

BIOGRAPHICAL SKETCH

Provide the following information for the key personnel in the order listed for Form Page 2.
Follow the sample format on preceding page for each person. **DO NOT EXCEED FOUR PAGES.**

NAME Steven R. Gwaltney		POSITION TITLE Assistant Professor, Department of Chemistry	
EDUCATION/TRAINING (<i>Begin with baccalaureate or other initial professional education, such as nursing, and include postdoctoral training.</i>)			
INSTITUTION AND LOCATION	DEGREE (if applicable)	YEAR(s)	FIELD OF STUDY
Indiana University, Bloomington, IN	B.S.	1992	Chemistry
University of Florida, Gainesville, FL	Ph.D.	1997	Physical Chemistry
University of California, Berkeley, CA	Post-Doc	1998-2002	Theoretical Chemistry

A. Positions and Honors.

Assistant Professor, Department of Chemistry and ERC Center for Computational Sciences, 2002-present

B. Selected peer-reviewed publications (in chronological order).

- Chakravorty, S.J., S.R. Gwaltney, E.R. Davidson, F.A. Parpia and C. Froese Fischer 1993. Ground-state correlation energies for atomic ions with 3 to 18 electrons. *Phys. Rev. A* 47:3649-3670.
- Gwaltney, S.R. and R.J. Bartlett 1993. Comment on: The relation between intensity and dipole moment for bending modes in linear molecules. *J. Chem. Phys.* 99:3151-3152.
- Song X., E.R. Davidson, S.R. Gwaltney and J.P. Reilly 1994. High-resolution zero kinetic energy photoelectron spectra of para-*n*-propylalanine. *J. Chem. Phys.* 100:5411-5421.
- Gwaltney, S.R. and R.J. Bartlett 1995. 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.
- Gwaltney, S.R., M. Nooijen and R.J. Bartlett 1996. Simplified methods for equation-of-motion coupled-cluster excited state calculations. *Chem. Phys. Lett.* 248:189-198.
- Watts, J.D., S.R. Gwaltney and R.J. Bartlett 1996. Coupled-cluster calculations of the excitation energies of ethylene, butadiene, and cyclopentadiene. *J. Chem. Phys.* 105:6979-6988.
- Sadeghi, R.R., S.R. Gwaltney, J.L. Krause, R.T. Skodje and P.M. Weber 1997. Structure and dynamics of the S₃ state of CS₂. *J. Chem. Phys.* 107:6570-6576.
- Gwaltney, S.R. and R.J. Bartlett 1998. Coupled-cluster calculations of the electronic excitation spectrum of free base porphyrin in a polarized basis. *J. Chem. Phys.* 108:6790-6798.
- Del Bene, J.E., S.R. Gwaltney and R.J. Bartlett 1998. Base properties of H₂CO in the excited ¹n? pi* state. *J. Phys. Chem. A* 102:5124-5127.
- Gwaltney, S.R. and R.J. Bartlett 1999. Gradients for the partitioned equation-of-motion coupled-cluster method. *J. Chem. Phys.* 110:62-71.
- Gwaltney, S.R., R.J. Bartlett, and M. Nooijen 1999. Gradients for the similarity transformed equation-of-motion coupled-cluster method. *J. Chem. Phys.* 111:58-64.
- Gwaltney, S.R. and M. Head-Gordon 2000. 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.
- Gwaltney, S.R., C.D. Sherrill, M. Head-Gordon, and A.I. Krylov 2000. 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.
- Kong, J., 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 2000. Q-Chem 2.0: a high-performance *ab initio* electronic structure program package. *J. Comp. Chem.* 21:1532-1548.
- Gwaltney, S.R. and M. Head-Gordon 2001. A second-order perturbative correction to the coupled-cluster singles and doubles method: CCSD(2). *J. Chem. Phys.* 115:2014-2021.
- Gwaltney, S.R. and M. Head-Gordon 2001. Calculating the equilibrium structure of the BNB molecule: Real vs. artifactual symmetry breaking. *Phys. Chem. Chem. Phys.* 3:4495-4500.
- Gwaltney, S.R., E.F.C. Byrd, T. Van Voorhis, and M. Head-Gordon 2002. A perturbative correction to the quadratic coupled-cluster doubles method for higher excitations. *Chem. Phys. Lett.* 353:359-367.

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- Beran, G.J.O., S.R. Gwaltney, and M. Head-Gordon 2002. Can coupled cluster singles and doubles be approximated by a valence active space model? *J. Chem. Phys.* 117:3040-3048.
- Gwaltney, S.R., S. V. Rosokha, M. Head-Gordon, and J.K. Kochi 2003. The 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.
- Beran, G.J.O., S.R. Gwaltney, and M. Head-Gordon. Approaching Closed-Shell Accuracy for Radicals. *Phys. Chem. Chem. Phys.* Accepted.

C. Research Support.

“Characterizing Organophosphates Computationally”

Principal Investigator: Steven R. Gwaltney, Ph.D.

Period: 1/01/2003 – 8/31/2003

Agency: National Institutes of Health

Type: COBRE Pilot Project

This project models the interactions of organophosphate insecticides with mouse acetylcholinesterase, in order to predict the binding affinity and rate of reaction of various organophosphates.