

Contact Information

Department of Chemistry
Yale University
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Professional Preparation

University of California – Berkeley	Berkeley, CA	Ph.D., Theoretical Chemistry	2008
Iowa State University	Ames, IA	B.S. with distinction, Chemistry	2003

Scientific Appointments

Post-Doctoral Associate	Aug 2008 – present
Department of Chemistry, Yale University Research group of Prof. John Tully	
Graduate Research Assistant	Aug 2003 – Aug 2008
Department of Chemistry, University of CA – Berkeley Research group of Prof. Martin Head-Gordon Thesis: <i>Dual-Basis Methods for Electronic Structure Theory</i>	
Graduate Student Instructor	
Department of Chemistry, University of CA – Berkeley Spring 2006 – Graduate Quantum Mechanics II with Prof. William H. Miller Fall 2004 – Head GSI, Introductory Chemistry with Prof. David Chandler Fall 2003 – Introductory chemistry with Dr. Michelle Douskey & Prof. Martin Head-Gordon	
Undergraduate Research Associate	May – Aug 2002
Georgia Institute of Technology Research group of Prof. C. David Sherrill	
Undergraduate Research Associate	Aug 2002 – May 2003
Iowa State University Research group of Prof. William S. Jenks	
Teaching Assistant	Aug 2002 – May 2003
Iowa State University Introductory Chemistry I & II with Prof. Thomas Greenbowe	

Honors & Awards

Teaching Effectiveness Award 2007 (1 of 13 University-wide)

Outstanding Graduate Student Instructor 2006

Berkeley Travel Award 2006

The Phi Beta Kappa Society

The Honor Society of Phi Kappa Phi

Mortar Board Honor Society

Golden Key International Honour Society

Tau Beta Pi Engineering Honor Society

Iowa State University Senior Chemistry Student of the Year

National Merit Scholar

Scholarships: Robert C. Byrd Dept. of Education, Iowa State University Merit, ConSern Corp., Alpha Chi Sigma Engineering, Millhone Scholar Engineering, Phillips Engineering, Kay Merit, Donald Delahunt, Harry O. Price.

Software and Development

Main development within the *Q-Chem* software package (back-end program for *Spartan*)

Journals Refereed

Journal of Chemical Physics

Physical Chemistry Chemical Physics

Journal of Chemical Theory and Computation

Molecular Physics

Presentations, Posters, Conferences

Poster: *The quantum structure of protonated methane (CH_5^+)*. Gordon Research Conference: Atomic and Molecular Collisions, New London, NH, Jul 2010.

Invited talk: *Protons: Nature's Nomads*. University of Alabama, Tuscaloosa, AL, Feb 2009.

Invited talk: *A riddle from the ionosphere reveals how water activation is controlled by the shape of an H-bonded network*. NSF/PIRE Workshop, Pisa, Italy, Jul 2009.

Poster: *Atmospheric water network activation: Delocalized protons and charge migration in $NO^+(H_2O)_{n=1-4}$ clusters*. Dynamics of Molecular Collisions, Snowbird, UT, Jul 2009.

Talk: *Dual basis methods: Energies, derivatives, and non-covalent interactions*. ACS National Meeting, New Orleans, LA, Apr 2008.

Poster: *Cation- π interactions in fullerene systems*. ACS National Meeting, New Orleans, LA, Apr 2008.

Talk: *Circumventing the basis set bottleneck: Dual-basis methods for non-covalent interactions*. MRS National Meeting, San Francisco, CA, Mar 2008.

Poster: *Dual-basis methods for electronic structure theory*. Molecular Quantum Mechanics – Analytic Gradients & Beyond (an international conference in honor of Peter Pulay), Budapest, Hungary, Jun 2007.

Invited Talk: *Recent improvements in SCF methods*. William A. Lester group, Berkeley, CA, Oct 2007.

Poster: *Dual-basis methods for electronic structure theory*. ACS National Meeting, San Francisco, CA, Sept 2006.

Poster: *Dual-basis methods for electronic structure theory*. American Conference on Theoretical Chemistry, Los Angeles, CA, Jul 2005.

Publications

1. *Mixed time slicing in path integral simulations.*
R. P. Steele, J. Zwickl, P. Shushkov, J. C. Tully.
J. Chem. Phys. **accepted** (2010).
2. *Accelerated ab initio molecular dynamics with response equation extrapolation.*
R. P. Steele, J. C. Tully.
Chem. Phys. Lett. **500**, 167 (2010).
3. *Ab initio molecular dynamics with dual-basis methods.*
R. P. Steele, M. Head-Gordon, J. C. Tully.
J. Phys. Chem. A. **114**, 11853 (2010).
4. *How the shape of an H-bonded network controls proton-coupled water activation in HONO formation.*
R. A. Relph, B. M. Elliott, R. P. Steele, T. L. Guasco, M. Z. Kamrath, A. B. McCoy, D. P. Schofield, K. D. Jordan, A. A. Viggiano, E. E. Ferguson, M. A. Johnson.
Science **327**, 5963 (2009).
5. *The 1,4-phenylenediisocyanide dimer: Gas-phase properties and insights into organic self-assembled monolayers.*
R. P. Steele, R. A. DiStasio, Jr., M. Head-Gordon.
Phys. Chem. Chem. Phys. **12**, 82 (2010).
6. *Potential energy curves for cation- π interactions: Off-axis configurations are also attractive.*
M. S. Marshall, R. P. Steele, K. S. Thanthiriwatte, C. D. Sherrill.
J. Phys. Chem. A. **113**, 13628 (2009).
7. *The initial and final states of electron and energy transfer processes: Diabatization as motivated by system-solvent interactions.*
J. E. Subotnik, R. J. Cave, R. P. Steele, N. Shenvi.
J. Chem. Phys. **130**, 234102 (2009).
8. *Non-covalent interactions with dual-basis methods: Pairings for augmented basis sets.*
R. P. Steele, R. A. DiStasio, Jr., M. Head-Gordon.
J. Chem. Theor. Comput. **5**, 1560 (2009).
9. *Direct observation of photoinduced bent nitrosyl excited-state complexes.*
K. R. Sawyer, R. P. Steele, E. A. Glascoe, J. F. Cahoon, J. P. Schlegel, M. Head-Gordon, C. B. Harris.
J. Phys. Chem. A. **112**, 8505 (2008).
10. *The analytical gradient of dual-basis resolution-of-the-identity second-order Moller-Plesset perturbation theory.*
R. A. DiStasio, Jr., R. P. Steele, M. Head-Gordon.
Mol. Phys. **105**, 2731 (2007).
11. *Dual-basis SCF methods: 6-31G* calculations with a minimal 6-4G basis.*
R. P. Steele, M. Head-Gordon.
Mol. Phys. **105**, 2455 (2007).
12. *An improved algorithm for analytical gradient evaluation in resolution-of-the-identity second-order Moller-Plesset perturbation theory: Application to the alanine tetrapeptide conformational energy analysis.*
R. A. DiStasio, Jr., R. P. Steele, Y. Shao, M. Head-Gordon.
J. Comput. Chem. **28**, 839 (2007).
13. *On the T-shaped structures of the benzene dimer*
R. A. DiStasio, Jr., G. von Helden, R. P. Steele, Y. Shao, M. Head-Gordon.
Chem. Phys. Lett. **437**, 227 (2007).
14. *Dual-basis analytic gradients: I. Self-Consistent Field Theory.*
R. P. Steele, Y. Shao, R. A. DiStasio, Jr., M. Head-Gordon.
J. Phys. Chem. A. **110**, 13915 (2006).

15. *Dual-Basis Second-Order Møller-Plesset Perturbation Theory: A reduced-cost reference for correlation calculations.*

R. P. Steele, R. A. DiStasio, Jr., Y. Shao, J. Kong, M. Head-Gordon.

J. Chem. Phys. **125**, 074108 (2006).

16. *Advances in methods and algorithms in a modern quantum chemistry program package. (Q-Chem software development reference)*

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. Dachsel, 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. Khaliulin, 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, M. Head-Gordon.

Phys. Chem. Chem. Phys. **8**, 3172 (2006).