximation", S.B. Trickey, Am. J. Phys. **38**, 529 (1970).

223. "Temperature Dependence of Debye θs for bcc ^{3}He and hcp ^{4}He", P.N. Henriksen, M.F. Panczyk, S.B. Trickey, and E.D. Adams, Phys. Rev. Lett. **23**, 518-520 (1969).

224. "Convergence and Energy Bounding Properties of the Nosanow Cluster Expansion", S.B. Trickey and J. Nuttall, J. Low Temp. Phys. **1**, 109-122 (1969).

225. "Relation Between the Brueckner-Frohberg and Nosanow Cluster Expansions", S.B. Trickey, Phys. Rev. **166**, 177-180 (1968).

B. Published Computer Codes

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).
2. "PUPIL - Program for User Package Interfacing and Linking", J. Torras, Y. He, C. Cao, K. Muralidharan, E. Deumens, H-P. Cheng, and S.B. Trickey, Open source (GPL) http://sourceforge.net/projects/pupil
3. "Profess@QuantumExpresso". V.V. Karasiev, T. Sjostrom, and S.B. Trickey, arXiv 1406.0835; Open source (GPL) http://www.qtp.ufl.edu/ofdft
4. "KGEC - Kubo-Greenwood Electrical Conductivity", L. Calderín, V.V. Karasiev, and S.B. Trickey, Open source (GPL) http://www.qtp.ufl.edu/ofdft

C. Thesis and Dissertation:
"A Calculation of the Rotational Constants of Ammonia", M.S. thesis, Texas A&M Univ., May 1966 (Prof. J.B. Coon)
"Studies in One Dimension of the Quantum Crystal Problem", Ph.D. dissertation, Texas A&M Univ., August 1968 (Profs. J.L. Gammel and J. Nuttall)

D. 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).

E. Editorships:

1. Specialist Editor for Condensed Matter Physics, *Computer Physics Communications* (1991–2016).
2. *Frontiers and Challenges in Warm Dense Matter*, F. Graziani, M.P. Desjarlais, R. Redmer and S.B. Trickey eds. (Springer Verlag, Heidelberg, 2014)
3. co-Editor, with R.J. Bartlett, of special issue of *Molecular Physics*, vol. 108, nos. 21-23 (2010) regarding 50 years of the Sanibel Symposium.
4. Guest Editor, *Journal of Computer Aided Materials Design*, vol. 13, nos. 1-3 (2006).
5. Special Editor, *Chemical Physics*, Notker Rösch Festschrift issue (vol. 309, no. 1, 2005).
6. 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
7. 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)
8. *Density Functional Theory of Many-Fermion Systems*, Vol. 21 Adv. Quantum Chem. (Academic, San Diego, 1990)
9. *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.
10. *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.
11. Member, Advisory Editorial Board, International J. Quantum Chemistry (1988-93)

Invited Talks and Seminars (Research)

1. "Free-energy Density Functional Theory for Matter under Extreme Conditions", *18th Internat. Meeting on Physics of Non-Ideal Plasmas*, Oxford UK, Sept. 16-19, 2024. [Invited]
2. "Meeting Exchange-correlation Challenges in Orbital-free DFT", *Towards Routine Orbital-Free Large-Scale Quantum Mechanical Modelling of Materials*, Banff Internat. Res. Station Workshop 24w5171, 8-13 Sept. 2024 (virtual). [Invited]
3. "Two Distinct Uses of Ensemble DFT: Spin-crossover and Free-energy Exchange-Correlation Functionals", *Psi-K Ensemble Density Functional Theory Workshop* , Durham UK, 22-25 July 2024. [Invited]
4. "Free-energy Density Functional Theory for Matter under Extreme Conditions", Physics Division Seminar, Lawrence Livermore National Laboratory, 03 July 2024.
5. "Predictive, High-throughput Computation of Spin-crossover", invited talk (F21.0002), Amer. Phys. Soc. (Minneapolis), 05 March 2024.
6. "Predictive, High-throughput Computation of Spin-crossover", invited talk, Sociedad Química de México annual meeting (virtual) 04 October 2023.

7. "Avoiding the Use of Orbitals", Invited talk, *50 Years of Density Functional Theory* meeting, Tulane Univ., 16 June 2023.

8. "Matter Under Extreme Conditions and Free Energy Density Functional Theory", Physics Dept. Colloquium, Rutgers University at Newark, 21 April 2023.

9. "Simplifying Density Functional Approximations for Challenging Materials Simulations", Physics Dept. Colloquium, Univ. Texas at El Paso, 24 March 2023.

10. "Warm Dense Matter and Orbital-free Finite-tempearature Density Functional Theory", invited talk A9, PsiK-2022, Lausanne Switzerland, 23 Aug. 2022.

11. "Hardness, Band Gaps, and Derivative Discontinuities from a Simple exchange-Correlation Functional", Seminar, Instiut of Materials Chemistry, Technische Universität Wien (Austria) 29 Aug. 2022.

12. "Funcionales de la Densidad Sencillos: ¿Hasta Donde Los Podemos Lllevar?", Reunión Mexicana Fisicoquímica Teórica XVIII, Toluca, México, 24-26 Oct. 2019.

13. "Speed and Insight from Pure Kohn-Sham Approximate Density Functionals", The Utah Workshop on Quantum Methods in Molecular and Solid-State Theory, Park City Utah, 22-27 Sept. 2019.

14. "Less is More - or - Back to Kohn-Sham", Current Topics in Theoretical Chemistry, Quito Ecuador 1-5 July 2019

15. "Essentials of Many-Fermion DFT and Their Relationship [or Lack Thereof] to Classical DFT", CECAM Workshop "Fundamentals of Density Functional Theory for T ¿ 0: Quantum Meets Classical", Lausanne Switzerland, 20 May 2019.

16. "Increasing the Accuracy of GGA Exchange Functionals Through Constraint Satisfaction", Symposium D.1, XVIIth Internat. Materials Research Congress, Cancún México, 21 Aug. 2018 (substitute for J.L. Gázquez)

17. "Free Energy Density Functional Theory for Matter Under Extreme Conditions", DOE Condensed Matter Theory Program PI meeting, Gaithersburg MD, 14 Aug. 2018.

18. "Free Energy Density Functional Theory for Matter Under Extreme Conditions", Lecture Series on Materials Theory and Computation, Xi'an Jiaotong Univ., Xi'an China, 30 June 2018.

19. "Seeking Simplicity for Accurate Approximate Density Functionals -A Story of Gators, Pan Dulce, and Electronic Structure Theory"; investiture lecture as Miembro Correspondiente (Corresponding Member), Academia Mexicana de Ciencias; at CINVESTAV - Zacatenco, Cd. de México, 16 April 2018.

20. "Atoms in Magnetic Fields - Challenges to Density Functional Theory", Facultad de Química, Univ. Autónoma Metropolitana - Iztapalapa, Cd. de México, 13 April 2018.

21. "Properly Constrained, Highly Accurate, Simple Exchange-Correlation Functionals", Facultad de Química, Univ. Nacional Autónoma de México, Cd. de Mexíco, 18 April 2018.

22. “Strategies for Removing Orbitals from meta-GGA Exchange-Correlation Functionals”, Seminar de Química Teorica, CINVESTAV - Zacatenco, Cd. de Mexíco, 19 April 2018.

23. “New Methods for Simulation of Matter Under Extreme Conditions”, Colloquium, Dept. of Physics, Tulane Univ., New Orleans LA, 04 Dec. 2017.

24. “New Methods for Simulation of Matter Under Extreme Conditions”, Seminario, Departamento de Química, CINVESTAV, Ciudad de México, México, 27 Oct. 2017.

25. “Revelations from Mel”, Fundamentals of Density Functional Theory: Mel Levy Workshop, City Univ. of New York, 19 May 2017.

26. “Finite-temperature Exchange-Correlation Functionals: Developments and Implications”, Warm Dense Matter 2017 Workshop; Vancouver B.C., 10-12 April 2017.

27. “Free Energy DFT with Cost-Effective Computational Scaling”, EMN Meeting on Computation and Nanotechnology, Las Vegas Nevada, 20-14 Oct. 2016.

28. “Density Functionals for Atoms Under Stringent External Specifications”, Current Topics in Theoretical Chemistry 2016, Trujillo Peru, 26-30 Sept. 2016.

29. “Primordial Quantum Statistical Mechanics - Modern Forms and Uses”, Beck-Seel Retirement Symposium, Dept. of Physics, Michigan Tech Univ. 16 May 2016.

30. “Back to the Future: Progress on Primordial Quantum Statistical Mechanics”, Colloquium, Dept. of Physics, Texas Tech Univ. Lubbock TX, 10 Sept. 2015.

31. “Ab Initio MD, Lower Rung Functionals, and Near-origin Misbehaviors from Pseudo-densities”, S.B. Trickey, Sympos. 4A, XXIV Internat. Materials Research Congress, Quintana Roo México, 16-20 Aug. 2015.

32. “Finite-temperature Density Functional Developments and Some Computational Consequences”, S.B. Trickey, Electronic Structure 2015, Univ. Washington, 21-24 June 2015.

33. “Pseudo-density-induced Functional Misbehavior”, 15th deMon Developers Workshop, Sofia Bulgaria, 27-30 May 2015.

34. “Density Functionals for Matter Under Extreme Conditions”, 55th Sanibel Symposium, 19 Feb. 2015, St. Simons Island, GA.

35. “Density Functionals for Systems Under Extreme Conditions”, 10th Congress World Assoc. Theoret. and Computational Chemists, 5-10 Oct. 2014, Santiago Chile.

36. “Geometry Optimization with One Orbital”, Symposium 1A, XXIII Internat. Materials Research Congress, Cancún México, 17-21 Aug. 2014.

37. “Density Functionals for Hot Matter”, Dept. of Energy Theoretical Condensed Matter Physics Program PIs meeting (invitation only), Gaithersburg MD, 11-13 Aug. 2014.

38. “Outlook for Lower-rung Exchange-Correlation Functionals for Faster Simulations”, 14th deMon Developers Workshop, Los Cabos México, 27-30 April 2014.

39. "Report on the Quest for Nearly Exact Thomas-Fermi-like Approximations", "March in November Symposium - Honoring N.H. March", Namur Belgium, 21 Nov. 2013.

40. "Fast ab initio MD with Non-empirical Orbital-free Density Functionals", CECAM Conference "Density Functional Theory: Learning From the Past, Looking to the Future", Berlin Germany 2-5 July 2013.

41. "Constraint-based, Finite-Temperature. Orbital-Free Density Functionals: Development and Application", XXII Internat. Materials Research Congress, Cancún México, 11-15 August 2013.

42. "Progress toward Orbital-free Many-Fermion Quantum Statistical Mechanics", Atomic-Biophysics-Condensed-Matter Seminar, Dept. of Physics, Univ. of Washington, 06 Nov. 2012.

43. "Design Criteria for Constraint-based, Single-point Orbital-free Density Functional Approximations", CECAM Workshop on Orbital-free Methods for High Energy Density Physics, Paris, 05-07 Sept. 2012.

44. "Constraint-based Development of Orbital-free Free Energy Density Functionals", 14th Conference on Physics of Non-Ideal Plasmas, Rostock Germany, 10-14 Sept. 2012.

45. " Topics, Issues, Questions - Quantum Simulations (mostly Workshop IV), IPAM Long Program, High Energy Density Plasmas" Institute of Pure and Applied Mathematics UCLA, Long Program on Computational Methods for High Energy Density Plasmas, Culminating Workshop, 11 June 2012.

46. "The Quantum Theory Landscape for Warm Dense Matter", Institute of Pure and Applied Mathematics UCLA, Long Program on Computational Methods for High Energy Density Plasmas, Workshop IV (Warm Dense Matter), 21 May 2012.

47. "The Highly Important Games of Temperature-dependent DFT and Hartree-Fock", Institute of Pure and Applied Mathematics UCLA, Long Program on Computational Methods for High Energy Density Plasmas, Tutorial Week, 16 March 2012.

48. "Many-electron Quantum Statistical Mechanics without Orbitals", Physics Dept. Colloquium, Michigan Tech Univ., 13 Oct. 2011.

49. "Temperature-Dependent Behavior of Confined Many-electron Systems in the Hartree-Fock Approximation", First International Workshop on Studies of Confined Quantum Systems, Mexico City, 7-9 Sept. 2011.

50. "Introductory Survey of Ground-state Density Functional Theory", "Brief Summary of Orbital-free DFT", "Localized Basis Set Methods for DFT Calculations on Two-Dimensionally Periodic Nano-structures", Complex 1, Computer Simulations on Nanotechnology for the Environment - the W.E. Heraeus Summer School for Physics 2011, Jacobs University, Bremen Germany, July 4 and 6, 2011.

51. "Coherent Approach to Orbital-free DFT", FCAM Workshop "The Orbital-free Alternative", Institut Henri Poincaré, Paris, 30-31 May 2011.

52. "Consistent Orbital-free DFT: Stalking an Ancient Prey", Université Pierre et Marie Curie (Paris 6), Laboratoire de Chimie Thórique, Jussieu, 01 June 2011.

53. "Many-electron Quantum Mechanics without Orbitals", Dept. of Physics and Engineering Physics Seminar, Tulane University, New Orleans LA, 10 Nov. 2010.

54. "New Approaches to Old Ideas", 19 Sept. 2010, Workshop on New Approaches to Many Electron Theory, organized by Mathematics Dept. Technische Universität Mainz and Max Planck Institut für Polymerforschung, Mainz Germany.

55. "Progress on Orbital-free Density Functional Theory", Molecular Simulation Group, Technische Universität Darmstadt (Germany), 16 Sept. 2010 and Center for Catalysis Research, Technische Universität München (Germany) 27 Sept. 2010.

56. "Improving Constraint-based GGA Exchange-correlation Functionals for Large Systems", 14 June 2010, Theory of Atomic and Molecular Clusters VI, Mexico City.

57. "Progress on Both Fronts of the Orbital-free DFT Agenda", "International Workshop on Density Functional Theory - Present and Future Challenges", 14-15 May 2010, Univ. Fed. Minas Gerais, Belo Horizonte, Brazil.

58. "Pursuit of an Ideal: Toward Orbital-free Density Functional Theory", 12 May 2010, Materials Simulation Seminar, Univ. Fed. ABC, Santo André, Brazil.

59. "Good Cheap Band Gaps from GGA Density Functionals?", Departamento de Química, Grupo de Química Teorica, Centro de Investigacion y Estudios Avanzados, México DF, México, 29 October 2009 and Departamento de Química, Universidad Metropolitana - Iztapalapa, México DF, México, 30 October 2009.

60. "Reworking the Second Rung of the Exchange-Correlation Ladder", Symposium on Density Functional Methods and Their Applications", Geburtstagfest für Prof. N. Rösch, Technische Universität München, 7 Nov. 2008.

61. "Tightening the Lieb-Oxford Bound in the PBE Exchange-Correlation Functional", Simposio de Teoría de Funcionales de la Densidad, Univ. Autónoma Metropolitana – Iztapalapa, México City, México, 17 October 2008.

62. "Física de Música y Música de Física", (in Spanish) Escuela de Laudería, Instituto Nacionál de Bellas Artes de México, Querétaro, Querétaro, México, 14 October 2008.

63. "Short Course on Density Functional Theory and Applications" 10 lectures, Dept. of Physics, Michigan Technological University, Houghton Michigan, Sept. 15–19, 2008.

64. "Novel Materials Properties from Gaussian Orbital DFT Methods", Tutorial Session on DFT-TDDFT, Div. of Chem. Educ., Amer. Chem. Society, Philadelphia PA, 19 Aug. 2008.

65. "Recent Progress on Orbital-free Kinetic Energy Density Functionals for Materials Simulations", Sixth Congress of the Internat. Soc. for Theoretical Chemical Physics, Vancouver B.C., 24 July 2008

66. "Orbital-free Density Functional Theory", Kolloquium für Physikalische und Theoretische Chemie, Technische Universität München, 16 April 2008.

67. "Density Functionals and Highly Anisotropic Systems: Graphite and Graphene", Pan American Workshop on Molecular and Materials Sciences, Cuernavaca México, Oct. 9-11, 2007.

68. "Stress, Fracture, and Hydrolytic Effects in Nanoscale Silica Systems", CECAM Workshop on Modelling the Structure and Reactivity of Silica and Water, Lyon France, Sept. 17-19, 2007.

69. "Prediction of Materials Properties via Local Basis Set DFT Methods", Pan American Advanced Scientific Institute on Electronic States and Excitations in Nanostructures, Zacatecas México, June 11-15, 2007.

70. "Approximate Kinetic Energy Density Functionals - A Sampler", Pan American Advanced Scientific Institute on Electronic States and Excitations in Nanostructures, Zacatecas México, June 11-15, 2007.

71. "Approximate Quantum Mechanics for Materials Simulations", Theoretical Chemistry Seminar, Dept. of Chemical Engineering, Universidad Politécnica de Catalunya, Barcelona Catalunya Spain, 24 May 2007.

72. "Orbital-free Density Functionals for Multi-scale Materials Simulations", Condensed Matter Physics Seminar (invited), Rice University, Mar. 19, 2007.

73. "Spin-Orbit Splitting in Graphene", QTP Seminar, Univ. of Florida, Feb. 14, 2007.

74. "Orbital-free Density Functionals for Materials Simulations", (in Spanish), 7 Dec. 2006, Lab. de Química Computacional y Teórica, Univ. de La Habana, Cuba, Dec. 7, 2006.

75. "Overview of Multi-scale Materials Simulation Techniques and Issues" and "Quantum Mechanical Methods in Multi-scale Materials Simulations", Two two-hour tutorial (advanced graduate student level) lectures at Cinvestav, Theoretical Chemistry Group, Mexico City, Oct. 23 and 25, 2006.

76. "Hydrolytic Weakening of Nanoscale Silica: Materials Simulation with Chemical Realism", Invited Talk, Symposium 19 (Nanoscience at the Intersection of Physics and Biology), XV Internat. Materials Research Congress, Academia Méxicana de Ciencía de Materiales, Cancún, México, 22 Aug. 2006.

77. "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).

78. "Quantum Mechanical Methods in Multi-scale Materials Simulations", DoE (PNNL) Multi-scale Mathematics in Materials Science Workshop, Tacoma, WA, 25-30 May 2006 (invited)

79. "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).

80. "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.

81. "Orbital-Free Density Functionals and Density Models for Driving Molecular Dynamics", DFTEM-2006 Conference, Vienna Austria, 20-22 April 2006 (invited)

82. "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).

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

84. "Progress on Approximate Density Functionals", Quantum Theory Project Seminar, Univ. Florida, 28 Sept. 2005 (invited).

85. "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).

86. "Prediction of Materials Properties Via Gaussian Orbital DFT Methods", 13th International Conference on Current Trends in Computational Chemistry, Jackson MS, 12 Nov. 2004 (invited).

87. "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).

88. "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)

89. "Tutorial on Plenary Sessions I - XI" 44th Sanibel Symposium graduate student tutorial session, Feb. 28, 2004

90. "Quantum Mechanics meets Classical Mechanics in Simulations", U. Florida Dept. of Physics Brown Bag Lunch talk, Nov. 5, 2003.

91. "Basics of the Art of Funding Research - Tutorial for Grad Students and Postdocs", Seminar, Quantum Theory Project, Univ. Florida, Oct. 15, 2003.

92. "Classical Potentials for Multi-scale Simulation of Fracture in Silica", Seminar, Institut für Physikalische und Theoretische Chemie, Technische Universität München, Germany, 20 May 2003.

93. "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).

94. "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.

95. "Multi-scale, Multi-pass Simulations from Molecules to Materials", NSF DMR Computational Materials Theory Review meeting, Univ. of Illinois Urbana-Champaign, June 19, 2002

96. "Constructive Approach to Density Functional Theory", Löwdin Memorial Symposium, Uppsala University (Sweden), invited talk, 25 Oct. 2000.

97. "Challenges and State of the Art in Simulation of Chemo-Mechanical Processes", 198th Meeting of Electrochemical Society, Phoenix AZ, invited talk, 23 Oct. 2000.

98. "Dielectric Functions in LiF", 20th Werner Brandt Workshop on Energy Deposition Phenomena, U. Florida, invited talk, 10-11 Feb. 2000.

99. "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.

100. "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.

101. "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.

102. "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.

103. "Calculated Momentum Densities - Properties and Uses", Invited lecture, 18th Werner Brandt Workshop on Energy Deposition Phenomena, U. Florida, 4-5 June 1998.

104. "Prediction of the Structure and Properties of Ordered Ultra-thin Films", Physics Department Colloquium, Iowa State University, Ames IA, 22 April 1998.

105. "Prediction of the Structure and Properties of Ordered Ultra-thin Films", Physics Department Colloquium, Texas Tech University, Lubbock TX, 26 Mar. 1998.

106. "First-Principles Systematics of Ordered Metallic Monolayers: 3D Transition Metals", Invited lecture, Fifth Chemical Congress of North American, Cancún, México, 11-15 Nov. 1997.

107. "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.

108. "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.

109. "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.

110. "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.

111. "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.

112. "A Partisan's View of Current Challenges in Density Functional Theory", Seminario de Depto. de Física Teorica, Atómica y Nuclear, Universidad de Valladolid, España. 15 Feb. 1996.

113. "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.

114. "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.

115. "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.

116. "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.

117. "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.

118. "Novel Uses of the Local Density Approximation", Invited paper, Symposium on 30th Anniversary of Density Functional Theory, Cracow Poland, 13-16 June 1994.

119. "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.

120. "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.

121. "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.

122. "Density Functional Methods for Extended Systems", Host lecture, Q.T.P. Latin American Workshop, Gainesville, FL 12 Mar. 1993.

123. "Thickness-Dependent Properties of Ultra-thin Metallic Films: Predictive Calculations", Molecular Astrophysics Seminar, Max Planck Institut für Astrophysik, München, 25 May 1992.

124. Physics Department Colloquium, Vanderbilt University, 10 Dec. 1990.

125. "Direct Kohn-Sham Theory for $n^{1/2}$?", Molecular Physics Seminar, Max-Planck Institut für Astrophysik, München, 16 Oct. 1990.

126. "Wave-Function versus Density-Functional Methods", Invited Panelist, South Eastern Theoretical Chemistry Assoc. Annual Meeting, 18–19 May 1990.

127. Physics Department Colloquium, Univ. of Alabama-Birmingham, 23 Feb. 1990.

128. "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).

129. "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.

130. Physics Department Colloquium, Univ. of Akron, 8 Feb. 1989.

131. "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).

132. "Static Quantum Size Effect in Ultra-thin Films", Molecular Physics Seminar, Max-Planck Institut für Astrophysik, München, 19 June 1986.

133. "Current Status of Density Functional Theory", Great Lakes Summer Workshop in Condensed Matter Research, 19 July 1985.

134. "Recent Research Problems in Density Functional Theory", T11/T4 Seminar, Los Alamos National Laboratory, 13 June 1985.

135. "Current Research Problems in Density Functional Theory", Seminar, Lehrstuhl für Theoretische Chemie, Technische Universität München, 14 May 1985.

136. "One-Electron Energies in Density Functional Theory", invited paper 25th Internat. Sanibel Symposium, 20 March 1985.

137. Physics Dept. Colloquium, Louisiana State Univ., 24 Jan. 1985.

138. 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.

139. 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.

140. Materials Science and Technology (MST-5) Seminar (May 9, 1984) and Center for Materials Science Seminar (May 10, 1984), Los Alamos National Laboratory.

141. Physics Dept. Colloquium, Michigan Tech Univ., Jan. 12, 1984.

142. Physics Dept. Colloquium, Texas Tech Univ., Dec. 10, 1982.

143. Center for Materials Science Seminar, Los Alamos National Lab, Dec. 9, 1982.

144. Physics Dept. Colloquium, Univ. Texas at Arlington, Dec. 7. 1982.

145. Physics Dept. Colloquium, Michigan Technological University, 27 May 1981.

146. Physics Dept. Colloquium, Louisiana Tech Univ., 23 Oct. 1978.

147. Physics Dept. Colloquium, Univ. of Southwestern Louisiana, 13 Oct. 1978.

148. Physics Dept. Colloquium, Texas Tech Univ., 16 May 1977.

149. Physics Dept. Colloquium, Washington State Univ., 24 Feb. 1977.

150. Physics Dept. Colloquium, North Texas State Univ., 23 Apr. 1976.

151. Physics Dept. Colloquium, Texas A&M Univ., 22 April 1976.

152. Physics Dept. Colloquium, Rice Univ., 20 April 1976.

153. Joint Stanford-Berkeley Theoretical Chemistry Seminar, Stanford Univ., 3 March 1976.

154. Department Seminar (Dept. K32), IBM Research, San Jose, Calif., 5 Dec. 1975.

155. "Superfluid ^{3}He - Recent Progress in Theory and Experiment", Invited Review Lecture, International Symposium on Quantum Chemistry and Solid State Physics, Dalseter, Norway, August 30, 1975.

156. Physics Department Colloquium, Univ. of Georgia, 24 April 1975.

157. "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).

158. "The Present Status of Calculational 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.

159. "Lattice Dynamics of Hard-Core, Highly Anharmonic Crystals", S.B. Trickey, N.M. Witriol, and G.L. Morley, Contribution to Conf. on Quantum Crystals, Banff, Canada, 6-10 Sept. 1971 (Invited Panelist).

Contributed Papers Presented (Research)

1. "Polymorphism of the Spin-crossover Fe(III) Complex [Fe^t(BuMeqsal)$_2$], Angel M. Albavera-Mata, Divya Kumar, Michael Shatruk, S.B. Trickey, and Richard G. Hennig, 64th Sanibel Symposium, 27 Feb. 2025.

2. "Equivariant Graph Neural Networks for Predicting Spin-Crossover Energy in Transition Metal Complexes", Angel Albavera Mata, R.G. Hennig, and S.B. Trickey, K60.00004, Amer. Physical Soc., Minneapolis Minn. 05 March 2024.

3. "Enhancing the Computational Efficiency of De-orbitalized metaGGA Exchange-Correlation Functionals", Héctor Francisco R., B39.00005, Amer. Physical Soc., Minneapolis Minn. 04 March 2024.

4. "Ensemble Hubbard U Correction for Improved Transition Temperatures for Spin-crossover Materials", Angel Albavera-Mata, Richard Hennig, and S.B. Trickey, Amer. Phys. Soc. March 2023 meeting, paper A28.00012.

5. “Deorbitalization of Two-indicator-function meta-GGA Exchange-correlation Functionals”, Héctor Francisco R., S.B. Trickey and A.C. Cancio, Amer. Phys. Soc. March 2023 meeting, paper B17.00008.

6. “Smoothing Techniques to Tame Laplacian-dependent Exchange-Correlation Functionals”, S.B. Trickey, Tun Sheng Tan, and A.C. Cancio, Amer. Phys. Soc. March 2023 meeting, paper B17.00009.

7. “Dureza de Moléculas y Banda Prohibida de Sólidos con el Funcional Tipo GGA NCAPR”, J. Carmona-Espíndola, A. Flores, A. Vela, and S.B. Trickey, Reunión Mexicana Fisicoquímica Teórica XX, 16-19 Nov. 2022.

8. “Hardness of Molecules and Band Gap of Solids from a Generalized Gradient Approximation Exchange Energy Functional”, J.L. Gázquez, J. Carmona-Espíndola, A. Flores, A. Vela, and S.B. Trickey, 61st Sanibel Symposium “Hot Topics” presentation, 15 Feb. 2022.

9. “Collective Effects on the Spin Crossover Energy”, Angel M. Albavera Mata, Sijin Ren, Richard G. Hennig and S.B. Trickey, paper D60.00007, Amer. Phys. Soc. March 2022 meeting, 14 March 2022.

10. “Dipole Switching by Intramolecular Electron Transfer in Single-Molecule Magnetic Complex [Mn12O12(O2CR)16(H2O)4]”, Dmitry Skachkov, Shuang-Long Liu, Jia Chen, George Christou, Arthur Hebard, Xiao-Guang Zhang, S.B. Trickey, and Hai-Ping Cheng, paper M54.00008, Amer. Phys. Soc. March 2022 meeting, 16 March 2022.

11. “Artifactual Liquid-liquid Hydrogen Phase Transition from a Machine-Learnt Potential”, S.B. Trickey, V.V. Karasiev, J. Hinz, and Suxing Hu, paper N49.00007, Amer. Phys. Soc. March 2022 meeting, 16 March 2022.

12. “Consistent Deorbitalization and New Deorbitalizers for Meta-GGA Exchange-correlation Functionals”, Hector Francisco Rodríguez, S.B. Trickey, and Antonio C. Cancio, paper T01.00004, Amer. Phys. Soc. March 2022 meeting, 17 March 2022

13. “Boost all-electron full-potential DFT calculation with the domain specific SIRIUS library”, Long Zhang, S.B. Trickey, and Hai-Ping Cheng; APS March meeting, F22.0009, 16 March 2021.

14. ”Spin-crossover in Molecules and Solids with a Low-cost, Well-behaved meta-GGA Density Functional”, S.B. Trickey and Daniel Mejía-Rodríguez, and Angel Albavera Mata; APS March meeting, L53.003, 17 March 2021.

15. “Methodological Choices for the Spin-Crossover Energy: Mn(taa) as an Example”, Angel Albavera Mata, Daniel Mejía-Rodríguez, Eric Fonseca, Dianteng Chen, H-P. Cheng, S.B. Trickey, and Richard Hennig; APS March meeting L53.0011, 17 March 2021.

16. “Solid Calculations with Meta-GGA Accuracy at Little more than GGA Cost Daniel Mejía-Rodríguez and S.B. Trickey; APS March meeting Y21.001, 19 March 2021.

17. “Performance of Generalized Gradient Approximations with Nearly Correct Asymptotic Potentials on Molecular and Solid-State Properties”, A. Vela, A. Albavera-Mata, K.B. Mancilla,

J. Carmona-Espíndola, S.B. Trickey, and J.L. Gázquez, Amer. Phys. Soc., March 5, 2019, paper H31.00004.

18. "A Generalized Gradient Approximation with Local Parameters", A. Albavera-Mata, K.B. Mancilla, D. Mejía-Rodríguez, S.B. Trickey, J.L. Gázquez, and A. Vela, Amer. Phys. Soc., March 7, 2019, paper S18.00003.

19. "SCAN-L extended to an exchange-correlation free- energy density functional for extreme conditions", D. Mejía-Rodríguez and S.B. Trickey, Amer. Phys. Soc., March 7, 2019, paper V17.00004.

20. "Fast First-Principles Predictions for Warm Dense Matter with Orbital-free Free Energy Density Functional Theory", K. Luo, V.V. Karasiev, and S.B. Trickey, Amer. Phys. Soc., March 7, 2019, paper V17.00005.

21. "Simplification of meta-GGA Exchange-Correlation Functionals", S.B. Trickey, Symposium D.1, XVIIth Internat. Materials Research Congress, Cancún México, 21 Aug. 2018.

22. "Deorbitalization of meta-GGA exchange correlation functionals", Daniel Mejía-Rodríguez and S.B. Trickey, Paper C02:04, APS March meeting, Los Angeles CA, 05 March 2018.

23. "CAP-DD: Improved Correct Asymptotic Potential GGA with Derivative Discontinuity Treatment", S.B. Trickey, J. Carmona-Espíndola, J.L. Gazquez, and A. Vela., Paper R02:11, APS March meeting, Los Angeles CA, 08 March 2018.

24. "van Leeuwen Theorem for Mixed States and Finite Temperature Density Response", J.W. Dufty, K. Luo, and S.B. Trickey, Paper S02.03, APS March meeting, Los Angeles CA, 08 March 2018.

25. "A Novel Generalized Gradient Approximation for the Non-interacting Kinetic Energy Density Functional", Kai Luo, V.V. Karasiev, and S.B. Trickey, Paper S02:13, APS March meeting, Los Angeles CA, 08 March 2018.

26. "Non-empirical Semi-local Free-Energy Density Functional for Warm Dense Matter", S.B.T., V.V. Karasiev, and J.W. Dufty, Paper L60.034, APS March meeting, Los Angeles CA, 09 March 2018.

27. "Kubo-Greenwood Electric Conductivity Tensor: Essentials and Open-source Implementation" Lázaro Calderín, V.V. Karasiev, J.W. Dufty and S.B. Trickey, Paper K2.00005, Amer. Phys. Soc. March Meeting, New Orleans LA, 16 Mar. 2017.

28. "Tunable Non-interacting Free-energy Functionals: Development and Applications to Low-density Aluminum", S.B. Trickey and V.V. Karasiev, Paper K2.00006, Amer. Phys. Soc. March Meeting, New Orleans LA, 16 Mar. 2017.

29. "Generalized Gradient Approximation for Exchange-Correlation Free Energy", V.V. Karasiev, J.W. Dufty, and S.B. Trickey, Paper L26.00004 Amer. Phys. Soc. March Meeting, New Orleans LA, 16 Mar. 2017.

30. "Thermal DFT Functionals and Software For Extreme Condition Material Simulations"; poster DOE PIs' meeting, 15-17 Aug. 2016.

31. “Study of the Large Reduced Density Gradient Limit for the Exchange Energy,” J.L. Gázquez, J. Carmona-Espíndola , A. Vela, and S.B. Trickey, contributed paper A31.00010, Amer. Phys. Soc. Baltimore MD, 14 March 2016.

32. “Influence of Exchange-correlation Temperature Effects on Electric Conductivity of Aluminum in WDM Regime,” V.V. Karasiev, L. Calderín, and S.B. Trickey, contributed paper V211.00011, Amer. Phys. Soc. Baltimore MD, 17 March 2016.

33. “Orbital-free Molecular Dynamics Simulations to Characterize the Liquid-vapor Critical Point of Aluminum” D. , V.V. Karasiev, and S.B. Trickey, contributed paper V211.00012, Amer. Phys. Soc. Baltimore MD, 17 March 2016.

34. “A PW91-like Exchange with a Simple Analytical Form”, J.C. Pacheco-Kato, J.L. Gázquez, S.B. Trickey, and A. Vela, contributed paper, 56th Sanibel Symposium, 16 Feb. 2016.

35. “Finite-temperature Orbital-free Density Functional Theory: Development, Implementation, and Applications”, V.V. Karasiev and S.B. Trickey, Poster, 56th Sanibel Symposium , 17 Feb. 2016.

36. “The Importance of the Finite-temperature Exchange-correlation for Warm Dense Matter Studies”, Valentin V. Karasiev and S.B. Trickey, Amer. Phys. Soc. March meeting S23-001, San Antonio TX, 05 Mar. 2015.

37. “Proper Finite-temperature Density Functionals and their Computational Implementation”, D. Chakraborty, J.W. Dufty, V.V. Karasiev, and S.B.Trickey, Internat. Conf. on Strongly Coupled Coulomb Systems, Santa Fe NM, 27 July - 01 August 2014.

38. “Constraint-based development of finite-temperature. orbital-free density functionals” S.B. Trickey and V.V. Karasiev, Warm Dense Matter 2013 (Saint Malo France) 23-26 June 2013.

39. “Orbital-free molecular dynamics for warm dense hydrogen and deuterium”, V.V. Karasiev, and S.B. Trickey, Warm Dense Matter 2013 (Saint Malo France) 23-26 June 2013.

40. “Finite-temperature Orbital-free GGA Molecular Dynamics for Warm Dense Matter”, V.V. Karasiev, T. Sjostrom, S.B. Trickey, Amer. Phys. Soc. March 2013 meeting (Mar. 18), paper A39.00006.

41. “Constraint-based Non-empirical Parameterization of Generalized Gradient Approximation Kinetic Energy Functionals”, D. Chakraborty, S.B. Trickey, and V.V. Karasiev, Amer. Phys. Soc. March 2013 meeting (Mar. 20), paper R24.00012.

42. “Revised Thomas-Fermi Functional for Singular Potentials”, J.W. Dufty and S.B. Trickey, Amer. Phys. Soc. March 2013 meeting (Mar. 20), paper R24.00013.

43. “A Generalized Gradient Approximation for the Coulomb Energy”, A. Vela, J.L. Rosas-Trigueros, S.B. Trickey, and J.L. Gázquez, Amer. Phys. Soc. March 2013 meeting (Mar. 20), paper R24.00007.

44. “Analysis of the Large Reduced density Gradient Limit for the Exchange Energy”, J.L. Gázquez,, J. Mártin del Campo, J. Pacheco-Kato, S.B. Trickey, and A. Vela, Amer. Phys. Soc. March 2013 meeting (Mar. 20), paper R24.00008.

45. "Orbital-free Molecular Dynamics: Application to Hydrogen and Deuterium Under Extreme Conditions", V.V. Karasiev and S.B. Trickey, 53rd Sanibel Symposium, 21 Feb. 2013.

46. "Non-empirical Constraint-based Parameterization of a Generalized Gradient Approximation for the Orbital-Free Kinetic Energy", D. Chakraborty, S.B. Trickey, and V.V. Karasiev, 53rd Sanibel Symposium, 21 Feb. 2013.

47. "Comparison of Finite Temperature Hartree-Fock and Density Functional Theory for Confined Systems", Travis Sjostrom, S.B. Trickey, and F.E. Harris, Amer. Phys. Soc. "March" 2012 meeting (Feb. 28), contributed paper L25.00002.

48. "Density Functional versus Thermal Hartree-Fock Approximations in Warm Dense Lithium", V.V. Karasiev, Travis Sjostrom, S.B. Trickey, Amer. Phys. Soc. "March" 2012 meeting (Feb. 28), contributed paper L25.00004.

49. "A Non-empirical Improvement of PBE and Its Hybrid PBE0", A. Vela, J.M. Del Campo, J.L. Gazquez, and S.B. Trickey, Amer. Phys. Soc. "March" 2012 meeting (Feb. 28), contributed paper L35.00008.

50. "Finite Temperature Scaling of the Free Energy Density Functional", James Dufty, V.V. Karasiev, and S.B. Trickey, Amer. Phys. Soc. "March" 2012 meeting (Feb. 29), contributed paper P35.00010.

51. "Construction of Generalized Gradient Approximation Free Energy Density Functionals", S.B. Trickey, V.V. Karasiev, and Travis Sjostrom, Amer. Phys. Soc. "March" 2012 meeting (Feb. 29), contributed paper P35.00011.

52. "A Non-empirical Improvement of PBE and Its Hybrid PBE0",J. Mártin del Campo, J.L. Gázquez, S.B. Trickey, and A. Vela, contributed paper, 52nd Sanibel Symposium, 20 Feb. 2012.

53. "Structure of Generalized Gradient Approximation Free Energy Density Functionals", V.V. Karasiev, T. Sjostrom, and S.B. Trickey, contributed paper, 52nd Sanibel Symposium, 22 Feb. 2012.

54. "Finite Temperature Hartree-Fock and Density Functional Theory Calculations on Confined Hydrogen Systems", T. Sjostrom, S.B. Trickey, and F.E. Harris, contributed paper, 52nd Sanibel Symposium, 22 Feb. 2012.

55. "Comparison of Density Functional Approximations and the Finite-Temperature Hartree-Fock Approximation: Warm Dense Lithium", S.B. Trickey, V.V. Karasiev, and T. Sjostrom, contributed paper, 52nd Sanibel Symposium, 22 Feb. 2012.

56. "Temperature-Dependent Behavior of Confined Many-electron Systems in the Hartree-Fock Approximation", T. Sjostrom, F.E. Harris, and S.B. Trickey, 53rd meeting Div. Plasma Physics, Amer. Phys. Soc., 18 Nov. 2011, contributed paper YM10.00003.

57. "Finite-Temperature Orbital-free Density Functional Calculations for Warm Dense Lithium", V.V. Karasiev, T. Sjostrom, and S.B. Trickey, 53rd meeting Div. Plasma Physics, Amer. Phys. Soc., 18 Nov. 2011, contributed paper YP9.00081.

58. "Finite-temperature Exchange and Correlation Functionals in Self-Consistent Calculations", T. Sjostrom, V.V. Karasiev, and S.B. Trickey, Amer. Phys. Soc. March 2011 meeting (Mar. 21), contributed paper D15.014

59. "Finite Temperature Scaling of the Non-interacting Free Energy Density Functional", J.W. Dufty, V.V. Karasiev, and S.B. Trickey, Amer. Phys. Soc. March 2011 meeting (Mar. 21), contributed paper D15.015.

60. "Better GGA and meta-GGA Functionals: VT84, meta-VMT, meta-VT84", A. Vela, J. Mártin del Campo, J.L. Gázquez, and S.B. Trickey, Amer. Phys. Soc. March 2011 meeting (Mar. 24), contributed paper W24.08

61. "All-Electron and Pseudopotential Orbital-Free Density Functional Calculations", V.V. Karasiev, T. Sjostrom, and S.B. Trickey, Amer. Phys. Soc. March 2011 meeting (Mar. 24), contributed paper W24.09

62. "Contributions to the Non-interacting Free Energy Density Functional", S.B. Trickey, J.W. Dufty, and T. Sjostrom, Amer. Phys. Soc. March 2011 meeting (Mar. 24), contributed paper W24.10

63. "Self-consistent Orbital-Free Density Functional Calculations", V.V. Karasiev, T. Sjostrom, and S.B. Trickey, 51st Sanibel Symposium, 28 Feb. 2011.

64. "Finite Temperature Scaling in Orbital Free Density Functional Theory", J.W. Dufty, V.V. Karasiev, and S.B. Trickey, 51st Sanibel Symposium, 26 Feb. 2011.

65. "Finite Temperature Exchange and Correlation Functionals in Self-consistent Calculations", T. Sjostrom, S.B. Trickey, and V.V. Karasiev, 51st Sanibel Symposium, 26 Feb. 2011.

66. "Makeup of the Non-interacting Free Energy Density Functional", S.B. Trickey, J.W. Dufty, and T. Sjostrom, 51st Sanibel Symposium, 25 Feb. 2011.

67. "Size Effects in the Catalytic Activity of Nano-particles: A DFT Study of CO Adsorption on Pd Clusters", R. Koitz, I.V. Yudanov, T.M. Soini, A. Genest, S.B. Trickey, and N. Rösch, 51st Sanibel Symposium, 26 Feb. 2011.

68. "Improved Constraint-based GGA Functionals in Extended Systems and Molecules", S.B. Trickey, A. Vela, and J. Pacheco Kato, Amer. Phys. Soc. March 2010 meeting, contributed paper T23-02.

69. "Quenched Lieb-Oxford Satisfaction and Improved Performance for PBE-type Functionals", S.B. Trickey, V. Medel, and A. Vela, Amer. Phys. Soc. March 2009 meeting, contributed paper X13-4.

70. "Constraint-based Single-point Approximate Kinetic Energy Density functionals", F.E. Harris, V.V. Karasiev, R.S. Jones, and S.B. Trickey, Amer. Phys. Soc. March 2009 meeting, contributed paper X13-2.

71. "Incorporating a New Parallel Quantum Mechanical Worker in the PUPIL System", Oscar Bertran, Juan Torras, and S.B. Trickey, 49th Sanibel Symposium, 26 Feb. – 3 March 2009.

72. "Tightening the Lieb Oxford Bound for Atoms, Molecules, and Solids", M.M. Odashima, K. Capelle, and S.B. Trickey, 49th Sanibel Symposium, 26 Feb. – 3 March 2009.

73. "Orbital-free Kinetic Energy Density Functionals of GGA Type with Positive-definite, Finite Pauli Potentials", S.B. Trickey, V.V. Karasiev, R.S. Jones, and Frank E. Harris, Amer. Phys. Soc. March 2008 meeting, contributed paper L13-10.

74. "Recent Advances in Developing Orbital-free Kinetic Energy Functionals", V.V. Karasiev, R.S. Jones, S.B. Trickey, and Frank E. Harris, 48th Sanibel Symposium, 21-26 Feb. 2008.

75. "Angelis' Salt Secomposition, a Multiscale Study", Gustavo de M. Seabra, J. Torras-Costa, Erik Deumens, S.B. Trickey3, and Adrian Roitberg, Amer. Chem. Soc., contributed paper COMP-104, March 27, 2007.

76. "Direct Calculation of Spin-orbit Gap in Graphene", J.C. Boettger and S.B. Trickey, 47th Sanibel Symposium, 22-27 Feb. 2007.

77. "Iterative Procedure to Determine Kohn-Sham Potentials from a Given Density: Application to All-electron and Pseudo-densities", V.V. Karasiev, R.S. Jones, S.B. Trickey, and F.E. Harris, 47th Sanibel Symposium, 22-27 Feb. 2007.

78. "Incorporating Existing Large Applications in the PUPIL System: Amber", S.B. Trickey, J. Torras Costa, G. de Miranda Seabra, and A. Roitberg, Amer. Phys. Soc. March 2007 meeting, contributed paper N11-11.

79. "Graded Sequence of Approximations: Quantum Mechanical Forces", K. Runge, D.E. Taylor, V.V. Karasiev, S.B. Trickey, and F.E. Harris, Amer. Phys. Soc. March 2007 meeting, contributed paper N11-10.

80. "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

81. "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

82. "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

83. "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

84. " 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

85. "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.

86. "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.

87. "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).

88. "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).

89. "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.

90. "Exact Current DFT Study of Hooke's Atom in Magnetic Fields", Wuming Zhu and S.B. Trickey, Amer. Physical Society March Meeting 2005, paper U32.0005.

91. "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.

92. "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.

93. "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.

94. "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.

95. "Quasi-spin Density Exchange-correlation Functionals", V.V. Karasiev, S.B. Trickey, and F.E. Harris, 45th Sanibel Symposium, March 5-11, 2005.

96. "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

97. "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

98. "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.

99. "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.

100. "Tests of Perturbative DFT Total Energy Estimates Implemented in a Gaussian Basis", W. Zhu and S.B. Trickey, 43rd Sanibel Symposium, Feb. 22, 2003.

101. "MD Simulations of SiO_2 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)

102. '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)

103. "Encoding First-principles Electronic Structure Information in Classical Potentials:SiO_2" - 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).

104. "Encoding First-principles Cluster Information in Semi-Empirical Potentials: SiO_2" - A.R. Al-Derzi, K. Runge, M. Cory, W. Zhu, and S.B. Trickey, 42nd Sanibel Symposium, Feb. 23, 2002.

105. "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.

106. "A Systematic Approach to Produce Approximate Time-dependent Density Functionals" - B. Weiner and S.B. Trickey, 41st Sanibel Symposium, March 1, 2001

107. "Molecular Shape and Chemical Hardness", 39th International Sanibel Symposium, contrib. poster, 27 Feb. - 05 Mar. 1999.

108. "Approach to Bulk Behavior from Ultrathin Layered Systems: Energy Deposition", S.P. Apell, J.R. Sabin, and S.B. Trickey, 35th Internat. Sanibel Symposium, contributed poster, 28 Feb. 1995.

109. "High Precision First Principles Prediction of the Aluminum Equation of State", J.C. Boettger and S.B. Trickey, 35th Internat. Sanibel Symposium, contributed poster, 28 Feb. 1995.

110. "Energy Loss Properties of Swift Protons in Allotropic Carbon Ultra-thin Layers" Jin Zhong Wu, J. R. Sabin, S.B. Trickeyu, and J.A. Nobel, 34th Internat. Sanibel Symposium, contributed poster, 17 Feb. 1994.

111. "Theoretical Ion Implantation Profiles for Low Energy Protons under Channeling Conditions", J.A. Nobel, J.R. Sabin, S.B. Trickey, and P.M. Echenique, 34th Internat. Sanibel Symposium, contributed poster, 17 Feb. 1994.

112. "Quantum Size Effects in Hexagonal Aluminum Films", J.C. Boettger, U. Birkenheuer, N. Rösch, and S.B. Trickey, 34th Internat. Sanibel Symposium, contributed poster, 17 Feb. 1994.

113. "Quasi-classical Simulation of Channeling in Extended Systems", J.A. Nobel, J.R. Sabin, S.B. Trickey, A. Arnau, and P. Echenique, 33rd Internat. Sanibel Symposium, contributed poster, 19 Mar. 1993.

114. "Electronic Stopping Power for Protons in an LiF Monolayer and an Isolated LiF Molecule", J. Z. Wu, J. R. Sabin and S.B. Trickey, 33rd Internat. Sanibel Symposium, contributed poster, 19 Mar. 1993.

115. "Calculation of the Electronic Properties of an Ionic Monolayer: LiF", J.Z. Wu, S.B. Trickey, J.R. Sabin, and J.C. Boettger, 32nd Internat. Sanibel Symposium, contrib. paper, 20 Mar. 1992.

116. "Density Decomposition Options in the Orbital Local Plasma Approximation", D. E. Meltzer, J. R. Sabin, and S.B. Trickey, 30th Internat. Sanibel Symposium, contrib. paper, 22 Mar. 1990.

117. "Structure of Hydrogen Thin Films", J.Z. Wu, J.R. Sabin, S.B. Trickey, and J.C. Boettger, 30th Internat. Sanibel Symposium, contrib. paper, 22 Mar. 1990.

118. "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.

119. "Calculation of Orbital Mean Excitation Energies and Stopping Cross Sections in the Local Plasma Approximation", D.E. Meltzer, J.R. Sabin, and S.B. Trickey, 29th Internat. Sanibel Symposium, contrib. paper, 7 April 1989.

120. "Theoretical Properties of Hexagonal Monolayer and Dilayer Films of Lithium", J.C. Boettger and S.B. Trickey, Bull. Am. Phys. Soc. **34**, 720 (1989).

121. "Pathological Behavior of the Kohn-Sham Direct Gap at a Metal-Insulator Transition", S.B. Trickey and R.S. Jones, 27th Internat. Sanibel Symposium, contrib. paper, March 21, 1987.

122. "Theoretical Confirmation of Highly Localized Electronic Surface States in Beryllium", S.B. Trickey and J.C. Boettger, 26th Internat. Sanibel Symposium, contrib. paper, 14 March 1986.

123. "Density Functional Theory of the Band Gap of a Model Insulating System", R.S. Jones and S.B. Trickey, Bull. Am. Phys. Soc. **31**, 302 (1986).

124. "Correlated Wavefunctions for Crystalline Solids: Metal-Insulator Transitions in the Electron Gas", R.S. Jones and S.B. Trickey, Bull. Am. Phys. Soc. **30**, 226 (1985).

125. "Avoiding Orthogonality Problems in the Application of the Alternant Molecular Orbital Method to Solids", R.S. Jones and S.B. Trickey, contrib. paper 25th Internat. Sanibel Symposium, 19 March 1985.

126. Physics Department Colloquium, Univ. of Cincinnati, Mar. 14, 1984.

127. "Electronic Properties of a Be Bilayer", J.C. Boettger, J.R. Sabin, and S.B. Trickey, 24th Internat. Sanibel Symposium, contrib. paper, Mar. 8, 1984.

128. "Correlated Wavefunctions for Crystalline Solids", R.S. Jones and S.B. Trickey, 24th Internat. Sanibel Symposium, contrib. paper, Mar. 6, 1984.

129. "Generator Coordinate Treatment of Some Model Periodic Systems", Contributed Paper, IVth Internat. Congress on Quantum Chemistry, Uppsala Sweden, 14-19 June 1982.

130. "Local Density Theories and Metallization in Crystalline Xenon", Contributed Paper, Conference on Local Density Approximations, Copenhagen, Denmark, 11-12 June 1982 .

131. "Monte Carlo Calculations on Heavy Methane - Some Preliminary Results", Post-deadline Paper, Internat. Conf. on Quantum Crystals, Colorado State Univ., Ft. Collins, Colo., 8-12 August 1977.

132. "Lattice Dynamics of Hard-Core Quantum Crystals via Point Transformation Theory", N.M. Witriol, S.B. Trickey, and G.L. Morley, Bull. Am. Phys. Soc. **18**, 23 (1973).

133. "Self-Consistent APW Calculation of the Cohesive Energy and Zero Temperature PV Relation for Solid Argon", S.B. Trickey and F.W. Averill, Bull. Am. Phys. Soc. **17**, 346 (1972).

134. "Difficulties in the $\mathbf{k}\cdot\mathbf{p}$ Method Induced by d Bands", S.B. Trickey, T.J. Kuebbing, K. Schwarz, and J.B. Conklin, Jr., Bull. Am. Phys. Soc. **16**, 637 (1971).

135. "Temperature Dependence of Debye θs for bcc ^{3}He and hcp ^{4}He", E.D. Adams, P.N. Henriksen, S.B. Trickey, and M.F. Panczyk, Bull. Am. Phys. Soc. **15**, 211 (1970).

136. "Transfer Integral Treatment of a Two-Dimensional Quantum Solid", Bull. Am. Phys. Soc. **14**, 528 (1969).

137. "Single Particle Functions in One-Dimensional Quantum Crystals", Bull, Am. Phys. Soc. **13**, 91 (1968).

138. "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 S.B. Trickey, Abstracts of the Symposium on Molecular Structure and Spectroscopy, Ohio State Univ. (Sept. 1966) , p. 67.

139. "Calculation of the Rotational Constants of Ammonia", J.B. Coon and S.B. Trickey, 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. Organizing Group [Dr. Felix Hummel and Prof. Andreas Grüneis (Technische Universität Wien), Dr. Valentin Karasiev (Lab. for Laser Energetics, Univ. Rochester), S.B. Trickey] CECAM Flagship Workshop Workshop on "Accurate Methods for Thermal and Excited Electrons " Bring together experts for intense discussion on pure-state and ensemble methods for systems in which the physics requires inclusion of multiple excited many-electron states. Awarded: 02 Dec. 2024, budget 12,000 CHF $\approx$ 12,960 €. 7-9 May 2025 inclusive, Lausanne Switzerland.

2. Organizing Group [J.W. Dufty, R. Evans, J. Lutsko, S.B. Trickey] CECAM Flagship Workshop Proposal "1756. Fundamentals of Density Functional Theory for T$>$ 0 : Quantum meets Classical", awarded 26 Nov. 2018; 19-23 May 2019 Lausanne Switzerland.

3. Organizing Committee (Jorge Martín del Campo, Noa Marom, Alberto Vela), Symposium D.1, "Computational Discovery of Advanced Materials", Internat. Materials Research Congress (Sociedad Mexicana de Materiales) 19-24 August 2018.

4. Organizing Committee, "'The 'March Meeting' - A Symposium in Honor of Norman March", Namur Belgium, 21-23 November 2013.

5. Program Committee, "Computational Challenges in Warm Dense Matter", Workshop IV of the Long Program on Computational Methods in High Energy Density Plasmas, Institute for Pure and Applied Mathematics, Univ. Calif. Los Angeles, 21-25 May 2012.

6. Sanibel Symposium co-Organizer (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/$\sim$sanibel/

7. QTP Pan-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; Cuernavaca MX, Oct. 9-11, 2007.

8. Program Committee, 2009 and 2010 March Meetings, Division of Computational Physics, American Physical Society.

9. 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).

10. 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

11. 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.

12. 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.

13. Program Co-Chair, Southern Computer Center Directors Conference (1996 and 1997 meetings).

14. Member, Scientific Committee, Third UNAM-Cray Supercomputing Conference, August 1996, México DF.

15. Advisory Committee, Symposium on 30th Anniversary of Density Functional Theory, Cracow Poland, 13 - 16 June 1994.

16. 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

17. 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.

18. Member, Local Organizing Committee, Quantum Fluids and Solids 1983, 10-15 April 1983, Sanibel Island Florida.

19. Member, Local Organizing Committee, International Symposium on Super-heavy Elements, Texas Tech Univ., 9-11 March 1978.

20. Member of Advisory Committee, International Conference on Quantum Crystals, Colorado State University, 8-12 Aug. 1977.

Teaching

- *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).

Current Graduate Commitees (Univ. of Florida)
Eric Fonseca (Materials Science and Eng.), graduated Aug. 2024

Texas Tech University None

Postdoctoral Associates Tun Sheng Tan (2020 - 2022), Héctor Francisco Rodríguez (2020 - present), Angel Martín Albavera Mata (2020 - present); Long Zhang (2018 - 2023); Daniel Mejía Rodríguez (2016 - 2020); Kai Luo (2017 - 2019); Jeffrey Wrighton (2016 - 2019); Lázaro Calderín (senior Postdoc 2015 - 2017); Debajit Chakraborty (2012 - 2016); Vivek Kapila (2011-2012); Támas Gál (senior Postdoc, 2011 - 2012); Travis Sjostrom (2009 - 2012); Valentin Karasiev (senior Postdoc, 2009-2016, 2004 - 2006; Asst. Scientist 2016-2017); Krishna Muralidharan (2004 - 2006); Juan Torras Costa (senior Postdoc, 2004 - 2006); Wuming Zhu (2005 - 2006); J. Ashley Alford (2003 - 2005 at UF; partial support 2006-2007 at ORNL); Andrew M. Kolchin (2002); Norbert Flocke (2000 - 2002); Richard J. Mathar (1995 - 1998); Jian Wang (1996 - 1997); Steven A. Alexander (1995); Jan A. Nobel (1988 - 1994); Jin Zhong Wu (1988 - 1994); Gary R. Bamford (1988); David E. Meltzer (1987-1990); Randall S. Jones (1982-1985); Jonathan C. Boettger (1981-1984); Asok K. Ray (1979-1981; deceased); Joseph P. Worth (1976-1977); Bernard C. Laskowski (1975-1976).

University Service

1. Departmental

   - Search Committee, Physics, Visiting Asst. Prof. in Quantum Information Sciences, May-July 2019.
   - Consulting member, Informatics Faculty Search Committee (2013-14)
   - 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 - 2007)
- Committee on Computational Sciences Curriculum [Chair], College of Liberal Arts and Sciences (2004 - 2006)
- High-Performance Computing Committee, College of Liberal Arts and Sciences (2003 - 2006)
- Steering Committee for Networked Writing Environment, College of Liberal Arts and Sciences (1997 - 1999)
- Steering Committee, Imaging Systems Sciences and Technologies Center Project (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 - 2010)
- 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, Microfabritech^{TM} (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

"QLCI Preliminary Proposal - Molecular Coherent Spin Platforms for Quantum Applications", Xg. Zhang, PI, H-P Cheng, M. Shatruk, L. Kim, and R.G. Hennig co-PIs; S.B.T. and 13 others as Senior Investigators, Nat. Sci. Foundation, $25,000,000 proposed for 6 years, beginning Sept. 2026. Pending; submitted 07 March 2025.

"Exploring Exascale Quantum Chemistry Methods for Transition Metal Chemistry", ASCR 2024 Leadership Computing Challenge Award, (Pacific Northwest National Lab.), D. Mejía Rodríguez PI. UF co-PIs: A. Albavera Mata, R.G. Hennig, S.B. Trickey. 313,442 node hours on Frontier (Oak Ridge N.L.); 145,628 node-hours on Aurora (Argonne N.L.). 01 July 2024 - 30 June 2025.

"Quantum Theory, Quantum Materials, Quantum Computing: Thematic Program for 63rd Sanibel Symposium", Xg. Zhang PI, J.F. Stanton, and S.B. Trickey co-PIs, U.S. Dept. of Energy Computational and Theoretical Chem. Program, $17,000 proposed, submitted 21 Sept. 2023; approved by Theoretical Cond. Matter Physics Program, 28 Dec. 2023. $17,000 for one year.

U.S. Dept. of Energy, Basic Energy Sciences, "Quantum Theory, Quantum Materials, Quantum Computing: Thematic Program for 61st Sanibel Symposium", H.-P. Cheng P.I., S.B. Trickey co-P.I., $15,000; 15 Jan. 2022 for one year.

U.S. National Science Foundation(Cond. Matter Materials Theory), "Pure Density Functionals for Efficient, Predictive Simulations", 3 years, $400,000, S.B. Trickey P.I., A. Cancio (Ball State U.) co-PI (subaward); DMR-1912618, 01 May 2020-30 April 2023, NCE to 31 Dec. 2024.

U.S. National Science Foundation, "QLCI-CG: Conceptualization of The Institute for Quantum Biology on Quantum Computers", Quantum Leap Challenge Institutes Conceptualization grant, 1 year, $149,999, Beverly Sanders P.I.; proposal OMA-1936853, awarded 14 Aug. 2019.

Joy McCann Foundation,"M^2QM Special Support", 2 years, $15,000; H-P. Cheng and M. Atherton (UF Foundation); drafted by S.B. Trickey, H-P. Cheng, and X. Zhang; awarded 16 Nov. 2018.

U.S. Dept. of Energy, Energy Frontier Research Center, grant DE-SC0019330, "Center for Molecular Magnetic Quantum Materials", H-P. Cheng PI, S.B. Trickey and 10 other co-PIs, $10,500,000, 01 August 2018 - 31 July 2022; renewal 01 August 2022 - 31 July 2026, $12,600,000.

U.S. Dept. of Energy (Basic Energy Sciences, Multi-Investigator Theory, Modeling, and Simulation Projects), DE-SC 0002139, "Orbital-free Quantum Simulation Methods for Application to Warm Dense Matter", S.B. Trickey PI, F.E. Harris, J.W. Dufty, and K. Runge co-PIs, $1,275,000, 01 Sept. 2009 - 31 Aug. 2013; renewal $765,000, 01 Sept. 2013 - 31 Aug. 2016. Renewal 01 Sept. 2016

- 31 August 2019 (S.B. Trickey PI, J.W. Dufty co-PI) $735,000; supplement 24 July 2018 $15,000. Renewal 01 sept. 2019 - 31 August 2023 (S.B. Trickey PI, J.W. Dufty co-PI) $360,000.

U.S. Dept. of Energy, Basic Energy Sciences,"Quantum Theory, Quantum Materials, Quantum Computing: Thematic Program for 60th Sanibel Symposium", 1 year, $15,000, H-P. Cheng P.I., S.B. Trickey co-PI, proposal 0000249279, awarded 10 Jan. 2020.

U.S. National Science Foundation (Cond. Matter and Materials Theory), "EAGER: Rung-reduced Density Functionals for Cost-capped ab initio Molecular Dynamics", S.B. Trickey PI, $160,844; award DMR-1515307, 01 Sept. 2015 - 31 Aug. 2018.

U.S. Dept. of Energy, Basic Energy Sciences, "Magnetism in Molecules, Interfaces, and Junctions - Thematic Program for 2018 Sanibel Symposium", H.-P. Cheng P.I., S.B. Trickey co-P.I., $15,000; 15 Jan. 2018 for one year.

Joy McCann Foundation, H-P. Cheng, X-G. Zhang and S.B. Trickey, $20,000 program support for Sanibel Symposium. Letter proposal 10 Nov. 2015, awarded 10 Dec. 2015.

U.S. Dept. of Energy, Basic Energy Sciences, Theoretical Condensed Matter Physics and Theoretical Chemistry Programs, "Partial Financial Support of the 54th Sanibel Symposium", H-P. Cheng and S.B. Trickey co-PIs, proposed one year $15,000, submitted Aug. 2013, awarded Dec. 2013.

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.

U.S. 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.

U.S. 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.

U.S. 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.

U.S. National Science Foundation KDI(DMR)-9980015 (1999-2003) $2,200,001 "Multi-scale Simulation Including Chemical Reactivity of Materials Behavior through Integrated Computational Heirarchies", R.J. Bartlett, PI, H-P. Cheng, J.H. Simmons, S.B. Trickey, and M.C. Zerner, co-PIs

U.S. 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.

U.S. 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.

U.S. 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.

U.S. 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.

U.S. 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.

U.S. 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.

U.S. 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).

U.S. 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, Univ. Florida, 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.

U.S. National Science Foundation, DMR8218498 (1983-86) $197,400, "Quantum Theory of Solids and Molecules", Co-Principal Investigators: S.B. Trickey and J.R. Sabin.

U.S. National Science Foundation, CHE84–02203 $11,255 "Symposium on Impact of Computers on Quantum Theory of Matter", Sanibel Symposia 1984, S.B. Trickey and N.Y. Öhrn.

U.S. National Science Foundation, 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, Univ. Florida, Seed Money Grant (1980-81) $1,600 "Rotational Ordering in Molecular Crystals", S.B. Trickey.

U.S. National Science Foundation, DMR79-09721 (1980-82) $195,200 "Quantum Theory of Solids and Molecules", Co-Principal Investigators: J.R. Sabin and S.B. Trickey.

U.S. National Science Foundation and Air Force of Scientific Research, $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.

U.S. National Science Foundation, 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).

U.S. National Science Foundation, 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

U.S. National Science Foundation, (1978) "International Symposium on Superheavy Elements", M.A.K. Lodhi and S.B. Trickey, $2,000.

Other Professional Service

- International Committee, Div. of Computational Physics, American Physical Society, 2011-2012.
- Scientific Oversight Commmittee for Computational Materials Science Network, U.S. Department of Energy, 2003-2010.
- Nominating Committee, Division of Computational Physics, American Physical Society (2003-06; Chair 2004-06)
- Program Committee (March Meeting), Division of Computational Physics, American Physical Society (2009, 2010 meetings)
- Panelist, Warm Dense Matter Sub-panel, High Energy Density Laboratory Plasmas Panel, Fusion Energy Science Div., US Dept. of Energy, Rockville MD, 14 - 18 Nov. 2009.
- INCITE ("Innovative and Novel Computational Impact on Theory and Experiment') Review Panel, US Dept. of Energy, Sept. 13-14, 2005; Nov. 2, 2006.
- Site Reviewer, Ames National Laboratory, (U.S. Dept. of Energy, Div. Basic Energy Sciences), Ames Iowa, 25-26 May 2010 (5 proposals)
- 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 between 6 & 10 total proposals and one panel 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, Fusion Energy Sciences Division.
  - Petroleum Research Fund of American Chemical Society.
  - Research Corporation
  - National Science and Engineering Research Council (Canada)
  - Austrian Science Fund (FWF)
  - Comisión Nacional de Investigación Cientfica y Tecnológia (Chile)
  - Research Council of Norway
  - Swiss State Secretariat for Education and Research

- Reviewer for: *Nature*, *Science*, *Reviews of Modern Physics*, *Physical Review Letters*, *Physical Review A*, *Physical Review B*, *Physical Review E*, *Physical Review X*, *Physical Review Materials*, *Journal of Physics A*, *Journal of Physics B*, *Journal of Physics Cond. Matter*, *Journal of Applied Physics*, *Journal of Chemical Physics*, *Computer Physics Communications*, *Surface Science*, *Modern Physics Letters B*, *Chemical Physics*, *Chemical Physics Letters*, *Molecular Physics*, *American Journal of Physics*, *Europhysics Letters*, *Computational Materials Science*, *High Energy Density Physics*, *New Journal of Physics*, *Journal of Molecular Modeling*, *Physica Scripta*, *Journal of Physics and Chemistry of Solids*, *Journal of Physical Chemistry C*, *Journal of Physical Chemistry Letters*, *Journal of Chemical Theory and Computation*, *Journal of the Mexican Chemical Society*, *Journal of the American Chemical Society*, *Physical Chemistry Chemical Physics*, *Journal of Theoretical and Computational Chemistry*, *Journal of Computational Chemistry*, *Advances in Quantum Chemistry*, *International Journal of Quantum Chemistry*, *Theoretical Chemistry Accounts*, *Journal of Computational and Theoretical Nanoscience*, *Modeling and Simulation in Materials Science and Engineering*, *Radiation Physics and Chemistry*, *Radiation Effects and Defects in Solids*, *Journal of Nuclear Materials*

- Coalition for Advanced Scientific Computing (formerly, Coalition for Academic Scientific Computing, Coalition of Academic Supercomputing Centers; "CASC"), 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); 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, Univ. Arizona, Peking Univ.

Involvement in the Life of the Wider Community

- Board of Directors and Executive Committee, National Farm Worker Ministry (President, 2001 - 2004; also variously Vice President, Treasurer, Secretary). Board member for more than 30 years.
- Co-founder, Board Member, and Corporate Secretary, Welcoming Gainesville Inc. (Jan. 2015 - Dec. 2018).
- Volunteer, Family Promise (ex Interfaith Hospitality Network) 2005 - present.
- 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 organ recital series, Westminster Presbyterian Church, Gainesville.
- Co-awardee, with Bill Powers, Wayzata Yacht Club, Apostle Islands Station, *Doc Sam Award*, 2009.
- Gulf Atlantic Yacht Club, Gainesville: Commodore (2004 - 2006); Vice Commodore (2001 - 2004), Secretary (1999 - 2001; 2019 - 2024), Race Committee Chair (1997 - 1999).