Curriculum Vitae

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Education

Indiana University, Honors B.S. with highest distinction, 1992, in Chemistry
University of Florida, Ph.D., 1997, in Physical Chemistry

Professional Preparation

1990-1992: Undergraduate Research, Department of Chemistry, Indiana University, under Prof. Ernest R. Davidson

1992-1997: Graduate Student, Department of Chemistry and the Quantum Theory Project, University of Florida, under Prof. Rodney J. Bartlett
Dissertation title: *Coupled-Cluster Based Methods for Excited State Energies and Gradients*.

1998-2002: Postdoctoral Fellow, Department of Chemistry, University of California, Berkeley, under Prof. Martin Head-Gordon

Professional Appointments

2002-2008: Assistant Professor, Department of Chemistry, Mississippi State University

2002-Present: Member, Center for Computational Sciences, Mississippi State University

2003-Present: Member, Center for Environmental Health Sciences, Mississippi State University

2008-2016: Associate Professor, Department of Chemistry, Mississippi State University

2016-Present: Professor, Department of Chemistry, Mississippi State University

2018-Present: Member, Advanced Composites Institute, Mississippi State University

Journal Articles (h index of 32)

1. S. J. Chakravorty, **S. R. Gwaltney**, E. R. Davidson, F. A. Parpia, and C. Froese Fischer, "Ground-state correlation energies for atomic ions with 3 to 18 electrons," Phys. Rev. A **47**, 3649-3670 (1993).
2. **S. R. Gwaltney** and R. J. Bartlett, "Comment on: The relation between intensity and dipole moment for bending modes in linear molecules," J. Chem. Phys. **99**, 3151-3152 (1993).
3. X. Song, E. R. Davidson, **S. R. Gwaltney**, and J. P. Reilly, "High-resolution zero kinetic energy photoelectron spectra of para-*n*-propylanaline," J. Chem. Phys. **100**, 5411-5421 (1994).
4. **S. R. Gwaltney** and R. J. Bartlett, "An application of the equation-of-motion coupled cluster method to the excited states of formaldehyde, acetaldehyde, and acetone," Chem. Phys. Lett. **241**, 26-32 (1995).
5. **S. R. Gwaltney**, M. Nooijen, and R. J. Bartlett, "Simplified methods for equation-of-motion coupled-cluster excited state calculations," Chem. Phys. Lett. **248**, 189-198 (1996).
6. J. D. Watts, **S. R. Gwaltney**, and R. J. Bartlett, "Coupled-cluster calculations of the excitation energies of ethylene, butadiene, and cyclopentadiene," J. Chem. Phys. **105**, 6979-6988 (1996).
7. R. R. Sadeghi, **S. R. Gwaltney**, J. L. Krause, R. T. Skodje, and P. M. Weber, "Structure and dynamics of the S_3 state of CS_2," J. Chem. Phys. **107**, 6570-6576 (1997).
8. **S. R. Gwaltney** and R. J. Bartlett, "Coupled-cluster calculations of the electronic excitation spectrum of free base porphin in a polarized basis," J. Chem. Phys. **108**, 6790-6798 (1998).
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10. **S. R. Gwaltney** and R. J. Bartlett, "Gradients for the partitioned equation-of-motion coupled-cluster method," J. Chem. Phys. **110**, 62-71 (1999).
11. **S. R. Gwaltney**, R. J. Bartlett, and M. Nooijen, "Gradients for the similarity transformed equation-of-motion coupled-cluster method," J. Chem. Phys. **111**, 58-64 (1999).
12. **S. R. Gwaltney** and M. Head-Gordon, "A second-order correction to singles and doubles coupled-cluster methods based on a perturbative expansion of a similarity-transformed Hamiltonian," Chem. Phys. Lett. **323**, 21-28 (2000).
13. **S. R. Gwaltney**, C. D. Sherrill, M. Head-Gordon, and A. I. Krylov, "Second order perturbation corrections to singles and doubles coupled-cluster methods: General theory and application to the valence optimized doubles model," J. Chem. Phys. **113**, 3548-3560 (2000).
14. J. Kong, C. A. White, A. I. Krylov, D. Sherrill, R. D. Adamson, T. R. Furlani, M. S. Lee, A. M. Lee, **S. R. Gwaltney**, T. R. Adams, C. Ochsenfeld, A. T. B. Gilbert, G. S. Kedziora, V. A. Rassolov, D. R. Maurice, N. Nair, Y. Shao, N. A. Besley, P. E. Maslen, J. P. Dombroski, H. Daschel, W. Zhang, P. P. Korambath, J. Baker, E. F. C. Byrd, T. Van Voorhis, M. Oumi, S. Hirata, C.-P. Hsu, N. Ishikawa, J. Florian, A. Warshel, B. G. Johnson, P. M. W. Gill, M. Head-Gordon, and J. A. Pople, "Q-Chem 2.0: a high-performance *ab initio* electronic structure program package," J. Comp. Chem. **21**, 1532-1548 (2000).
15. **S. R. Gwaltney** and M. Head-Gordon, "A second-order perturbative correction to the coupled-cluster singles and doubles method: CCSD(2)," J. Chem. Phys. **115**, 2014-2021 (2001).
16. **S. R. Gwaltney** and M. Head-Gordon, "Calculating the equilibrium structure of the BNB molecule: Real *vs*. artifactual symmetry breaking," Phys. Chem. Chem. Phys. **3**, 4495-4500

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18. G. J. O. Beran, **S. R. Gwaltney**, and M. Head-Gordon, "Can coupled cluster singles and doubles be approximated by a valence active space model?", J. Chem. Phys. **117**, 3040-3048 (2002).
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21. K. S. Thanthiriwatte and **S. R. Gwaltney**, "Excitation Spectra of Dibenzoborole Containing π-Electron Systems: Controlling the Electronic Spectra by Changing the $p_\pi - \pi^*$ Conjugation," J. Phys. Chem. A **110**, 2434-2439 (2006).
22. G. J. O. Beran, M. Head-Gordon, and **S. R. Gwaltney**, "Second order correction to perfect pairing: An inexpensive electronic structure method for the treatment of strong electron-electron correlations," J. Chem. Phys. **124**, 114107 (2006) (15 pages).
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35. T. Pechan and **S. R. Gwaltney**, "Calculations of relative intensities of fragment ions in the MSMS spectra of doubly charged penta-peptide," BMC Bioinformatics **13**(Suppl 15), S13 (2012) (DOI: 10.1186/1471-2105-13-S15-S13).
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47. S. Chen, S. Sun, C. Li, C. U. Pittman Jr., T. E. Lacy, S. Hu, and **S. R. Gwaltney**, "Behavior of protruding lateral plane graphene sheets in liquid dodecane: molecular dynamics simulations," J. Nanopart. Res. **18**, 317 (2016) (DOI: 10.1007/s11051-016-3645-1).
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Embedded-Atom Method with Bond Order (MEAM-BO)," J. Phys. Chem. A **121**, 1502-1524 (2017) (DOI: 10.1021/acs.jpca.6b11343).

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51. M. A. Tschopp, B. C. Rinderspacher, S. Nouranian, M. I. Baskes, **S. R. Gwaltney**, and M. F. Horstemeyer, "Quantifying Parameter Sensitivity and Uncertainty for Interatomic Potential Design: Application to Saturated Hydrocarbons," ASME J. Risk Uncertainty Part B **4**, 011004 (2018) (17 pages) (DOI: 10.1115/1.4037455).
52. R. C. Fortenberry and **S. R. Gwaltney**, "NeON+: An Atom *and* a Molecule," ACS Earth Space Chem **2**, 491-495 (2018) (DOI: 10.1021/acsearthspacechem.8b00019).
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54. D. Dickel, **S. R. Gwaltney**, S. Mun, M. I. Baskes, and M. F. Horstemeyer, "A Dispersion-Corrected Modified Embedded-Atom Method Bond Order Interatomic Potential for Sulfur," J. Phys. Chem. A **122**, 9572-9578 (2018) (DOI: 10.1021/acs.jpca.8b07410).
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56. D. Jinasena, J. Bowleg, R. Simmons, Y. Zhang, **S. R. Gwaltney**, and N. C. Fitzkee, "Using Histone H1 Derived Peptides to Investigate Binding Affinity and Inter-Domain Dynamics in Human Pin1," Biophys. J. **116**, 463a (2019) (DOI: 10.1016/j.bpj.2018.11.2500).
57. A. Bowman, S. Mun, S. Nouranian, **S. R. Gwaltney**, B. D. Huddleston, M. Baskes, and M. F. Horstemeyer, "Free Volume and Internal Structural Evolution During Creep in Amorphous Polyethylene by Molecular Dynamics Simulations," Polymer **170**, 85-100 (2019) (DOI: 10.1016/j.polymer.2019.02.060).
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C. N. Scott, "Thienylpiperidine donor NIR xanthene-based dye for photoacoustic imaging," Org. Lett. **23,** 7640-7644 (2021) (DOI: 10.1021/acs.orglett.1c02862).

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64. R. M. O. Nayanathara, W. Leng, S. D. Liyanage, X. Wang, L. Wang, J. Wang, Z. Tian, C. U. Pittman Jr., **S. R. Gwaltney**, X. Zhang, "A general Metal-Ion-Modification route for preparing hydrophobic paper and tableware from lignocellulose fibers," Chem. Eng. J. **459**, 141596 (2023) (DOI: 10.1016/j.cej.2023.141596).
65. C. S. L. Rathnamalala, S. Hernandez, M. Y. Lucero, C. B. Swartchick, A. K. Shaik, N. I. Hammer, A. K. East, **S. R. Gwaltney**, J. Chan, and C. N. Scott, "Xanthene-based nitric oxide-responsive nanosensor for photoacoustic imaging in the SWIR window," Angew. Chem. **135**, e202214855 (2023) (DOI: 10.1002/anie.202214855).
66. J. L. Bowleg, C. G. Mikek, and **S. R. Gwaltney**, "Computed interactions of Berenil with restricted foldamers of c-MYC DNA G-quadruplexes," J. Biomol. Struct. Dyn. **42**, 2162-2169 (2024) (DOI: 10.1080/07391102.2023.2217913).
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68. S. D. Liyanage, J. L. Bowleg, and **S. R. Gwaltney**, "Computational modeling to understand the Interaction of TMPyP4 with a G- Quadruplex," J. Biomol. Struct. Dyn. (submitted).

Book Chapters

1. M. Head-Gordon, M. Lee, P. Maslen, T. Van Voorhis, and **S. Gwaltney**, "Tensors in Electronic Structure Theory: Basic Concepts and Applications to Electron Correlation Models," in *Modern Methods and Algorithms of Quantum Chemistry Proceedings, Second Edition*, NIC Series Vol. 3, edited by J. Grotendorst (John von Neumann Institute for Computing, Jülich, 2000), pp. 593-638.
2. M. Head-Gordon, T. Van Voorhis, **S. R. Gwaltney**, and E. F. C. Byrd, "Coupled Cluster Methods for Bond-Breaking," in *Low-Lying Potential Energy Surfaces*, ACS Symposium Series No. 828, edited by M. R. Hoffmann and K. G. Dyall (American Chemical Society, Washington DC, 2002), pp. 93-108.
3. **S. R. Gwaltney**, G. J. O. Beran, and M. Head-Gordon, "Partitioning Techniques in Coupled-Cluster Theory," in *Fundamental World of Quantum Chemistry: A Tribute to the Memory of Per-Olav Löwdin*, Vol. 1, edited by E. J. Brändas and E. S. Kryachko (Kluwer Academic Publishers, Dordrecht, 2003), pp. 433-457.
4. T. E. Lacy, **S. Gwaltney**, C. U. Pittman, Jr., H. Toghiani, C. Jang, S. Nouranian, and J. Yu, "Some Key Issues in Multi-Scale Modeling of Thermoset Nanocomposites/Composites," in *Tools, Models, Databases, and Simulation Tools Developed and Needed to Realize the Vision of Integrated Computational Materials Engineering*, edited by S.M. Arnold and T. Wong

(ASM International, Materials Park, OH, 2011) pp. 128-140.
5. H. U. Rehman and **S. R. Gwaltney**, "Structure and Energetics of Polyhedral Oligomeric Silsesquioxane (T_8, T_{10}, T_{12}–POSS) cages with Atomic and Ionic Lithium Species," in *Practical Aspects of Computational Chemistry III*, edited by J. Leszczynski and M. Shukla (Springer, New York, 2014), pp. 151-165 (DOI: 10.1007/978-1-4899-7445-7_5).
6. D. Dickel, S. Mun, M. Baskes, **S. Gwaltney**, R. K. Prabhu, and M. F. Horstemeyer, "Density functional theory and bridging to classical interatomic force fields," in *Multiscale Biomechanical Modeling of the Brain*, edited by R. K. Prabhu and M. F. Horstemeyer (Academic Press, London, 2022), pp. 39-52 (DOI: 10.1016/B978-0-12-818144-7.00007-4).

Invited Talks

1. "Quantum Chemistry for the Hard Problems," Indiana University, Bloomington, IN, October 5, 2000.
2. "Inner Sphere Electron Transfer Complexes," National Institute of Standards and Technology, Gaithersburg, MD, November 27, 2001.
3. "Inner Sphere Electron Transfer Complexes," University of Southern California, Los Angeles, CA, June 25, 2002.
4. "The Role of Electron Transfer in Nitration and Nitrosation," University of Mississippi, Oxford, MS, November 7, 2002.
5. "Breaking Bonds Perturbatively," American Chemical Society National Meeting, New York, NY, September 9, 2003.
6. "A Powerful Perturbation Procedure for a Perfect Pairing Parameterization," The Systematic Treatment of Electronic Correlation. A Celebration of the Science of Rodney J. Bartlett, St. Simons Island, GA, April 24, 2004.
7. "The Mechanism of Aromatic Nitration," Southeastern Theoretical Chemistry Association (SETCA) 04, Oxford, MS, May 21, 2004.
8. "The Mechanism of Aromatic Nitration," Jackson State University, Jackson, MS, October 22, 2004.
9. "Multi-Step Model for the Molecular Mechanism of Organophosphates Binding with Acetylcholinesterase," American Chemical Society National Meeting, Washington, DC, August 29, 2005.
10. "Molecular Modeling to Understand Pesticide Toxicity," Waterways Experiment Station, Vicksburg, MS, October 18, 2006.
11. "Molecular Modeling to Understand Pesticide Toxicity," University of Alabama Huntsville, Huntsville, AL, November 17, 2006.
12. "A Molecular Mechanism for Decreased Activity in Mutant pnb CE Enzymes," Southeastern Theoretical Chemistry Association (SETCA) 08, Tuscaloosa, AL, May 23, 2008.
13. "An Overview of Computational Chemistry," Bioscience Review 2008 breakout session, Hunt Valley, MD, June 5, 2008.
14. "Implicit Solvation Models for Coupled-Cluster Theory," The Sixth Congress of the International Society for Theoretical Chemical Physics (ISTCP-VI), Vancouver, BC, July 21, 2008.
15. "Substrate Specificity in Carboxylesterate Binding," Theory and Application of Computational Chemistry (TACC), Shanghai, China, September 27, 2008.
16. "Capturing External Correlation in Reduced Orbital Space Approaches," Southeastern

Theoretical Chemistry Association (SETCA) 2010, Columbia, SC, May 22, 2010.
17. "Computational Chemistry for Designing Better Reactivators", Mississippi Biophysical Consortium, Jackson, MS, June 3, 2010.
18. "Understanding Differences in Activities of Oxime Reactivators through Molecular Dynamics," Southeastern Regional Meeting of the American Chemical Society (SERMACS), New Orleans, LA, December 2, 2010.
19. "Better Ways to Counter Nerve Gases through Computational Chemistry," Auburn University, Auburn, AL, October 6, 2011.
20. "Molecular Dynamics Simulations of Vinyl Ester Resin Monomers Interacting with Vapor-Grown Carbon Nanofibers," Mississippi Academy of Sciences, Hattiesburg, MS, February 24, 2012.
21. "Better Ways to Counter Nerve Gases through Computational Chemistry," Jackson State University, Jackson, MS, May 4, 2012.
22. "Why Does Entropy Have to be so Hard?" Southeastern Theoretical Chemistry Association (SETCA) 2012, Athens, GA, May 19, 2012.
23. "Why Does Entropy Have to be so Hard?" Mississippi College, Clinton, MS, October 15, 2012.
24. "Why Does Entropy Have to be so Hard?" Current Trends in Computational Chemistry (CCTCC), Jackson, MS, November 9, 2012.
25. "The Character of the Interphase Region between a Vinyl Ester and Graphene," Polymer Composites and High Performance Materials, Santa Rosa, CA, July 23, 2013.
26. "The Character of the Interphase Region between a Vinyl Ester and Graphene," ACS Southwest Regional Meeting, Waco, TX, November 17, 2013.
27. "Novel Nucleophiles to Negate Nerve Agents," Sanibel Symposium, St. Simons Island, GA, February 16, 2016.
28. "Novel Nucleophiles to Negate Nerve Gases," Southeastern Theoretical Chemistry Association (SETCA) 2016, Tallahassee, FL, May 14, 2016.
29. "Novel Nucleophiles to Negate Nerve Gases," Southern School on Computational Chemistry and Materials Science, Jackson, MS, July 28, 2016.
30. "Novel Nucleophiles to Negate Nerve Gases," Mississippi College, Clinton, MS, December 1, 2016.
31. "Reduced Active Spaces and External Correlation," Sanibel Symposium, St. Simon's Island, GA, February 24, 2017.
32. "Novel Nucleophiles to Negate Nerve Agents," US Army Engineer Research and Development Center (ERDC), Computational Chemistry/Computational Modeling Meeting, Vicksburg, MS, September 12, 2017.
33. "Using Computer Modeling to Understand how Drugs Bind to DNA," Tougaloo College, Jackson, MS, January 28, 2019.
34. "The Structure of Diminazene Binding to G-Quadruplex DNA," 35th Southern Biomedical Engineering Conference, Hattiesburg, MS, February 23, 2019.