

## Steven E. Wheeler, Ph.D.

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### Education

**Ph.D. Physical Chemistry** Center for Computational Quantum Chemistry 2006  
University of Georgia, Athens, Georgia  
Advisor: Henry F. Schaefer III  
Dissertation Title: *Accurate Thermochemistry of Key Soot Formation Intermediates*

- Computed definitive thermochemical parameters for key intermediates in the combustion of hydrocarbon fuels and formation of soot
- Examined the underlying causes of oscillatory and divergent Møller-Plesset perturbation energy series
- Provided the first study of high-order Z-averaged perturbation theory (ZAPT) energies
- Derived and implemented third and fourth order ZAPT (ZAPT3 and ZAPT4)
- Computed benchmark geometries, atomization energies, and ionization potentials for small lithium clusters and hydrogenated lithium clusters
- Provided accurate ionization potentials for linear and cyclic carbon clusters, enabling the identification of isomers in molecular beam experiments
- Studied the isomerization potential energy surface of HSCO<sup>+</sup> through the systematic extrapolation of *ab initio* energies
- Developed a stochastic search algorithm (SASS) exploiting point group symmetry for the efficient exploration of quantum mechanical potential energy surfaces

**B.A. Chemistry and Physics** New College of Florida, Sarasota, Florida 2002  
Thesis Advisor: Donald C. Colladay  
Thesis Title: *Implementation of Density Functional Theory and Application of DFT to the Chlorine/Benzene Adduct*

- Wrote a stand-alone density functional theory code
- Examined the Cl/Benzene adduct using DFT methods
- Studied 3-D quantum wavepacket scattering from various spherical potentials
- Used a genetic algorithm approach to derive optimal chirped laser pulses for multiphoton excitation of HF to selected vibrational levels (with Shih-I Chu, University of Kansas)

### Academic Honors and Awards

NIH NRSA Postdoctoral Fellowship (Ruth L. Kirschstein, F32)	National Institute of General Medical Sciences	2007-2009
Presidential Fellowship	University of Georgia	2002-2006
Robert S. Mulliken Fellowship	Center for Computational Quantum Chemistry	2002-2006
Summer Undergraduate Research Fellowship	Center for Computational Quantum Chemistry	2001
NSF Research Experiences for Undergraduates Fellowship	University of Kansas	2000
New College Foundation Scholarship	New College of Florida	1998-2002

## Professional Experience

**NIH NRSA Postdoctoral Fellow**      Department of Chemistry and Biochemistry      12/2008-present  
 University of California, Los Angeles      8/2007-8/2008  
 Advisor: K. N. Houk

- Developing new models of substituent effects in non-covalent interactions with aryl rings ( $\pi$ - $\pi$ , C-H/ $\pi$ , and cation/ $\pi$ )
- Examining substituent effects in molecular electrostatic potentials of substituted arenes
- Studying the role of  $\pi$ -stacking interactions in the intercalation of polycyclic aromatic diol epoxides into DNA
- Exploring antibody-DNA interactions in anti-DNA autoantibodies
- Quantifying role of  $\pi$ -stacking interactions in enzyme active sites
- Predicting barriers of enzyme catalyzed reactions of natural and computationally designed enzymes
- Benchmarking DFT functionals for organocatalyzed reactions

**Visiting Scientist and Graduate Instructor**      Center for Computational Quantum Chemistry      8/2008-12/2008  
 University of Georgia, Athens, Georgia

- Taught CHEM8930: Introduction to Quantum Chemistry
- Computed accurate thermochemical parameters of the HOSO radical, a key intermediate in fossil fuel combustion

**Postdoctoral Scholar**      Department of Chemistry and Biochemistry      10/2006-8/2007  
 University of California, Los Angeles  
 Advisor: K. N. Houk

- Examined stereoselective Diels-Alder reactions mediated by  $\pi$ -stacking interactions
- Developed a new model for substituent effects in  $\pi$ -stacking interactions
- Benchmarked DFT functionals for the description of substituent effects in  $\pi$ - $\pi$  stacking interactions
- Introduced a hierarchy of homodesmotic reaction types that result in systematic cancellation of errors in computed reaction energies
- Provided definitive reaction thermochemistry for the 1,3-dipolar cycloadditions of ozone with acetylene and ethylene, pinpointing the source of errors in commonly employed composite *ab initio* approaches for these reactions
- Co-Taught C145/C245: Theoretical and Computational Organic Chemistry

## Teaching Experience

Introduction to Quantum Chemistry      University of Georgia      2008

- CHEM8930: Introduction to Quantum Chemistry
- Graduate course covering topics in molecular quantum mechanics, including introductory quantum mechanics through modern electronic structure theory
- Overall Instructor Rating: 1.3/5.0 (1 = Excellent, 5 = Poor)

Theoretical and Computational Organic Chemistry      University of California, Los Angeles      2007  
 co-taught with K. N. Houk

- C145/C245: Theoretical and Computational Organic Chemistry
- Developed and delivered lectures on *ab initio* electronic structure theory and density functional theory to graduate students and advanced undergraduates

Advanced Quantum Chemistry      University of Georgia      2006  
Teaching Assistant      Supervisor: Wesley D. Allen

- Lectured on the use of Mathematica for solving problems in molecular quantum mechanics to advanced graduate students
- Answered questions about course material and problem sets
- Graded problem sets and exams

Summer Program Lecturer      Center for Computational Quantum Chemistry      2003-2006

- Wrote and delivered lectures to undergraduates and beginning graduate students on Computational Chemistry, Hartree-Fock Theory, and Møller-Plesset Perturbation Theory

Summer Research Program      Center for Computational Quantum Chemistry      2004, 2005  
co-Director

- Recruited top undergraduates for intensive, highly selective 10 week research program
- Organized lecture series on methods of electronic structure theory
- Supervised research of undergraduates

### Funding Sources

“Towards the *ab initio* Prediction of Catalytic Proficiencies of Enzymes”      \$96,472  
National Institute of General Medical Sciences – F32GM082114      8/2007-11/2009

### Current Research Interests

$\pi$ -stacking interactions in enzyme catalysis and computational enzyme design

Substituent effects in non-covalent interactions with aromatic rings ( $\pi$ - $\pi$ , CH/ $\pi$ , cation/ $\pi$ )

Origin of sequence selectivity in anti-DNA autoantibodies (lupus)

DNA intercalation of polycyclic aromatic diol epoxides

### Scholarly Activities

Active reviewer for the following journals:

*Journal of the American Chemical Society*

*Accounts of Chemical Research*

*Journal of Physical Chemistry*

*Physical Chemistry Chemical Physics*

*Journal of Organic Chemistry*

*Molecular Physics*

*Journal of Physical Organic Chemistry*

Member: American Chemical Society

## Scientific Collaborators

Paul v. R. Schleyer	University of Georgia
Wesley D. Allen	University of Georgia
Michael A. Duncan	University of Georgia
Anne J. McNeil	University of Michigan, Ann Arbor
Vladimir V. Popik	University of Georgia

## Scientific Publications

1. "Binding Energies of Small Lithium Clusters ( $\text{Li}_n$ ) and Hydrogenated Lithium Clusters ( $\text{Li}_n\text{H}$ )", **S. E. Wheeler**, K. W. Sattelmeyer, P. v. R. Schleyer, and H. F. Schaefer, *J. Chem. Phys.* **120**, 4683-4689 (2004).
2. "The Vinyl Radical and Fluorinated Vinyl Radicals,  $\text{C}_2\text{H}_{3-n}\text{F}_n$  ( $n = 0-3$ ), and Corresponding Anions: Comparison with the Isoelectronic Complexes  $[\text{X}\cdots\text{YC}\equiv\text{CZ}]^-$ ", A. C. Simmonett, **S. E. Wheeler**, and H. F. Schaefer, *J. Phys. Chem. A* **108**, 1608-1615 (2004).
3. "Thermochemistry of Disputed Soot Formation Intermediates  $\text{C}_4\text{H}_3$  and  $\text{C}_4\text{H}_5$ ", **S. E. Wheeler**, W. D. Allen, and H. F. Schaefer, *J. Chem. Phys.* **121**, 8800-8813 (2004).
4. "Electron Affinities of the Radicals Derived from Cytosine", Q. Luo, J. Li, Q. S. Li, S. Kim, **S. E. Wheeler**, Y. Xie, and H. F. Schaefer, *Phys. Chem. Chem. Phys.* **7**, 861-865 (2005).
5. "Ionization Potentials of Small Lithium Clusters ( $\text{Li}_n$ ) and Hydrogenated Lithium Clusters ( $\text{Li}_n\text{H}$ )", **S. E. Wheeler** and H. F. Schaefer, *J. Chem. Phys.* **122**, 204328 (2005).
6. "The Extremely Flat Torsional Potential Energy Surface of Oxalyl Chloride", S. Kim, **S. E. Wheeler**, N. J. DeYonker, and H. F. Schaefer, *J. Chem. Phys.* **123**, 234313 (2005).
7. "On the Møller-Plesset Critical Point", A. V. Sergeev, D. Z. Goodson, **S. E. Wheeler**, and W. D. Allen, *J. Chem. Phys.* **123**, 064105 (2005).
8. "The Pentacyanocyclopentadienyl System: Structures and Energetics", R. L. Lord, **S. E. Wheeler**, and H. F. Schaefer, *J. Phys. Chem. A* **109**, 10084-10091 (2005).
9. "Protonated Carbonyl Sulfide: Prospects for the Spectroscopic Identification of the Elusive  $\text{HSCO}^+$  Isomer", **S. E. Wheeler**, Y. Yamaguchi, and H. F. Schaefer, *J. Chem. Phys.* **124**, 044322 (2006).
10. "The Remarkable Electron Accepting Properties of the Simplest Benzenoid Cyanocarbons: Hexacyanobenzene, Octacyanonaphthalene, and Decacyano-anthracene", X. Zhang, Q. Li, J. B. Ingels, A. C. Simmonett, **S. E. Wheeler**, Y. Xie, R. B. King, H. F. Schaefer, and F. A. Cotton, *Chem. Commun.*, 758-760 (2006).
11. "The Deprotonated Guanine-Cytosine Base Pair", M. C. Lind, P. P. Bera, N. A. Richardson, **S. E. Wheeler**, and H. F. Schaefer, *Proc. Natl. Acad. Sci. USA* **103**, 7554-7559 (2006).
12. "Microsolvation Effects on the Electron Capturing Ability of Thymine: Thymine-Water Complexes", S. Kim, **S. E. Wheeler**, and H. F. Schaefer, *J. Chem. Phys.* **124**, 204310 (2006).
13. "SASS: A Symmetry Adapted Stochastic Search Algorithm Exploiting Site Symmetry", **S. E. Wheeler**, P. v. R. Schleyer, and H. F. Schaefer, *J. Chem. Phys.* **126**, 104104 (2007).
14. "Thermochemistry of Key Soot Formation Intermediates: Isomers of  $\text{C}_3\text{H}_3$ ", **S. E. Wheeler**, K. A. Robertson, W. D. Allen, H. F. Schaefer, Y. J. Bomble, and J. F. Stanton, *J. Phys. Chem. A* **111**, 3819-3830 (2007).
15. "The Renner-Teller Bending Frequencies of the  $\tilde{A}^2\Pi$  State of  $\text{OCS}^+$ ", **S. E. Wheeler**, A. C. Simmonett, and H. F. Schaefer, *J. Phys. Chem. A* **111**, 4551-4555 (2007).

16. "Hydrogen Abstracted Adenine-Thymine Radicals with Interesting Transferable Properties", M. C. Lind, N. A. Richardson, **S. E. Wheeler**, and H. F. Schaefer, *J. Phys. Chem. B* **111**, 5525-5530 (2007).
17. "Ionization Thresholds of Small Carbon Clusters: Tunable VUV Experiments and Theory", L. Belau, **S. E. Wheeler**, B. W. Ticknor, M. Ahmed, S. R. Leone, W. D. Allen, H. F. Schaefer, and M. A. Duncan, *J. Am. Chem. Soc.* **129**, 10229-10243 (2007).
18. "Thinking Out of the Black Box: Accurate Barrier Heights of 1,3-Dipolar Cycloadditions of Ozone with Acetylene and Ethylene", **S. E. Wheeler**, D. H. Ess, and K. N. Houk, *J. Phys. Chem. A* **112**, 1789-1807 (2008).
19. "On the Convergence of Z-Averaged Perturbation Theory (ZAPT)", **S. E. Wheeler**, W. D. Allen, and H. F. Schaefer, *J. Chem. Phys.* **128**, 074107 (2008).
20. "Substituent Effects in the Benzene Dimer are Due to Direct Interactions of the Substituents with the Unsubstituted Benzene Ring", **S. E. Wheeler** and K. N. Houk, *J. Am. Chem. Soc.* **130**, 10854-10855 (2008).
21. "Bifurcations on Potential Energy Surfaces of Organic Reactions", D. H. Ess, **S. E. Wheeler**, Robert G. Iafe, Lai Xu, N. Çelebi-Ölçüm, and K. N. Houk, *Angew. Chem. Int. Ed.* **47**, 7592-7601 (2008).
22. "Origin of Substituent Effects in Edge-to-Face Aryl-Aryl Interactions", **S. E. Wheeler** and K. N. Houk, *Mol. Phys.* **107**, 749-760 (2009).
23. "A Hierarchy of Homodesmotic Reactions for Thermochemistry", **S. E. Wheeler**, K. N. Houk, P. v. R. Schleyer, and W. D. Allen, *J. Am. Chem. Soc.* **131**, 2547-2560 (2009).
24. "Substituent Effects in Cation/ $\pi$  Interactions and Electrostatic Potentials above Substituted Benzenes Are Due Primarily to through-Space Effects of the Substituents", **S. E. Wheeler** and K. N. Houk, *J. Am. Chem. Soc.* **131**, 3126-3127 (2009).
25. "Thermochemistry of the HOSO Radical, a Key Intermediate in the Combustion of Fossil Fuels", **S. E. Wheeler** and H. F. Schaefer, *J. Phys. Chem. A* **113**, 6779-6788 (2009).
26. "Through-Space Effects of Substituents Dominate Molecular Electrostatic Potentials of Substituted Arenes", **S. E. Wheeler** and K. N. Houk, *J. Chem. Theory Comput.* **5**, 2301-2312 (2009). (Journal Cover)
27. "Accurate Reaction Enthalpies and Sources of Error in DFT Thermochemistry for Aldol, Mannich, and  $\alpha$ -Aminoxylation Reactions", **S. E. Wheeler**, A. Moran, S. N. Pieniazek, and K. N. Houk, *J. Phys. Chem. A* **113**, 10376-10384 (2009).

### Submitted Manuscripts

28. "Probing Substituent Effects in Aryl-Aryl Interactions Using Stereoselective Diels-Alder Cycloadditions", **S. E. Wheeler**, A. J. McNeil, P. Müller, T. M. Swager, and K. N. Houk, *J. Am. Chem. Soc.* (submitted).
29. "Non-Covalent Interactions of a Benzo[a]pyrene Diol Epoxide with DNA Base Pairs: Insight into the DNA Intercalation of (+)-BaP DE-2", J. C. Hargis, H. F. Schaefer, K. N. Houk, and **S. E. Wheeler**, *Proc. Natl. Acad. Sci. USA* (submitted).

### Presentations and Abstracts

1. "Small Lithium Clusters and Hydrogenated Lithium Clusters", **S. E. Wheeler**, K. W. Sattelmeyer, P. v. R. Schleyer, and H. F. Schaefer, Southeastern Theoretical Chemistry Association (SETCA) Conference, Clemson University (2003).

2. "Thermochemistry of  $C_4H_3$  and  $C_4H_5$  Soot Formation Intermediates", **S. E. Wheeler**, W. D. Allen, and H. F. Schaefer, Southeastern Theoretical Chemistry Association (SETCA) Conference, University of Mississippi (2004).
3. "In Pursuit of Subchemical Accuracy in Computational Thermochemistry", W. D. Allen, M. Schuurman, **S. Wheeler**, J. P. Kenny, and H. F. Schaefer, Abstracts of Papers of the Am. Chem. Soc. **228**, U508-U509.
4. "Thermochemistry of Disputed Soot Formation Intermediates  $C_4H_3$  and  $C_4H_5$ ", **S. E. Wheeler**, W. D. Allen, and H. F. Schaefer, Molecular Quantum Mechanics: The No-Nonsense Path to Progress, Cambridge University, England (2004). (Poster)
5. "Thermochemistry of Disputed Soot Formation Intermediates  $C_4H_3$  and  $C_4H_5$ ", **S. E. Wheeler**, W. D. Allen, and H. F. Schaefer, World Congress of Theoretically Oriented Chemists, Cape Town, South Africa (2005). (Poster)
6. "Protonated Carboynyl Sulfide: Prospects for the Spectroscopic Identification of the Elusive  $HSCO^+$  Isomer", **S. E. Wheeler**, Y. Yamaguchi, and H. F. Schaefer, Southeastern Theoretical Chemistry Association (SETCA) Conference, University of Tennessee (2005). (Poster)
7. "In Search of Sub-chemically Accurate  $C_3H_3$  Thermochemical Parameters via Computational Focal-Point Extrapolation", K. A. Robertson, **S. Wheeler**, and W. D. Allen, Abstracts of Papers of the Am. Chem. Soc. **231**, 1076-CHED (2006).
8. "Microsolvation Effects on Electron Affinities of Pyrimidine DNA Bases", S. Kim, **S. E. Wheeler**, and H. F. Schaefer, Southeastern Theoretical Chemistry Association Conference, Emory University (2006). (Poster)
9. "The Deprotonated Guanine-Cytosine Base Pair", M. C. Lind, P. P. Bera, N. A. Richardson, **S. E. Wheeler**, and H. F. Schaefer, Southeastern Theoretical Chemistry Association (SETCA) Conference, Emory University (2006). (Poster)
10. "Substituent Effects in  $\pi$ - $\pi$  Stacking Interactions: Performance of New DFT Functionals and an Experimental Probe", **S. E. Wheeler**, A. J. McNeil, T. M. Swager, and K. N. Houk, Abstracts of Papers of the Am. Chem. Soc. (2007).
11. "Unraveling the Origin of Substituent Effects in the Benzene Dimer", **S. E. Wheeler** and K. N. Houk, Southeastern Theoretical Chemistry Association (SETCA) Conference, University of Alabama (2008).
12. "Unraveling the Origin of Substituent Effects in  $\pi$ -stacking Interactions", **S. E. Wheeler** and K. N. Houk, Abstracts of Papers of the Am. Chem. Soc. (2008).
13. "Through-Space Effects of Substituents on Non-Covalent Interactions and Molecular Electrostatic Potentials of Arenes", **S. E. Wheeler** and K. N. Houk, Southeastern Theoretical Chemistry Association (SETCA) Conference, Duke University (2009).
14. "Non-Covalent Interactions between a Polycyclic Aromatic Diol Epoxide and DNA Base Pairs", J. C. Hargis, **S. E. Wheeler**, K. N. Houk, and H. F. Schaefer, Southeastern Theoretical Chemistry Association (SETCA) Conference, Duke University (2009). (Poster)
15. "Through-Space Effects of Substituents on Non-Covalent Interactions and Molecular Electrostatic Potentials of Arenes", **S. E. Wheeler** and K. N. Houk, Southern School of Materials Science and Computational Chemistry, Jackson State University (2009). (Poster)
16. "Non-Covalent Interactions, Molecular Electrostatic Potentials, and Lupus", **S. E. Wheeler**, Natural Sciences Seminar, New College of Florida (2009). (Invited Lecture)

**Professional References**

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