

**Dr. Gregory S. Tschumper, AAAS Fellow**

Donald L. Castleman/FCR Missouri Endowed Professor of Discovery  
 Department of Chemistry, Missouri University of Science and Technology

**I. Educational Background**

Ph. D. Theoretical Chemistry (Advisor: Henry F. Schaefer III)	University of Georgia Athens, GA	1999
B.S. Chemistry and Mathematics (Advisor: C. B. William Ng)	Winona State University Winona, MN	1995

**II. Professional Experience**

Castleman/FCR Endowed Professor (Chemistry)	Missouri S&T Rolla, MO	2024–present
Professor and Chair (Chemistry and Biochemistry)	University of Mississippi University, MS	2017–2024
Professor (Chemistry and Biochemistry)	University of Mississippi University, MS	2013–2017
Associate Professor (Chemistry and Biochemistry)	University of Mississippi University, MS	2007–2013
Assistant Professor (Chemistry and Biochemistry)	University of Mississippi University, MS	2001–2007
Postdoctoral Research Associate (Advisor: Keiji Morokuma)	Emory University Atlanta, GA	2000–2001
Postdoctoral Research Associate (Advisor: Martin Quack)	ETH-Zentrum Zürich, Switzerland	1999–2000

**III. Scholarly Activity and Bibliographic Indices**

126	Peer-reviewed journal publications (72 undergrad co-authors as university professor)
14	Journal covers/artwork featuring research
5,822	Total citations (9/2/24 via Google Scholar)
40	h-index (9/2/24 via Google Scholar)
80	i10-index (9/2/24 via Google Scholar)
117	Invited lectures at scientific meetings, colleges, universities and research institutions
>\$3M	External funding for my research lab
>\$25M	External research funding through leadership roles in multi-PI awards
>\$40M	Total external funding from all awards as PI, co-PI, senior personnel, etc.

**IV. Select Awards and Honors**

39th Annual Robert S. Mulliken Lecture, University of Georgia	2023
Featured in “Professor Appreciation” section of Fall 2021 <i>University of Mississippi Honors Report</i> (pages 16–26) from Sally McDonnell Barksdale Honors College	2021
University of Mississippi Distinguished Research and Creative Achievement Award	2021
SEC Faculty Achievement Award	2021

Elected Fellow of AAAS	2020
Elected Full Member of Sigma Xi	2020
PLATO Pioneer Award (Personalized Learning & Adaptive Teaching Opportunities)	2017
University of Mississippi Faculty Achievement Award	2015
Who's Who in America	2005, 2011
University of Mississippi Cora Lee Graham Award for Outstanding Teacher of Freshmen	2009
Who's Who of Emerging Leaders	2007
Mississippi Academy of Sciences Outstanding Presentation in Division	2005
University of Mississippi Faculty Research Fellow	2003, 2004
Graduated <i>summa cum laude</i> from University of Georgia	1999
ACS Local Section No. 427 Outstanding Graduate Student Award	1999
University of Georgia Graduate Honors Assistantship	1997–1999
ACS Local Section No. 427 Outstanding Chemistry Teaching Assistant of the Year	1996
Graduated <i>summa cum laude</i> from Winona State University	1995
ACS Local Section No. 537 Outstanding Graduating Chemistry Major	1995
Who's Who Among Students in American Universities and Colleges	1994
Ray C. Houtz Chemistry Scholarship at Winona State University	1994
ACS Local Section No. 537 Outstanding Freshman Chemistry Student	1992

## V. Select Professional Activities and Service

Co-editor of special issue in <i>International Journal of Molecular Sciences</i> Noncovalent Interactions: New Developments in Experiment and Theory	2022–2024
Invited Panelist for Mississippi NSF Day in Starkville, MS	21 November 2022
University of Mississippi representative on NSF Impact Panel	
Co-editor of special issue in <i>Inorganics</i> Halogen Bonding: Fundamentals and Applications	2018–2019
Host and co-organizer of annual conference for SETCA in Oxford, MS Southeast Theoretical Chemistry Association	18–20 May 2017
Associate Editor, Journal of Atomic and Molecular Sciences (JAMS)	2009–2017
Mississippi EPSCoR Computational Chemistry Research Group Leader	2009–2016
Co-organizer (with Nathan Hammer) of symposium on chemical physics at joint SE/SW Regional Meeting of the American Chemical Society in Memphis, TN	4–6 Nov. 2015
Co-organizer (with Troy Van Voorhis) of symposium on non-covalent interactions at 245th American Chemical Society National Meeting in New Orleans, LA	7–11 April 2013
Organizer of the 2011 MS EPSCoR Fall Research Forum in Oxford, MS with keynote lecture by 1981 Nobel Laureate Professor Roald Hoffmann	20 Sept. 2011
Quantum Chemistry Section Editor, Annual Reports in Computational Chemistry	2008–2014
Consultant to the Mississippi Center for Supercomputing Research	2004–2024
Host and organizer of annual conference for SETCA in Oxford, MS Southeast Theoretical Chemistry Association	21–22 May 2004
Chair of the Ole Miss local section of the American Chemical Society	2003–2004

## VI. External Research Grants and Fellowships

01/02–12/06	Research Corporation Research Innovation Award (PI) <i>Toward the Automated Theoretical Determination of Chemical Reactions with Systematically Guided Reaction Path Searches</i>	\$35,000
05/02–04/06	NSF EPS-0132618 (Senior Personnel) <i>Mississippi Computational Cluster</i>	Award total: \$6,200,000 PI total: \$195,000
07/05–06/08	Wolfram Research Inc. (PI) <i>Mathematica Academic Grant</i>	\$10,000
08/05–07/09	NSF CHE-0517067 (PI) <i>Probing Protein-Based Molecular Recognition through Computation and Simulation: Multicentered Hybrid Methods for the Reliable Characterization <math>\pi \cdots \pi</math> Interactions</i>	\$375,000
01/06–12/06	NASA NNG05GJ72H (co-PI) <i>Predicting Gas Solubility and Diffusivity in Room Temperature Ionic Liquids for the Design of Separating Agents for Carbon Dioxide Management</i>	\$30,000
05/06–10/09	NSF EPS-0556308 (Senior Personnel) <i>Innovations Through Computational Science</i>	Award total: \$7,125,000 PI total: \$221,334
08/09–07/10	Oak Ridge National Laboratories (PI) <i>Sabbatical Project at Oak Ridge National Laboratories</i>	\$100,964
09/09–08/16	NSF EPS-0903787 (CompChem Focus Area Leader) <i>Modeling and Simulation of Complex Systems</i>	Award total: \$23,000,000 PI total: \$950,338
07/10–06/13	NSF CHE-0957317 (PI) <i>Development and Application of Multicentered Integrated Methods for Weakly Bound Clusters</i>	\$363,173
09/10–08/12	NSF EPS-1006983 (co-PI) <i>Broadening Workstation Connectivity to Enhance Research Productivity and Student Preparation in Computational Sciences</i>	Award total: \$1,176,470 PI total: \$256,591
08/12–07/16	NSF CHE-1256713 (co-PI) <i>REU Site: Ole Miss Physical Chemistry Summer Research Program</i>	\$300,000
09/13–10/17	NSF CHE-1338056 (PI) <i>MRI: Acquisition of a GPU Cluster for Computational Science in Mississippi</i>	\$300,000
08/14–07/17	NSF IIA-1430364 (Senior Personnel, UM lead investigator) <i>Track-2: The Smart MATerial Design, Analysis, and Processing (SMATDAP) consortium</i>	Award total: \$2,699,753 PI total: \$320,428
08/15–07/18	NSF CHE-1460568 (co-PI) <i>REU Site: Ole Miss Physical Chemistry Summer Research Program</i>	\$270,000
08/17–07/22	NSF CHE-1664998 (PI) <i>Computational Characterization of Non-covalent Clusters with New &amp; Existing Methods</i>	\$374,939
09/18–08/22	NSF CHE-1757888 (co-PI) <i>REU Site: Ole Miss Physical Chemistry Summer Research Program</i>	\$299,682
08/22–07/25	NSF CHE-2154403 (PI) <i>Computational Characterization of Inter and Intramolecular NonCovalent Interactions</i>	\$484,922

## VII. Mentoring

76	Former undergraduate research assistants (REU participants, chemistry majors, etc.)
2	Former high school researchers
13	Ph.D. dissertations completed (9 women)
1	Ph.D. dissertation in progress
5	M.S. theses completed (3 women)
20	Undergraduate honors theses completed (13 women)
27	Student talks at scientific meetings, colleges and universities
238	Student posters at scientific meetings
2	Former post-doctoral researchers (1 woman)
1	Current post-doctoral researcher

## VIII. Select University Activities and Service

Department Chair	2017–2024
Research Space Analysis Task Force	2022–2024
Honors Council for Sally McDonnell Barksdale Honors College	2017–2024
School of Engineering Dean Search Committee	2022–2023
Promotion and Tenure, Innovation and Entrepreneurship (PTIE) committee	2020–2022
College of Liberal Arts Distinguished Professor Committee	2017–2022
Big Data Flagship Constellation Planning Committee	2018–2019
Chair of Research Momentum Task Force	2016–2018
Faculty Excellence Task Force	2016–2017
University Research Board	2013–2019
College of Liberal Arts Tenure and Promotion Review Committee	2015–2017
Department Representative on Faculty Senate	2015–2016
Chair of Biochemistry Faculty Search Committee	2015–2016
Co-Director of NSF-funded REU Summer Program	2013–2023
Academic Freedom and Faculty Responsibility Committee	2011–2015
Coulter Hall Annex Planning Committee	2012–2016
College of Liberal Arts Teaching Award Selection Committee	2010–2013
Co-Director of Chemistry Summer Research Program	2009–2012
Instructional Technology Standing Committee	2009–2012
Chair of Physical Chemistry Faculty Search Committee	2005–2006
University Research Board	2004–2007
External Seminar Program Coordinator for Department	2003–2009

## IX. Professional Societies

Sigma Xi, The Scientific Research Honor Society	2020–present
American Association for the Advancement of Science (AAAS)	2015–present

Mississippi Academy of Sciences (MAS) lifetime member 2005  
World Association of Theoretical and Computational Chemists (WATOC) lifetime member 2004  
American Chemical Society (ACS) 1993–present

## X. Graduate Dissertations (13) and Theses Directed(5)

Brian W. Hopkins, Ph.D. 13 April 2006  
*Ab Initio Studies of Intermolecular Interactions: Hydrogen Bonding, van der Waals Interactions, and the Multicentered Approach to Integrated Quantum Mechanical Calculations*

Abby Jones Weldon, M.S. 22 March 2007  
*A Quantum Chemical Examination of the Intrinsic Conformational Preferences of Oxaspirocyclic Model Systems and Substituted Cyclohexane, Tetrahydropyran, and Silocyclohexane*

Julie A. Anderson, Ph.D. 26 April 2007  
*Highly Accurate Computational Characterization of Weak Interactions in Biologically Relevant Prototypes: From Hydrogen Bonding in the Water Trimer to Stacking in Protein/Ligand Binding*

Adel M. ElSohly, M.S. 12 July 2007  
*Theoretical Investigations of Perfluorocycloalkanes, Prototyping  $\pi \cdots \pi$  Interactions, Implementation of Gradients into MC ONIOM Formalism, and Analysis of Polarization Consistent Basis Sets for Correlated Methods*

Ginger S. Mitchell, M.S. 15 November 2010  
*Characterizing the Structures, Energetics, and  $\pi$ -Type Interactions of  $(HC\equiv CH)_2$ ,  $(N\equiv N)_2$  and  $N\equiv N/HC\equiv CH$  van der Waals Dimers*

Desiree M. Bates, Ph.D. 22 March 2011  
*Theoretical Characterization of Non-covalent Weakly Bound Clusters Through the Application of Sophisticated Computational Quantum Chemistry Methodologies and the Development of Integrated Fragmentation Techniques*

Emily J. Carrell, M.S. 8 August 2011  
*Characterization of Intermolecular  $\pi$ -Type Interactions with Sophisticated Quantum Mechanical Electronic Structure Computations*

Kari L. Copeland, Ph.D. 11 April 2012  
*On the Nature of Weak Intermolecular Forces: A First Principles Approach to Hydrogen Bonding and Pi-Type Interactions*

Eric Van Dornshuld, Ph.D. 19 August 2014  
*Characterizing Non-covalent Interactions and Peptide Bond Formation with Electronic Structure Theory*

J. Coleman Howard, Ph.D. 1 December 2015  
*Accurate Computation of Molecular Properties from Novel Applications of Quantum Mechanical Wavefunction Methods*

Katelyn M. Dreux, Ph.D. 11 October 2018  
*Probing Noncovalent Interactions and Dative Bonding Using Electronic Structure Theory*

Thomas L. Ellington, Ph.D. 26 November 2018  
*Probing the Structures, Energetics, and Vibrational Signatures of Noncovalently Bound Complexes using Quantum Chemical Computations*

Sarah N. (Johnson) Arradondo, Ph.D. 13 May 2019

*Characterization of Hydrogen Bonding, Halogen Bonding and Argyrophilic Interactions using Computational Modeling*

Ben E. Smith, M.S.

14 October 2019

*Intramolecular Hydrogen Bonding in Epoxide, Thiirane, Aziridine and Phosphirane Containing Cyclopentanols*

Morgan A. Perkins, Ph.D.

2 November 2022

*Exploring Non-Covalent Interactions with Quantum Chemical Tools*

Kayleigh R. Barlow, Ph.D.

3 May 2023

*Computational Investigation of the Structures and Vibrational Spectra of Isolated and Hydrated Ions*

Carly A. Rock, Ph.D.

25 July 2023

*Characterization of Inter- and Intramolecular Non-Covalent Interactions through Computational Quantum Chemistry*

Jacquelyn J. Mosely, Ph.D.

19 July 2024

*Characterizing Cooperative Effects in Halogen Bonding and Ionic Hydrogen Bonding with Computational Quantum Chemistry*

## **XI. Undergraduate Honors Research Theses Directed (20)**

Adel M. ElSohly

May 2007

*Computational and ESR Studies of Perfluorocycloalkanes: Reliable Electron Affinities and Structures Determined from  $^{13}\text{C}$  and  $^{19}\text{F}$  Hyperfine Coupling Constants*

Macey L. Renault

May 2008

*Examination of Cooperative Effects in  $\pi$ -Stacking*

J. Coleman Howard

May 2011

*Structures, Energetics and Vibrational Spectra of Hydrated Pyrimidine*

Josh R. Smith

May 2011

*A Comparison and Cooperative Utilization of Møller-Plesset perturbation theory and B3LYP Density Functional Theory on Weakly Bound Structures*

Lance R. Ezell

May 2014

*Non-Covalent Interactions, Dative Bonding, and Electron Affinities: A Multi-Method Computational Study of Boron Tetrahalides*

Amanda Hardwick

May 2014

*Examination of Harmonic Vibrational Frequency Convergence to the Complete Basis Set Limit in Water Dimers and Hydrogen Fluoride Dimers*

Christina M. Holy

May 2014

*Anchoring the Potential Energy Surfaces of Homogeneous and Heterogeneous Dimers of Formaldehyde and Thioformaldehyde*

Cara M. Thorne

May 2014

*Evaluating the Efficacy of Small Basis Sets and the Counterpoise Procedure to Reproduce Complete Basis Set Limit Higher-Order Correlation Corrections for Weakly Bound Molecular Clusters*

Emily N. Hugo

May 2016

*A Computational Study of High Energy Density Materials and Their Detection Using Surface-Enhanced Raman Spectroscopy*

Laura M. Cline	May 2016
<i>Conformational Analysis of a Furan, Thiophene Alternating <math>\pi</math> System</i>	
Suhwan Paul Lee	May 2018
<i>Energetics and Vibrational Signatures of Nucleobase Argrophilic Interactions</i>	
Katarina M. Pittman	May 2018
<i>Computational Investigation on Electronic Structures and Properties of 4,6-bis(nitroimino)-1,3,5-triazinan-2-one: An Insensitive Munitions Compound</i>	
Hailey B. Reed	May 2018
<i>Investigations of Vibrational Signatures of Nitrobenzenes Enhanced by Argrophilic Interactions</i>	
Yasmeen Abdo	May 2019
<i>Structures, Energetics, and Vibrational Frequencies of Microhydrated Hexafluorophosphate, <math>PF_6^-(H_2O)_{n=1,2}</math> from DFT and Ab Initio Computations</i>	
Caroline A. Rader	May 2019
<i>Benchmark Structures and Harmonic Vibrational Frequencies of Hydrated Halide Ions: <math>X^-(H_2O)_n</math>, <math>X = F, Cl, Br, \text{ and } I</math> (where <math>n = 1-4</math>)</i>	
Carly A. Rock	May 2019
<i>Solvation of Isoelectronic Halide and Alkali Metal Ions by Noble Gas Atoms</i>	
Johnny Yang	May 2021
<i>A Theoretical Study of Concerted Proton Transfer in <math>(HF)_n</math>, <math>(H_2O)_n</math>, and <math>(HCl)_n</math> where <math>n = 3, 4, 5</math></i>	
Rachel Huynh	May 2022
<i>Microhydration of the Superhalogen Beryllium Trifluoride Anion, <math>BeF_3^-(H_2O)_{n=1-3}</math></i>	
Qihang (Jeffrey) Wang	May 2022
<i>Relative Energy Comparison for Water Clusters using MP2, df-MP2, and CCSD(T):MP2 Methods</i>	
Anna Robertson	May 2023
<i>Microhydration of Hexachlorophosphate Anion</i>	

## XII. Publications (126 Peer-Reviewed Journal Articles)

Publications include 72 undergraduate co-authors\* and 1 high school co-author†.

### A. Refereed Review Articles

- 1 J.C. Rienstra-Kiracofe, G.S. Tschumper, H.F. Schaefer, S. Nandi, and G.B. Ellison, *Chem. Rev.*, **102**, 231–282 (2002). “Atomic and Molecular Electron Affinities: Photoelectron Experiments and Theoretical Computations” <http://doi.org/10.1021/cr990044u>
- 2 G.S. Tschumper, in *Reviews in Computational Chemistry*, K.B. Lipkowitz and T.R. Cundari, Eds., Wiley-VCH, Inc., Hoboken, NJ, **26**, 39–90 (2009). “Reliable Electronic Structure Computations for Weak Non-Covalent Interactions in Clusters” <http://doi.org/10.1002/9780470399545.ch2>
- 3 J.C. Howard and G.S. Tschumper, *WIREs Comput. Mol. Sci.*, **4**, 199–224 (2014). “Wavefunction methods for the accurate characterization of water clusters” <http://doi.org/10.1002/wcms.1168>

### B. Other Refereed/Peer-Reviewed Publications

- 4 G.S. Tschumper, J.T. Fermann, and H.F. Schaefer, *J. Chem. Phys.*, **104**, 3676–3683 (1996). “Structures, thermochemistry, and electron affinities of the  $PF_n$  and  $PF_n^-$  series,  $n = 1 - 6$ ” <http://doi.org/10.1063/1.471538>

- 5 J.T. Fermann, B.C. Hoffman, G.S. Tschumper, and H.F. Schaefer, *J. Chem. Phys.*, **106**, 5102–5108 (1997). “The hydroperoxyl radical dimer: Triplet ring or singlet string?” <http://doi.org/10.1063/1.473530>
- 6 G.S. Tschumper, Y. Yamaguchi, and H.F. Schaefer, *J. Chem. Phys.*, **106**, 9627–9633 (1997). “A high level theoretical investigation of the cyclic hydrogen fluoride trimer” <http://doi.org/10.1063/1.473861>
- 7 G.S. Tschumper and H.F. Schaefer, *J. Chem. Phys.*, **107**, 2529–2541 (1997). “Predicting electron affinities with density functional theory: Some positive results for negative ions” <http://doi.org/10.1063/1.474593>
- 8 G.S. Tschumper and H.F. Schaefer, *J. Chem. Phys.* **108**, 7511–7515 (1998). “A comparison between the CISD[TQ] wave function and other highly correlated methods: Molecular geometry and harmonic vibrational frequencies of MgH<sub>2</sub>” <http://doi.org/10.1063/1.476183>
- 9 G. S. Tschumper, M. D. Kelty, and H. F. Schaefer, *Mol. Phys.* **96**, 493–504 (1999). “Subtle basis set effects on hydrogen bonded systems” <http://doi.org/10.1080/002689799165350>
- 10 R.A. Provencal, J.B. Paul, K. Roth, C. Chapo, R.N. Caseas, R.J. Saykally, G.S. Tschumper, and H.F. Schaefer, *J. Chem. Phys.*, **110**, 4258–4267 (1999). “Infrared cavity ringdown spectroscopy of methanol clusters: Single donor hydrogen bonding” <http://doi.org/10.1063/1.478309>
- 11 N.R. Brinkmann, G.S. Tschumper, and H.F. Schaefer, *J. Chem. Phys.*, **110**, 6240–6245 (1999). “Electron affinities of the oxides of aluminum, silicon, phosphorus, sulfur, and chlorine” <http://doi.org/10.1063/1.478528>
- 12 G.S. Tschumper, J.M. Gonzales, and H. F. Schaefer, *J. Chem. Phys.*, **111**, 3027–3034 (1999). “Assignment of the infrared spectra of the methanol trimer” <http://doi.org/10.1063/1.480263>
- 13 R.A. Provencal, R.N. Casaes, K. Roth, J.B. Paul, C.N. Chapo, R.J. Saykally, G.S. Tschumper, and H.F. Schaefer, *J. Phys. Chem. A*, **104**, 1423–1429 (2000). “Hydrogen Bonding in Alcohol Clusters: A Comparative Study by Infrared Cavity Ringdown Laser Absorption Spectroscopy” <http://doi.org/10.1021/jp9919258>
- 14 R. Berger, M. Quack, and G.S. Tschumper, *Helv. Chim. Acta* (Albert Eschenmoser special issue) **83**, 1919–1950 (2000). “Electroweak Quantum Chemistry for Possible Precursor Molecules in the Evolution of Biomolecular Homochirality” <http://quantum.chem.olemiss.edu/pub011HCAdirect.html>
- 15 G.S. Tschumper, *J. Chem. Phys.*, **114**, 225–230 (2001). “Chemically accurate conformational energies for aziridine-2-carbonitrile” <http://doi.org/10.1063/1.1329888>
- 16 G.S. Tschumper, M.L. Leininger, B.C. Hoffman, E.F. Valeev, H.F. Schaefer, and M. Quack, *J. Chem. Phys.*, **116**, 690–701 (2002). “Anchoring the water dimer potential energy surface with explicitly correlated computations and focal point analyses” <http://doi.org/10.1063/1.1408302>
- 17 G.S. Tschumper and M.R. Hoffman, *J. Math. Chem.*, **31**, 105–120 (2002). “Superconvergent Perturbation Theory for an Anharmonic Oscillator.” <http://doi.org/10.1023/A:1015438514814>



- 18 R.G. Carter, D.E. Graves, M.A. Gronemeyer\*, and G.S. Tschumper, *Org. Lett.*, **4**, 2181–2184 (2002). “Synthesis of the ABC Ring System of Azaspiracid. 2. A Systematic Study into the Effect of C<sub>16</sub> and C<sub>17</sub> Substitution on Bis-spirocyclization” <http://doi.org/10.1021/ol026034o>
- 19 G.S. Tschumper, M.C. Heaven, and K. Morokuma, *J. Phys. Chem. A*, **106**, 8453–8460 (2002). “An *ab Initio* Excursion on the Lowest 18 Electronic Surfaces of the NCl + NCl System: Some Insight into the Long-Range Self-Quenching Pathways of the First Excited State of NCl” <http://doi.org/10.1021/jp025692n>
- 20 G.S. Tschumper and K. Morokuma, *J. Mol. Struct. (THEOCHEM)*, **592**, 137–147 (2002). “Gauging the applicability of ONIOM (MO/MO) methods to weak chemical interactions in large systems: hydrogen bonding in alcohol dimers” [http://doi.org/10.1016/S0166-1280\(02\)00234-8](http://doi.org/10.1016/S0166-1280(02)00234-8)
- 21 G.S. Tschumper, M.C. Heaven, and K. Morokuma, *Chem. Phys. Lett.*, **370**, 418–424 (2002). “Concerning the stability of dichlorodiazene.” [http://doi.org/10.1016/S0009-2614\(03\)00129-5](http://doi.org/10.1016/S0009-2614(03)00129-5)
- 22 B.W. Hopkins and G.S. Tschumper, *J. Comput. Chem.*, **24**, 1563–1568 (2003). “A multicentered approach to integrated QM/QM calculations. Applications to multiply hydrogen bonded systems” <http://doi.org/10.1002/jcc.10319>
- 23 P. Zhang, S. Irle, K. Morokuma, and G.S. Tschumper, *J. Chem. Phys.*, **119**, 6524–6538 (2003). “*Ab Initio* theoretical studies of potential energy surfaces in the photodissociation of the vinyl radical. I.  $\tilde{A}$  state dissociation” <http://doi.org/10.1063/1.1604378>
- 24 N.R. Brinkmann, G.S. Tschumper, G. Yan, and H.F. Schaefer, *J. Phys. Chem. A*, **107**, 10208–10216 (2003). “An Alternative Mechanism for the Dimerization of Formic Acid” <http://doi.org/10.1021/jp031043f>
- 25 B.W. Hopkins and G.S. Tschumper, *Int. J. Quantum Chem.*, **96**, 294–302 (2004). “Extending the ONIOM Integrated MO/MO Approach to Hydrogen Bonding in Biological Systems: Serine-Water and Threonine-Water Dimers” <http://doi.org/10.1002/qua.10725>
- 26 N.J. Russ, T.D. Crawford, and G.S. Tschumper, *J. Chem. Phys.*, **120**, 7298–7306 (2004). “Real versus artifactual symmetry-breaking effects in Hartree–Fock, density-functional, and coupled-cluster methods” <http://doi.org/10.1063/1.1687336>
- 27 B.W. Hopkins and G.S. Tschumper, *J. Phys. Chem. A*, **108**, 2941–2948 (2004). “*Ab Initio* Studies of  $\pi \cdots \pi$  Interactions: The Effects of Quadruple Excitations” <http://doi.org/10.1021/jp0369084>
- 28 J.A. Anderson, K. Crager\*, L. Fedoroff\*, and G.S. Tschumper, *J. Chem. Phys.*, **121**, 11023–11029 (2004). “Anchoring the potential energy surface of the cyclic water trimer” <http://doi.org/10.1063/1.1799931>
- 29 B.W. Hopkins and G.S. Tschumper, *Mol. Phys.*, **103**, 309–315 (2005). “Multicentred QM/QM methods for overlapping model systems” <http://doi.org/10.1080/00268970512331317291>
- 30 B.W. Hopkins and G.S. Tschumper, *Chem. Phys. Lett.*, **407**, 362–367 (2005). “Integrated quantum mechanical approaches for extended  $\pi$  systems: Multicentered QM/QM studies of the cyanogen and diacetylene trimers” <http://doi.org/10.1016/j.cplett.2005.03.115>

- 31 A.M. ElSohly\*, G.S. Tschumper, R.A. Crocombe, J.T. Wang, and T.F. Williams, *J. Am. Chem. Soc.*, **127**, 10573–10583 (2005). “Computational and ESR Studies of Electron Attachment to Octafluorocyclobutane and Hexafluorocyclopropane: Electron Affinities of the Molecules and the Structures of their Stable Negative Ions as Determined from  $^{13}\text{C}$  and  $^{19}\text{F}$  Hyperfine Coupling Constants” <http://doi.org/10.1021/ja0505898>.
- 32 A. Jones Weldon, T.L. Vickrey, and G.S. Tschumper, *J. Phys. Chem. A*, **109**, 11073–11079 (2005). “Intrinsic Conformational Preferences of Substituted Cyclohexanes and Tetrahydropyrans Evaluated at the CCSD(T) Complete Basis Set Limit: Implications for the Anomeric Effect” <http://doi.org/10.1021/jp0550311>
- 33 A.M. ElSohly\*, M.L. Renault\*, and G.S. Tschumper, *J. Phys. Chem. A*, **110**, 1975–1977 (2006). “Reliable Electron Affinities of Perfluorocyclopropane and Perfluorocyclobutane from Convergent *ab Initio* Computations” <http://doi.org/10.1021/jp0557722>
- 34 J.A. Anderson and G.S. Tschumper, *J. Phys. Chem. A*, **110**, 7268–7271 (2006). “Characterizing the Potential Energy Surface of the Water Dimer with DFT: Failures of Some Popular Functionals for Hydrogen Bonding” <http://doi.org/10.1021/jp0613889>
- 35 G.S. Tschumper, *Chem. Phys. Lett.*, **427**, 185–191 (2006). “Multicentered integrated QM:QM methods for weakly bound clusters: An efficient and accurate 2-body:many-body treatment of hydrogen bonding and van der Waals interactions” <http://doi.org/10.1016/j.cplett.2006.06.021>
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- 112 C.A. Rock, S.N. Arradondo and G.S. Tschumper, *J. Phys. Chem. A*, **125**, 10524–10531 (2021). “Solvation of Isoelectronic Halide and Alkali Metal Ions by Argon Atoms” <http://dx.doi.org/10.1021/acs.jpca.1c08069>
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- 114 M.A. Perkins and G.S. Tschumper, *J. Phys. Chem. A*, **126**, 3688–3695 (2022). “Characterization of Competing Halogen- and Hydrogen-Bonding Motifs in Simple Mixed Dimers of HCN and HX (X = F, Cl, Br, and I)” <http://dx.doi.org/10.1021/acs.jpca.2c02041>
- 115 L.E. McNamara, E.C. Lambert\*, D.N. Reinemann, H. Valle, T.K. Hollis, G.S. Tschumper and N.I. Hammer, *Chem. Phys. Lett.*, **805**, 139928 (2022). “Raman spectroscopic, computational, and X-ray crystallographic investigation of intermolecular interactions in trimethylamine N-oxide (TMAO) and TMAO-d<sub>9</sub>” <http://dx.doi.org/10.1016/j.cplett.2022.139928>
- 116 K.R. Barlow and G.S. Tschumper, *Int. J. Quantum. Chem.*, **123**, e27075 (2023). “Conformational comparison of urea and thiourea near the CCSD(T) complete basis set limit” <http://dx.doi.org/10.1002/qua.27075>
- 117 A.L. Dorris, J. Watson, J.J. Mosely, E.C. Lambert, G.S. Tschumper, J.H. Delcamp and N.I. Hammer, *J. Phys. Chem. B*, **127**, 649–659 (2023). “Effects of Proaromaticity on Excited-State Lifetimes and Charge Separation in Near-Infrared Sensitizer Dyes in Solution and on TiO<sub>2</sub>” <http://dx.doi.org/10.1021/acs.jpcc.2c06906>
- 118 M.A. Perkins and G.S. Tschumper, *Chem. Phys*, **568**, 111843 (2023). “Characterization of competing halogen-bonding and hydrogen-bonding motifs in the acetonitrile/hydrogen iodide dimer” <http://dx.doi.org/10.1016/j.chemphys.2023.111843>
- 119 L.E. McNamara, E.C. Lambert\*, D.N. Reinemann, H. Valle, T.K. Hollis, G.S. Tschumper and N.I. Hammer, *Chem. Phys. Lett.*, **816**, 140369 (2023). Corrigendum to “Raman spectroscopic, computational, and X-ray crystallographic investigation of intermolecular interactions in trimethylamine N-oxide (TMAO) and TMAO-d<sub>9</sub>” <http://dx.doi.org/10.1016/j.cplett.2023.140369>
- 120 K.R. Barlow, and G.S. Tschumper, *Mol. Phys.*, **122**, e2262621 (2023). “Fundamental vibrational frequencies of pnictogen (*Pn*) containing linear triatomic anions:  $OCPn^-$  and  $SCPn^-$  where *Pn* = N, P, As and Sb” <http://dx.doi.org/10.1080/00268976.2023.2262621>
- 121 L.N. Olive, E.V. Dornshuld, H.F. Schaefer and G.S. Tschumper, *J. Phys. Chem. A*, **127**, 8806 (2023). “Competition Between Solvent/Solvent and Solvent/Solute Interactions in the Microhydration of the Tetrafluoroborate Anion,  $BF_4^- (H_2O)_{n=1,2,3,4}$ ” <http://dx.doi.org/10.1021/acs.jpca.3c04014>
- 122 C.A. Rock and G.S. Tschumper, *Int. J. Mol. Sci.*, **24**, 17480 (2023). “Insight into the Binding of Argon to Cyclic Water Clusters from Symmetry-Adapted Perturbation Theory” <http://dx.doi.org/10.3390/ijms242417480>
- 123 Y. Xue, T.M. Sexton, J. Yang\* and G.S. Tschumper, *PCCP*, **26**, 12483 (2024). “Systematic Analysis of Electronic Barrier Heights and Widths for Concerted Proton Transfer in Cyclic Hydrogen Bonded Clusters:  $(HF)_n$ ,  $(HCl)_n$  and  $(H_2O)_n$  where  $n = 3, 4, 5$ ” <http://dx.doi.org/10.1039/D4CP00422A>
- 124 M.A. Saucier, N.A. Kruse, B.E. Seidel, N.I. Hammer, G.S. Tschumper and J.H. Delcamp, *J. Org. Chem.*, **89**, 9092 (2024). “Phospha-RosIndolizine Dye with Shortwave Infrared (SWIR) Absorption and Emission” <http://dx.doi.org/10.1021/acs.joc.4c00741>
- 125 J.J. Mosely and G.S. Tschumper, *J. Phys. Chem. A*, **128**, 5637 (2024). “Probing the Effects of Size and Charge on the Monohydration and Dihydration of  $SiF_5^-$  and  $SiF_6^{2-}$  via Comparisons with  $BF_4^-$  and  $PF_6^-$ ” <http://dx.doi.org/10.1021/acs.jpca.4c03430>

- 126 W.E. Meador, M.A. Saucier, M.R. Tucker, N.A. Kruse, A.J. Mobley\*, C.R. Brower, S.R. Parkin, K.M. Clark, N.I. Hammer, G.S. Tschumper and J.H. Delcamp, *Chem. Sci.*, **15**, 12349 (2024). “Extended shortwave infrared absorbing antiaromatic fluorenum-indolizine chromophores” <https://doi.org/10.1039/D4SC00733F>

### C. Publications not Refereed/Peer-Reviewed

- 127 G. S. Tschumper and N. I. Hammer, *J. Am. Chem. Soc.* **132**, 9512 (2010). “Non-Covalent Interactions: Theory and Experiment” (Book Review). <http://.doi.org/10.1021/ja104759m>
- 128 G. S. Tschumper “The Great Anion Project” in *Molecular Quantum Mechanics: From Methylene to DNA and Beyond, Selected Papers of Henry F. Schaefer III*, R. J. Bartlett, T. D. Crawford, M. Head-Gordon and C. D. Sherrill, Eds. Brandon’s Printing, Atlanta, GA, Ch. 22, 245–247 (2010).

## XIII. Scientific Presentations

### A. Invited Lectures at Universities, Colleges and Professional Meetings

- 1 Department of Chemistry, Winona State University, Winona, MN, 16 Oct. 2000.
- 2 Department of Chemistry and Biochemistry, University of Mississippi, Oxford, MS, 18 Jan. 2001.
- 3 Center for Theoretical Studies of Physical Systems, Clark Atlanta University, Atlanta, GA, 18 Apr. 2002.
- 4 School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA, 19 Apr. 2002.
- 5 Department of Physical Sciences, University of West Alabama, Livingston, AL, 24 Oct. 2002.
- 6 Department of Chemistry, Hendrix College, Conway, AR, 18 Nov. 2002.
- 7 Department of Chemistry, University of Wisconsin-LaCrosse, LaCrosse, WI, 21 Nov. 2002.
- 8 Department of Chemistry, Winona State University, Winona, MN, 22 Nov. 2002.
- 9 Department of Chemistry, St. Mary’s University, Winona, MN, 22 Nov. 2002.
- 10 Polymer Science Research Center, University of Southern Mississippi, Hattiesburg, MS, 2 Mar. 2003.
- 11 Department of Chemistry and Biochemistry, Mississippi College, Clinton, MS, 3 Mar. 2003.
- 12 32nd Meeting of the Southeast Theoretical Chemistry Association, Clemson University, Clemson, SC, 24 May 2003.
- 13 Department of Chemistry, University of Alabama at Birmingham, Birmingham, AL, 25 Sept. 2003.
- 14 Department of Chemistry, Murray State University, Murray, KY, 26 Jan. 2004.
- 15 Department of Chemistry, University of Tennessee, Knoxville, TN, 13 May 2004.
- 16 Computational Chemical Sciences Group, Oak Ridge National Laboratory, Oak Ridge, TN, 14 May 2004.

- 17 Computational Center for Molecular Structure and Interactions, Jackson State University, Jackson, MS, 19 Jul. 2004.
- 18 228th National Meeting of the American Chemical Society, Philadelphia, PA, 26 Aug. 2004.
- 19 Department of Chemistry, University of Georgia, Athens, GA, 24 Sept. 2004.
- 20 Department of Chemistry, Winona State University, Winona, MN, 22 Nov. 2004.
- 21 Department of Chemistry, University of Wisconsin-LaCrosse, LaCrosse, WI, 23 Nov. 2004.
- 22 7th World Congress of the World Association of Theoretically Oriented Chemists, Cape Town, South Africa, 16–21 Jan. 2005.
- 23 230th National Meeting of the American Chemical Society, Washington, DC, 28 Aug. – 1 Sept. 2005.
- 24 2005 International Chemical Congress of Pacific Basin Societies (PACIFICHEM), Honolulu, Hawaii, 15–20 Dec. 2005.
- 25 231st National Meeting of the American Chemical Society, Atlanta, GA, 26–30 Mar. 2006.
- 26 Department of Chemistry, University of Memphis, Memphis, TN, 8 Sept. 2006.
- 27 Department of Chemistry and Biochemistry, University of Southern Mississippi, Hattiesburg, MS, 22 Sept. 2006.
- 28 Department of Chemistry, University of Central Arkansas, Conway, AR, 26 Oct. 2006.
- 29 Department of Chemistry, Mississippi State University, Starkville, MS, 19 Jan. 2007.
- 30 Department of Chemistry, Union University, Jackson, TN, 23 Mar. 2007.
- 31 Department of Physical Sciences, University of West Alabama, Livingston, AL, 19 Apr. 2007.
- 32 36th Meeting of the Southeast Theoretical Chemistry Association, Virginia Tech, Blacksburg, VA, 18-19 May 2007.
- 33 Molecular Quantum Mechanics: Analytic Gradients and Beyond. An International Conference in Honor of Peter Pulay, Budapest, Hungary, 29 May – 3 June 2007.
- 34 Mississippi Center for Supercomputing Research Symposium, Oxford, MS, 6–7 Sept. 2007.
- 35 Department of Chemistry and Biochemistry, Mississippi State University, Starkville, MS, 28 Sept. 2007.
- 36 Department of Chemistry, Tulane University, New Orleans, LA, 22 Oct. 2007.
- 37 Department of Chemistry, University of New Orleans, New Orleans, LA, 23 Oct. 2007.
- 38 235th National Meeting of the American Chemical Society, New Orleans, LA, 6–10 Apr. 2008.
- 39 8th Southern School on Computational Chemistry, Jackson, MS, 25–26 Apr. 2008.
- 40 236th National Meeting of the American Chemical Society, Philadelphia, PA, 17–21 Aug. 2008.

- 41 Latsis–Symposium, "Intramolecular Dynamics, Symmetry and Spectroscopy" ETH Zurich, Switzerland, 6-10 Sept. 2008.
- 42 8th International Congress of the World Association of Theoretical and Computational Chemists, Sydney, Australia, 14–19 Sept. 2008.
- 43 49th Sanibel Symposium, St. Simons Island, GA, 26 Feb.–3 March 2009.
- 44 Department of Chemistry, Western Carolina University, Cullowhee, NC, 13 Feb. 2009.
- 45 Department of Chemistry, Winona State University, Winona, MN, 23 Mar. 2009
- 46 Department of Chemistry and Biochemistry, Auburn University, Auburn, AL, 22 Oct. 2009
- 47 Department of Chemistry, Murray State University, Murray, KY, 23 Nov. 2009
- 48 Department of Chemistry, Georgia College and State University, Milledgeville, GA, 29 Jan. 2010
- 49 Department of Chemistry, Winona State University, Winona, MN, 22 Mar. 2010
- 50 Molecular Quantum Mechanics 2010: An International Conference in Honor of Professor Henry F. Schaefer III, University of California, Berkeley, CA, 24–29 May 2010
- 51 Mississippi Center for Supercomputing Research Mini-Camp, Oxford, MS, 11-12 July 2010
- 52 Department of Chemistry and Physics, Southeastern Louisiana University, Hammond, LA, 22 Oct. 2010
- 53 62nd Southeastern Regional Meeting of the American Chemical Society (Joint Meeting with 66th Southwest Regional Meeting), New Orleans, LA, 30 Nov.–4 Dec. 2010.
- 54 Department of Chemistry and Biochemistry, Jackson State University, Jackson, MS, 28 Jan. 2011
- 55 Department of Physics and Astronomy, University of Mississippi University, MS, 1 Mar. 2011
- 56 241st National Meeting of the American Chemical Society, Anaheim, CA, 27–31 Mar. 2011.
- 57 40th Meeting of the Southeast Theoretical Chemistry Association, Mississippi State University, Starkville, MS, 13–14 May 2011.
- 58 Department of Chemistry and Biochemistry, University of Lethbridge, Lethbridge, AB, Canada, 24 Aug. 2011.
- 59 Summer Talks in Santiago: Recent Developments in Quantum Chemistry at Pontificia Universidad Católica de Chile, Santiago, Chile, 9–13 Jan. 2012.
- 60 Department of Chemistry, University of Memphis, Memphis, TN, 27 Jan. 2012.
- 61 Department of Chemistry and Biochemistry, Huntingdon College Montgomery, AL, 30 Jan. 2012.
- 62 41st Meeting of the Southeast Theoretical Chemistry Association, University of Georgia, Athens, GA, 17–19 May 2012.
- 63 11th MERCURY Conference for Undergraduate Computational Chemistry, Bucknell University, Lewisburg, PA, 26–28 July 2012.

- 64 53rd Sanibel Symposium, St. Simons Island, GA, 17–22 Feb. 2013
- 65 42nd Meeting of the Southeast Theoretical Chemistry Association, Auburn University, Auburn, AL, 9–11 May 2013.
- 66 Department of Chemistry, University of Alabama at Birmingham, Birmingham, AL, 24 Oct. 2013.
- 67 Department of Chemistry, University of South Alabama, Mobile AL, 25 Oct. 2013.
- 68 Department of Chemistry and Biochemistry, University of Mississippi, Oxford, MS, 31 Oct. 2013.
- 69 2013 Southwest Regional Meeting (SWRM) of the American Chemical Society, Waco, TX, 16–19 Nov. 2013.
- 70 Department of Sciences and Mathematics, Mississippi University for Women, Columbus, MS, 22 Jan. 2014.
- 71 Department of Chemistry and Biochemistry, Mississippi College, Clinton, MS, 23 Jan. 2014.
- 72 Department of Chemistry and Biochemistry, University of Southern Mississippi, Hattiesburg, MS, 24 Jan. 2014.
- 73 25th Austin Symposium on Molecular Structure and Dynamics at Dallas (ASMD@D), Dallas, TX, 1–4 Mar. 2014.
- 74 College of Liberal Arts Common Reading Experience, University of Mississippi, 9 Sept. 2014.
- 75 14th Southern School on Computational Chemistry and Materials Science (SSCCMS), Jackson, MS, 24–15 July 2014.
- 76 10th International Congress of the World Association of Theoretical and Computational Chemists, Santiago, Chile, 5–10 Oct. 2014.
- 77 Department of Chemistry, Belhaven University Jackson, MS, 23 Jan. 2015.
- 78 Department of Chemistry and Biochemistry, Samford University Birmingham, AL, 5 Feb. 2015.
- 79 44th Meeting of the Southeast Theoretical Chemistry Association, University of Central Florida, Orlando, FL, 14–16 May 2015.
- 80 14th MERCURY Conference for Undergraduate Computational Chemistry, Bucknell University, Lewisburg, PA, 23–25 July 2015.
- 81 Intermolecular Interactions: New Challenges for ab initio Theory (Telluride Science Research Center workshop), Telluride, CO 6–11 July 2015.
- 82 Department of Chemistry, Johns Hopkins University, Baltimore, MD, 20 Oct. 2015.
- 83 2015 Joint Southeast/Southwest Regional Meeting of the American Chemical Society (SERMACS/SWRM), Memphis, TN, 4–7 Nov. 2015.
- 84 2015 International Chemical Congress of Pacific Basin Societies (PACIFICHEM), Honolulu, Hawaii, 15–20 Dec. 2015.
- 85 Department of Chemistry, Mississippi State University, Starkville, MS, 29 Jan. 2016.

- 86 Department of Chemistry and Biochemistry, Texas Woman's University, Denton, TX, 4 March 2016.
- 87 26th Austin Symposium on Molecular Structure and Dynamics at Dallas (ASMD@D), Dallas, TX, 5–7 Mar. 2016.
- 88 Electronic Structure: Concepts & Applications Symposium at 68th Southeastern Regional meeting of the American Chemical Society (SERMACS): Columbia, SC, 23–26 Oct. 2016
- 89 Cope Symposium: Molecules to Functional Supramolecular Materials at 68th Southeastern Regional meeting of the American Chemical Society (SERMACS): Columbia, SC, 23–26 Oct. 2016
- 90 Department of Chemistry and Biochemistry, Georgia Southern University, Statesboro, GA, 27 Oct. 2016
- 91 Department of Chemistry and Physics, Armstrong State University, Savannah, GA, 28 Oct. 2016
- 92 Chemistry Department, Truman State University, Kirksville, MO, 11 Nov. 2016
- 93 Center for Computational Quantum Chemistry, University of Georgia, Athens, GA, 9 Mar. 2017
- 94 Nanomaterials: Computation, Theory, and Experiment (Telluride Science Research Center Workshop), Telluride, CO 11–15 July 2017.
- 95 US Army ERDC Computational Chemistry/Computational Modeling Meeting, Vicksburg, MS 9 Sept. 2017.
- 96 Contemporary Computational Chemistry Symposium at 69th Southeastern Regional meeting of the American Chemical Society (SERMACS), Charlotte, NC, 7–11 Nov. 2017
- 97 Department of Chemistry and Biochemistry, Baylor University, Waco, TX, 12 Jan. 2018
- 98 Department of Chemistry and Biochemistry, Tulane University, New Orleans, LA, 19 Feb. 2018
- 99 27th Austin Symposium on Molecular Structure and Dynamics at Dallas, Dallas, TX, 3–5 March 2018
- 100 Current State of Environmental Contamination Research: Theory & Experiment Symposium at 255th National Meeting of the American Chemical Society (ACS), New Orleans, LA, 18–22 March 2018
- 101 47th Meeting of the Southeast Theoretical Chemistry Association, Louisiana State University, Baton Rouge, Louisiana, 18–19 May 2018.
- 102 US Army ERDC Computational Chemistry/Computational Modeling Meeting, Vicksburg, MS, 7 Aug. 2018.
- 103 Chemistry Department, Henderson State University, Arkadelphia, AR, 27 Sept. 2018.
- 104 Department of Chemistry, Xavier University, New Orleans, LA, 25 Oct. 2018.
- 105 Computational Quantum Chemistry: From Promise to Prominence Symposium at 258th National Meeting of the American Chemical Society (ACS), San Diego, CA, 25–29 Aug. 2019

- 106 US Army ERDC Computational Chemistry/Computational Modeling Meeting, Vicksburg, MS, 24 Sept. 2019.
- 107 Department of Chemistry, Southern Methodist University, Dallas, TX, 18 Oct. 2019.
- 108 Department of Chemistry, Virginia Tech, Blacksburg, VA, 5 Mar. 2020.
- 109 Department of Chemistry and Biochemistry, University of Mississippi, Oxford, MS (Virtual Coulter Grad Recruiting Seminar Series), 25 Oct. 2021.
- 110 2021 International Chemical Congress of Pacific Basin Societies (PACIFICHEM), Honolulu, Hawaii (virtual), 16–20 Dec. 2021.
- 111 12th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2020), Vancouver, BC, 3–8 July 2022
- 112 28th Austin Symposium on Molecular Structure and Dynamics at Dallas, Dallas, TX, 17–20 February 2023
- 113 2023 MERCURY Conference for Undergraduate Computational Chemistry, Furman University, Greenville, SC, 19–21 July 2023.
- 114 Department of Chemistry and Center for Computational Quantum Chemistry, University of Georgia, Athens, GA, 3 Oct. 2023
- 115 Department of Chemistry, Furman University, Greenville, SC, 5 Oct. 2023
- 116 Department of Chemistry and Biochemistry, University of California, Merced, Merced, CA, 27 Oct. 2023
- 117 Department of Chemistry, Missouri University of Science and Technology, Rolla, MO, 2 April 2024

## **B. Contributed Lectures at Professional Meetings**

- 1 Centennial Meeting of the American Physical Society, Atlanta, GA, 20–26 March 1999.
- 2 2nd Southern School on Computational Quantum Chemistry, Orange-Beach, AL, 23 Mar. 2002.
- 3 225th National Meeting of the American Chemical Society, New Orleans, LA, 24 Mar. 2003.
- 4 55th Southeast Regional Meeting of the American Chemical Society, Atlanta, GA, 16–19 Nov. 2003.
- 5 4th Southern School on Computational Quantum Chemistry, Orange-Beach, AL, 22–23 Mar. 2004.
- 6 69th Meeting of the Mississippi Academy of Sciences, Oxford, MS, 17–18 Feb. 2005.
- 7 34th Meeting of the Southeast Theoretical Chemistry Association, University of Tennessee, Knoxville, TN, 17–19 June 2005.
- 8 Spring 2008 National Meeting of the American Chemical Society, New Orleans, LA, 6–10 Mar. 2008.
- 9 9th World Congress of the World Association of Theoretically Oriented and Computational Chemists, Santiago de Compostela, Spain 17–22 July, 2011.

- 10 2013 Southeast Regional Meeting of the American Chemical Society (SERMACS), Atlanta, GA, 12–16 Nov. 2013.
- 11 248th American Chemical Society National Meeting, San Francisco, CA, 10–14 Aug. 2014.
- 12 2015 International Chemical Congress of Pacific Basin Societies (PACIFICHEM), Honolulu, Hawaii, 15–20 Dec. 2015.
- 13 Computational Studies of Water Symposium at 255th National Meeting of the American Chemical Society (ACS), New Orleans, LA, 18–22 March 2018
- 14 Physical Chemistry of Ionic Liquids Symposium at 255th National Meeting of the American Chemical Society (ACS), New Orleans, LA, 18–22 March 2018
- 15 ScotCHEM 2018 Computational Chemistry Symposium, St. Andrews Scotland, 14–15 June 2018
- 16 Computational Studies of Water Symposium at 256th National Meeting of the American Chemical Society (ACS), Boston, MA, 19–23 August 2018
- 17 59th Sanibel Symposium, St. Simons Island, GA, 17–22 Feb. 2019
- 18 Hydration from the Gas to the Condensed Phase Symposium at 258th National Meeting of the American Chemical Society (ACS), San Diego, CA, 25–29 Aug. 2019
- 19 New Developments in Hybrid QM/QM, QM/MM, and Fragmentation Methods Symposium at Spring National Meeting of the American Chemical Society (ACS), San Diego, CA, 20–24 March 2022
- 20 Synergy of Theory and Experiment: A Symposium in Honor of Prof. John F. Stanton at Spring National Meeting of the American Chemical Society (ACS), San Diego, CA, 20–24 March 2022
- 21 76th International Symposium on Molecular Spectroscopy, Urbana-Champaign, IL, 19–23 June, 2023
- 22 63rd Sanibel Symposium, St. Augustine Beach, FL, 25 Feb. – 1 Mar. 2024
- 23 Fritz Fest 2024: Symposium Honoring Prof. Henry F. Schaefer III on the Occasion of His 80th Birthday, Atlanta, GA, 7 June 2024
- 24 77th International Symposium on Molecular Spectroscopy, Urbana-Champaign, IL, 17–21 June, 2024

### **C. Posters and Other Presentations at Professional Meetings**

- 1 63rd Annual Meeting of the Minnesota Academy of Science, University of Minnesota Morris, MN, 29 April 1995.
- 2 Molecular Quantum Mechanics: Methods and Applications. An International Conference in Memory of Samuel Francis Boys and in Honor of Isaiah Shavitt, University of Cambridge, Cambridge, England, 3–7 September 1995.
- 3 37th Sanibel Symposium, St. Augustine, FL, 3 March 1997.
- 4 26th Meeting of the Southeast Theoretical Chemistry Association, University of Alabama at Birmingham, Birmingham, AL, 17 May 1997.



- 5 27th Meeting of the Southeast Theoretical Chemistry Association, Florida State University, Tallahassee, FL, 28–30 May 1998.
- 6 Structural and Mechanistic Organic Chemistry: An International Conference in Honor of Professor Norman L. Allinger, University of Georgia, Athens, GA, 3–7 June 1997.
- 7 5th World Congress of the World Association of Theoretically Oriented Chemists, Imperial College, London, England, 1–6 August 1999.
- 8 40th Sanibel Symposium, St. Augustine, FL, 28 Feb. 2000.
- 9 10th Current Trends in Computational Quantum Chemistry, Jackson, MS, 1-3 Nov. 2001.
- 10 31st Meeting of the Southeast Theoretical Chemistry Association, Georgia Institute of Technology, Atlanta, GA, 24–25 May 2002.
- 11 6th World Congress of the World Association of Theoretically Oriented Chemists, Lugano, Switzerland, 4–9 Aug. 2002.
- 12 15th Current Trends in Computational Quantum Chemistry, Jackson, MS, 3–4 Nov. 2006.
- 13 16th Current Trends in Computational Quantum Chemistry, Jackson, MS, 2–3 Nov. 2007.
- 14 13th International Congress of Quantum Chemistry, Helsinki, Finland, 22–27 June 2009.
- 15 50th Sanibel Symposium, St. Simons Island, GA, 24 February–2 March 2010.
- 16 2010 International Chemical Congress of Pacific Basin Societies (PACIFICHEM), Honolulu, Hawaii, 15–20 December 2010.
- 17 20th Current Trends in Computational Quantum Chemistry, Jackson, MS, 27–29 October 2011.
- 18 Molecular Quantum Mechanics: Electron Correlation: The Many-Body Problem at the Heart of Chemistry. An International Conference in Honour of Rodney J. Bartlett Lugano, Switzerland, 2–7 June 2013.

#### **XIV. Current Research Assistants**

Yuan (Mike) Xue

Postdoctoral Research Associate

Max Tucker

Ph.D. student