

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-
Outstanding Senior B.S. Chemistry, Indiana University, 1992
National Science Foundation Fellowship for Graduate Study, 1992-1995

Professional Experience

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

Graduate Student, Quantum Theory Project, University of Florida: 1992-1997 under Prof. Rodney J. Bartlett

The title of my dissertation was *Coupled-Cluster Based Methods for Excited State Energies and Gradients*.

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

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

Associate Director, Mississippi State University ERC Center for Computational Sciences: 2004-present

Papers

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).

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.

Invited Talks

1. “Quantum Chemistry for the Hard Problems,” Indiana University, October 5, 2000.
2. “Inner Sphere Electron Transfer Complexes,” National Institute of Standards and Technology, November 27, 2001.
3. “Inner Sphere Electron Transfer Complexes,” University of Southern California, June 25, 2002.
4. “The Role of Electron Transfer in Nitration and Nitrosation,” University of Mississippi, November 7, 2002.
5. “Breaking Bonds Perturbatively,” ACS 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, October 22, 2004.

Funded Grants

1. "Characterizing Organophosphates Computationally," NIH COBRE Pilot Project, Mississippi State University, December 2002, from 1/1/03 to 8/31/03 for \$19,276.
2. "A Computational Screen for Organophosphate Insecticides," NIH COBRE Pilot Project, Mississippi State University, August 2003, from 9/1/03 to 8/31/04 for \$14,224.
3. "The Mechanism of Organophosphate Insecticide Interactions with Acetylcholinesterase," NIH COBRE project, Mississippi State University, December 2004, from 2/11/05 to 6/31/07 for \$165,265