Kevin B. Moore III, Ph.D

Postdoctoral Appointee with Stephen J. Klippenstein
Chemical Sciences and Engineering Division, Argonne National Lab
9700 S. Cass Ave — Lemont, IL 60439 — 904-910-5718 — kmoore@anl.gov

Education

University of Georgia — Athens, GA
Doctor of Philosophy, Chemistry — Aug. 2013–May 2018

University of North Florida — Jacksonville, FL
Bachelors of Science, Chemistry and Mathematics — Aug. 2008–Apr. 2013

Research Background

Chemical Sciences and Engineering Division, Argonne National Lab — Lemont, IL
Postdoctoral Appointee with Stephen J. Klippenstein — Jun. 2018–Present

Center for Computational Quantum Chemistry, University of Georgia — Athens, GA
Graduate Research Assistant to Professor Henry F. Schaefer III — Aug. 2013–May 2018

Department of Chemistry, University of North Florida — Jacksonville, FL
Undergraduate Research Assistant to Professor Thomas J. Mullen III — Aug. 2012–Apr. 2013
Undergraduate Research Assistant to Professor Robert A. Vergenz — May 2009–Aug. 2012

Teaching Background

Department of Chemistry, University of Georgia — Athens, GA
Teaching Assistant for Organic Chemistry I Laboratory — Jan. 2014–Apr. 2014
Teaching Assistant for General Chemistry I Laboratory — Aug. 2013–Dec. 2013

Academic Center for Excellence, University of North Florida — Jacksonville, FL
Chemistry, Mathematics, and Physics Tutor — Aug. 2009–Apr. 2013
Undergraduate Orientation Academic Advisor — Summers: 2010, 2011, 2012

Department of Chemistry, University of North Florida — Jacksonville, FL
Grader and Teaching Assistant for General Chemistry I & II — Aug. 2009–Apr. 2013
Grader for Biochemistry — Jan. 2013–Apr. 2013

Department of Mathematics & Statistics, University of North Florida — Jacksonville, FL
Grader for Calculus I — Aug. 2011–Dec. 2011

Publications

In Press/Submitted

1. Weidman, J. D.; Allen, R. T.; Moore, K. B.; and Schaefer, H. F. High-level *Ab initio* Characterization of the Vinoxy Radical + O_2 Reaction. *J. Chem. Phys.* **2018**, *148*, 184308.

2. Misiewicz, J. P.; Elliott, S. N.; Moore, K. B.; and Schaefer, H. F. Re-Examining Ammonia Addition to the Criegee Intermediate: Converging to Chemical Accuracy. *Phys. Chem. Chem. Phys.* **2018**, *20*, 7479–7491.

3. Sun, Z.; Moore, K. B.; Hill, J. G.; Peterson, K. A.; Schaefer, H. F.; and Hoffmann, R. Alkali Metal Trihalides: $M^+X_3^-$ Ion Pair or MX–X_2 Complex? *J. Phys. Chem. B* **2017**, *122*, 3339–3353.

4. Zun, Z.; Moore, K. B.; and Schaefer, H. F. Communication: The $Al + CO_2 \longrightarrow AlO + CO$ Reaction: Experiment vs. Theory. *J. Chem. Phys.* **2017**, *147*, 171101.

5. Moore, K. B.; Sadeghian, K.; Sherrill, C. D.; Ochsenfeld, C.; and Schaefer, H. F. $C{-}H\cdots O$ Hydrogen Bonding. The Prototypical Methane-Formaldehyde System: A Critical Assessment. *J. Chem. Theory Comput.* **2017**, *13*, 5379–5395.

6. Moore, K. B.; Turney, J. M; and Schaefer, H. F. The Fate of the *Tert*-Butyl Radical in Low-Temperature Autoignition Reactions. *J. Chem. Phys.* **2017**, *146*, 194304.

7. Leavitt, C. M.; Moore, K. B.; Raston, P. L.; Agarwal, J.; Moody, G. H.; Shirley, C. C.; Schaefer, H. F.; and Douberly, G. E. Liquid Hot NAGMA Cooled to 0.4 Kelvin: Benchmark Thermochemistry of a Gas-Phase Peptide. *J. Phys. Chem. A* **2014**, *118*, 9692–9700.

8. Drexler, C. I.; Moore, K. B.; Causey, C. P.; Mullen, T. J. Atomic Force Microscopy Characterization and Lithography of Cu-Ligated Mercaptoalkanoic Acid "Molecular Ruler" Multilayers. *Langmuir* **2014**, *30*, 7447–7455.

9. Moore, K. B.; Migues, A. N.; Schaefer, H. F.; and Vergenz, R. A. Streptococcal Hyaluronate Lyase Reveals the Presence of a Structurally Significant $C{-}H\cdots O$ Hydrogen Bond. *Chem. Eur. J.* **2014**, *20*, 990–998.

In Progress

1. Moore, K. B.; Franke, P. R.; Douberly, G. E.; and Schaefer, H. F. *Ab initio* Characterization of the Vibrational Spectra for the Ground and First Excited States of the *Tert*-butyl Peroxy Radical.

2. Moore, K. B.; Vandezande, J. E.; Elliot, S. N.; and Schaefer, H. F. Theory Predicts New Binuclear Transition-Metal Oxo and Carboxylato Photooxidation Products of $Mn_2(CO)_{10}$, $Fe_2(CO)_9$, and $Co_2(CO)_8$.

3. Zhang, B.; Moore, K. B.; and Schaefer, H. F. Controlling the Spin-spate of Carbenes with Non-covalent Interactions.

4. Estep, M. L.; Moore, K. B.; and Schaefer, H. F. Assessing the Viability of the $CH_3SO^{\cdot} + O_3$ Reaction.

5. Misiewicz, J. P.; Morgan, W. J.; Moore, K. B.; and Schaefer, H. F. Initial High-level Computation of the Fundamental Vibrational Frequencies of the Elusive Sulfurous Acid (H_2SO_3).

Presentations

1. Moore, K. B.; Mullen, T.J., "Scanning Probe Lithography of Multilayer Films for Multifunctional Templates." *University of North Florida Natural Sciences Poster Session*, Jacksonville, FL; Oct. 19, **2012**.

2. Moore, K. B.; Vergenz, R. A.; Migues, A. N.; Sirmans, A. "Identification and Characterization of methyl donated hydrogen bonds in Hyaluronate Lyase". *52nd Annual Sanibel Symposium*, St. Simon's Island, GA; Feb. 23, **2012**.

3. Moore, K. B.; Vergenz, R. A.; Migues, A. N.; Sirmans, A. "Identification and Characterization of methyl donated hydrogen bonds in Hyaluronate Lyase". *University of North Florida Natural Sciences Poster Session*, Jacksonville, FL; Oct. 14, **2011**.

4. Moore, K. B.; Migues, A. N.; Timmins, N.; Vergenz, R. A. "Effects of methyl donated hydrogen bonds on tertiary structure and function of hyaluronate lyase". *ACS Florida Annual Meeting and Exposition*, Tampa, FL; May 13, **2011**.

5. Moore, K. B.; Migues, A. N.; Timmins, N.; Vergenz, R. A. "Effects of methyl donated hydrogen bonds on tertiary structure and function of hyaluronate lyase". *University of North Florida Students Transforming Academic Research Symposium*, Jacksonville, FL; Apr. 15, **2011**.

6. Moore, K. B.; Migues, A. N.; Vergenz, R. A.; "On the Existence of methyl donated hydrogen bonds and their effect in Hyaluronate Lyase". University of North Florida *Natural Sciences Poster Session*, Jacksonville, FL; Sep. 18, **2010**.

7. Vergenz, R. A.; Migues, A. N.; Dudenkov, D.; Nix, A. J.; Carrasquillo, M.; Moore, K. B.; Bruno, P.; Gray, J.; Qazizada, H. "Can methyl-donated hydrogen bonds in proteins affect tertiary structure and function?" *50th Annual Sanibel Symposium*, St. Simon's Island, GA; Feb. 28, **2010**.

8. Vergenz, R. A.; Moore, K. B.; Migues, A. N., "Methyl donated hydrogen bond effects in spnHL through coordinate system analysis." *University of North Florida Natural Sciences Poster Session*, Jacksonville, FL; Oct. 16, **2009**.

Society Membership

American Chemical Society 2012—Present

Awards

1. Ashland-Hercules Scholarship ($500), University of North Florida, 2012
2. Superior Undergraduate Student Presentation ($100), 52nd Annual Sanibel Symposium, 2012
3. Summer Research Grant ($2000), University of North Florida, 2011