

Curriculum Vitae

Steven R. Gwaltney

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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

Honors

Member, Phi Beta Kappa, 1991-present

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 28)

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*-propylaniline," *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 S₃ state of CS₂," *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 porphyrin in a polarized basis," *J. Chem. Phys.* **108**, 6790-6798 (1998).
9. J. E. Del Bene, **S. R. Gwaltney**, and R. J. Bartlett, "Base properties of H₂CO in the excited ¹n→π* state," *J. Phys. Chem. A* **102**, 5124-5127 (1998).
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 (2001).

17. **S. R. Gwaltney**, E. F. C. Byrd, T. Van Voorhis, and M. Head-Gordon, "A perturbative correction to the quadratic coupled-cluster doubles method for higher excitations," *Chem. Phys. Lett.* **353**, 359-367 (2002).
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).
19. **S. R. Gwaltney**, S. V. Rosokha, M. Head-Gordon, and J. K. Kochi, "Charge-Transfer Mechanism for Electrophilic Aromatic Nitration and Nitrosation via the Convergence of (ab Initio) Molecular-Orbital and Marcus-Hush Theories with Experiments," *J. Am. Chem. Soc.* **125**, 3273-3283 (2003).
20. G. J. O. Beran, **S. R. Gwaltney**, and M. Head-Gordon, "Approaching closed-shell accuracy for radicals using coupled cluster theory with perturbative triple substitutions," *Phys. Chem. Chem. Phys.* **5**, 2488-2493 (2003).
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).
23. Y. Shao, L. Fusti-Molnar, Y. Jung, J. Kussmann, C. Ochsenfeld, S. T. Brown, A. T. B. Gilbert, L. V. Slipchenko, S. V. Levchenko, D. P. O'Neill, R. A. Distasio Jr., R. C. Lochan, T. Wang, G. J. O. Beran, N. A. Besley, J. M. Herbert, C. Y. Lin, T. Van Voorhis, S. H. Chien, A. Sodt, R. P. Steele, V. A. Rassolov, P. E. Maslen, P. P. Korambath, R. D. Adamson, B. Austin, J. Baker, E. F. C. Byrd, H. Daschel, R. J. Doerksen, A. Dreuw, B. D. Dunietz, A. D. Dutoi, T. R. Furlani, **S. R. Gwaltney**, A. Heyden, S. Hirata, C.-P. Hsu, G. Kedziora, R. Z. Khalliulin, P. Klunzinger, A. M. Lee, M. S. Lee, W. Liang, I. Lotan, N. Nair, B. Peters, E. I. Proynov, P. A. Pieniazek, Y. M. Rhee, J. Ritchie, E. Rosta, C. D. Sherrill, A. C. Simmonett, J. E. Subotnik, H. L. Woodcock III, W. Zhang, A. T. Bell, A. K. Chakraborty, D. M. Chipman, F. J. Keil, A. Warshel, W. J. Hehre, H. F. Schaefer III, J. Kong, A. I. Krylov, P. M. W. Gill, and M. Head-Gordon, "Advances in methods and algorithms in a modern quantum chemistry program package," *Phys. Chem. Chem. Phys.* **8**, 3172-3191 (2006).
24. N. Binbuga, J. K. Hasty, **S. R. Gwaltney**, W. P. Henry, and T. P. Shultz, "Determination of the stability constants for the binding of sulfonated morin with Fe^{2+} ," *Inorg. Chim. Acta* **360**, 2339-2344 (2007).
25. S. Adhikaria, S. Fernando, **S. R. Gwaltney**, S. D. F. To, R. M. Bricka, P. H. Steele, and A. Haryanto, "A thermodynamic analysis of hydrogen production by steam reforming of glycerol," *Int. J. Hydrogen Energy* **32**, 2875-2880 (2007).
26. D. Hossain, C. U. Pittman Jr., and **S. R. Gwaltney**, "Structures and stabilities of copper encapsulated within silicon nano-clusters: $Cu@Si_n$ ($n = 9-15$)," *Chem. Phys. Lett.* **451**, 93-97 (2008).
27. T. M. Streit, A. Borazjani, S. E. Lentz, M. Wierdl, P. M. Potter, **S. R. Gwaltney**, and M. K. Ross, "Evaluation of the 'side-door' in carboxylesterase-mediated catalysis and inhibition," *Biol. Chem.* **389**, 149-162 (2008).
28. D. Hossain, **S. R. Gwaltney**, C. U. Pittman Jr., and S. Saebø, "Insertion of transition metal atoms and ions into the nanoscale dodecahedral silsesquioxane (T_{12} -POSS) cage: Structures, stabilities and electronic properties," *Chem. Phys. Lett.* **467**, 348-353 (2009).

29. J. A. Yancey, M. A. Novotny, and **S. R. Gwaltney**, “Small Pure Carbon Molecules with Small World Networks using Density Functional Theory Simulations,” *Int. J. Modern Phys. C* **20**, 1345-1356 (2009).
30. C. Liyanapatirana, **S. R. Gwaltney**, and K. Xia, “Transformation of Triclosan by Fe(III)-Saturated Montmorillonite,” *Environ. Sci. Technol.* **44**, 668-674 (2010).
31. S. Nouranian, C. Jang, T. E. Lacy, **S. R. Gwaltney**, H. Toghiani, and C. U. Pittman, Jr., “Molecular dynamics simulations of vinyl ester resin monomer interactions with a vapor-grown carbon nanofiber and their implications for composite interphase formation,” *Carbon* **49**, 3219-3232 (2011).
32. C. Jang, S. Nouranian, T. E. Lacy, **S. R. Gwaltney**, H. Toghiani, and C. U. Pittman, Jr., “Molecular dynamics simulations of oxidized vapor-grown carbon nanofiber surface interactions with vinyl ester resin monomers,” *Carbon* **50**, 748-760 (2012) (DOI: 10.1016/j.carbon.2011.09.013).
33. X. Yu, S. C. Sigler, D. Hossain, M. Wierdl, **S. R. Gwaltney**, P. M. Potter, and R. M. Wadkins, “Global and local molecular dynamics of a bacterial carboxylesterase provide insight into its catalytic mechanism,” *J. Mol. Model.* **18**, 2869-2883 (2012) (DOI: 10.1007/s00894-011-1308-9).
34. C. Jang, T. E. Lacy, **S. R. Gwaltney**, H. Toghiani, and C. U. Pittman, Jr., “Relative Reactivity Volume Criterion for Crosslinking: Application to Vinyl Ester Resin Molecular Dynamics Simulations,” *Macromolecules* **45**, 4876-4885 (2012) (doi: 10.1021/ma202754d), Errata: **45**, 5619-5619 (2012) (DOI: 10.1021/ma301156u).
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).
36. M. Bhavaraju and **S. R. Gwaltney**, “A Comparison of Substituent Effects on Aromatic Compounds,” *Int. J. Quantum Chem.* **113**, 1171-1179 (2013) (DOI: 10.1002/qua.24231).
37. C. Jang, T. E. Lacy, **S. R. Gwaltney***, H. Toghiani, and C. J. Pittman, Jr., “Interfacial shear strength of cured vinyl ester resin-graphene sheets from molecular dynamics simulations,” *Polymer* **54**, 3282-3289 (2013) (DOI: 10.1016/j.polymer.2013.04.035).
38. N. Bandara, C. N. Ratnaweera, **S. R. Gwaltney**, and W. P. Henry, “Isolation and Structure of the *anti,anti* isomer and a DFT study of it and the *syn,anti* isomer of bis[tricarbonylchromium]dibenzo[*a,e*]-cyclooctatetraene. Evidence for an attractive electrostatic interaction between carbonyl oxygen atoms and Cr(CO)₃-coordinated arene carbon atoms,” *J. Organomet. Chem.* **745-746**, 86-92 (2013) (DOI: 10.1016/j.jorganchem.2013.06.029).
39. D. Hossain, C. U. Pittman, Jr., and **S. R. Gwaltney**, “Structures and Stabilities of the Metal Doped Gold Nano-Clusters: M@Au₁₀ (M = W, Mo, Ru, Co),” *J. Inorg. Organomet. Polym.* **24**, 241-249 (2014) (DOI: 10.1007/s10904-013-9995-6).
40. S. Nouranian, M. A. Tschopp, **S. R. Gwaltney**, M. I. Baskes, M. F. Horstemeyer, “An interatomic potential for saturated hydrocarbons based on the modified embedded-atom method,” *Phys. Chem. Chem. Phys.* **16**, 6233-6249 (2014) (DOI: 10.1039/C4CP00027G).
41. J. E. Chambers, H. W. Chambers, E. C. Meek, K. E. Funck, M. Bhavaraju, **S. R. Gwaltney**, and R. B. Pringle, “Novel Nucleophiles Enhance the Human Serum Paraoxonase 1 (PON1)-mediated Detoxication of Organophosphates” *Toxicol. Sci.* **143**, 46-53 (2015) (DOI: 10.1093/toxsci/kfu205).
42. Y. Shao, Z. Gan, E. Epifanovsky, A. T. B. Gilbert, M. Wormit, J. Kussmann, A. W. Lange,

- A. Behn, J. Deng, X. Feng, D. Ghosh, M. Goldey, P. R. Horn, L. D. Jacobson, I. Kaliman, R. Z. Khaliullin, T. Kuś, A. Landau, J. Liu, E. I. Proynov, Y. M. Rhee, R. M. Richard, M. A. Rohrdanz, R. P. Steele, E. J. Sundstrom, H. L. Woodcock III, P. M. Zimmerman, D. Zuev, B. Albrecht, E. Alguire, B. Austin, G. J. O. Beran, Y. A. Bernard, E. Berquist, K. Brandhorst, K. B. Bravaya, S. T. Brown, D. Casanova, C.-M. Chan, Y. Chen, S. H. Chien, K. D. Closser, D. L. Crittenden, M. Diedenhofen, R. A. DiStasio Jr., H. Do, A. D. Dutoi, R. G. Edgar, S. Fatehi, L. Fusti-Molnar, A. Ghysels, A. Golubeva-Zadorozhnaya, J. Gomes, M. W. D. Hanson-Heine, P. H. P. Harbach, A. W. Hauser, E. G. Hohenstein, Z. C. Holden, T.-C. Jagau, H. Ji, B. Kaduk, K. Khistyayev, J. Kim, J. Kim, R. A. King, P. Klunzinger, D. Kosenkov, T. Kowalczyk, C. M. Krauter, K. U. Lao, A. Laurent, K. V. Lawler, S. V. Levchenko, C. Y. Lin, F. Liu, E. Livshits, R. C. Lochan, A. Luenser, P. Manohar, S. F. Manzer, S.-P. Mao, N. Mardirossian, A. V. Marenich, S. A. Maurer, N. J. Mayhall, E. Neuscamman, C. M. Oana, R. Olivares-Amaya, D. P. O'Neill, J. A. Parkhill, T. M. Perrine, R. Peverati, A. Prociuk, D. R. Rehn, E. Rosta, N. J. Russ, S. M. Sharada, S. Sharma, D. W. Small, A. Sodt, T. Stein, D. Stück, Y.-C. Su, A. J. W. Thom, T. Tsuchimochi, V. Vanovschi, L. Vogt, O. Vydrov, T. Wang, M. A. Watson, J. Wenzel, A. White, C. F. Williams, J. Yang, S. Yeganeh, S. R. Yost, Z.-Q. You, I. Y. Zhang, X. Zhang, Y. Zhao, B. R. Brooks, G. K. L. Chan, D. M. Chipman, C. J. Cramer, W. A. Goddard III, M. S. Gordon, W. J. Hehre, A. Klamt, H. F. Schaefer III, M. W. Schmidt, C. D. Sherrill, D. G. Truhlar, A. Warshel, X. Xu, A. Aspuru-Guzik, R. Baer, A. T. Bell, N. A. Besley, J.-D. Chai, A. Dreuw, B. D. Dunietz, T. R. Furlani, **S. R. Gwaltney**, C.-P. Hsu, Y. Jung, J. Kong, D. S. Lambrecht, W. Z. Liang, C. Ochsenfeld, V. A. Rassolov, L. V. Slipchenko, J. E. Subotnik, T. Van Voorhis, J. M. Herbert, A. I. Krylov, P. M. W. Gill, and M. Head-Gordon, "Advances in molecular quantum chemistry contained in the Q-Chem 4 program package," *Mol. Phys.* **113**, 184-215 (2015) (DOI: 10.1080/00268976.2014.952696).
43. S. Nouranian, **S. R. Gwaltney**, M. I. Baskes, M. A. Tschopp, and M. F. Horstemeyer, "Simulations of Tensile Bond Rupture in Single Alkane Molecules Using Reactive Interatomic Potentials," *Chem. Phys. Lett.* **635**, 278-284 (2015) (DOI: 10.1016/j.cplett.2015.06.071).
44. S.-H. Chen, S.-Q. Sun, **S. R. Gwaltney**, C.-L. Li, X.-M. Wang, and S.-Q. Hu, "Molecular Dynamics Simulations of the Interaction between Carbon Nanofiber and Epoxy Resin Monomers," *Acta Polymerica Sinica* **2015**, 1158-1164 (2015) (DOI: 10.11777/j.issn1000-3304.2015.15053).
45. H. U. Rehman and **S. R. Gwaltney**, "The Role of Mutations at the Side Door on the Thermal Stability and Structural Flexibility of the pnbCE Enzyme," *Z. Phys. Chem.* **230**, 837-849 (2016) (DOI: 10.1515/zpch-2015-0708).
46. M. A. Murphy, M. F. Horstemeyer, **S. R. Gwaltney**, T. Stone, M. LaPlaca, J. Liao, L. Williams, and R. Prabhu, "Nanomechanics of phospholipid bilayer failure under strip biaxial stretching using molecular dynamics," *Model. Simul. Mater. Sci. Eng.* **24**, 055008 (2016) (DOI: 10.1088/0965-0393/24/5/055008).
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).
48. S. Mun, A. L. Bowman, S. Nouranian, **S. R. Gwaltney**, M. I. Baskes, and M. F. Horstemeyer, "Interatomic Potential for Hydrocarbons on the Basis of the Modified Embedded-Atom Method with Bond Order (MEAM-BO)," *J. Phys. Chem. A* **121**, 1502-1524

- (2017) (DOI: 10.1021/acs.jpca.6b11343).
49. S. Chen, Q. Lv, Z. Wang, C. Li, C. U. Pittman Jr., **S. R. Gwaltney**, S. Sun, and S. Hu, "Effect of graphene dispersion on the equilibrium structure and deformation of graphene/eicosane composites as surrogates for graphene/polyethylene composites: a molecular dynamics simulation," *J. Mater. Sci.* **52**, 5672-5685 (2017) (DOI: 10.1007/s10853-017-0802-6).
 50. S. Chen, S. Sun, C. Li, C. U. Pittman Jr., T. E. Lacy, S. Hu, and **S. R. Gwaltney**, "Molecular dynamics simulations of the graphene sheet aggregation in dodecane," *J. Nanopart. Res.* **19**, 195 (2017) (11 pages) (DOI: 10.1007/s11051-017-3893-8).
 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).
 53. S. Chen, S. Sun, C. Li, C. U. Pittman Jr., T. E. Lacy, S. Hu, and **S. R. Gwaltney**, "Molecular dynamics simulations of the aggregation behavior of overlapped graphene sheets in linear aliphatic hydrocarbons," *Mol. Simul.* **44**, 947-953 (2018) (DOI: 10.1080/08927022.2018.1465569).
 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).
 55. 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).
 56. M. A. Murphy, S. Mun, M. F. Horstemeyer, M. I. Baskes, A. Bakhtiary, M. C. LaPlaca, **S. R. Gwaltney**, L. N. Williams, and R. Prabhu, "Molecular dynamics simulations showing 1-palmitoyl-2-oleoyl-phosphatidylcholine (POPC) membrane mechanoporation damage under different strain paths," *J. Biomolecular Struct. Dyn.* **37**, 1346-1359 (2019) (DOI: 10.1080/07391102.2018.1453376).
 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).
 58. I Rajapaksha, H. Chang, Y. Xoing, S. Marder, **S. Gwaltney**, and C. Scott, "A new design strategy towards NIR I xanthene-based dyes," *J. Org. Chem.* (in press) (DOI: 10.1021/acs.joc.0c01242).
 59. V. Le, K. von Maltzman, J. Dettler, E. Lewis, **S. Gwaltney**, M. Bhavaraju, L. Shack, B. Nanduri, W. Tan, and S. Pruet, "Ethanol at relevant concentrations changes the conformation of mouse and human toll-like receptor 3 (TLR3) bound to ligand: Evidence for an ethanol binding site," *Alcohol Clin. Exp. Res.* (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 (T₈, T₁₀, T₁₂-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).

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 Carboxylesterase 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.