Curriculum Vitae August 2025

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

128	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)
122	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 *University of Mississippi Honors Report* (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 *summa cum laude* 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 *summa cum laude* 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 *International Journal of Molecular Sciences* Noncovalent Interactions: New Developments in Experiment and Theory	2022–2024
Invited Panelist for Mississippi NSF Day in Starkville, MS University of Mississippi representative on NSF Impact Panel	21 November 2022
Co-editor of special issue in *Inorganics* 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) *Toward the Automated Theoretical Determination of Chemical Reactions with Systematically Guided Reaction Path Searches*	$35,000
05/02–04/06	NSF EPS-0132618 (Senior Personnel) *Mississippi Computational Cluster*	Award total: $6,200,000 PI total: $195,000
07/05–06/08	Wolfram Research Inc. (PI) *Mathematica Academic Grant*	$10,000
08/05–07/09	NSF CHE-0517067 (PI) *Probing Protein-Based Molecular Recognition through Computation and Simulation: Multicentered Hybrid Methods for the Reliable Characterization $\pi \cdots \pi$ Interactions*	$375,000
01/06–12/06	NASA NNG05GJ72H (co-PI) *Predicting Gas Solubility and Diffusivity in Room Temperature Ionic Liquids for the Design of Separating Agents for Carbon Dioxide Management*	$30,000
05/06–10/09	NSF EPS-0556308 (Senior Personnel) *Innovations Through Computational Science*	Award total: $7,125,000 PI total: $221,334
08/09–07/10	Oak Ridge National Laboratories (PI) *Sabbatical Project at Oak Ridge National Laboratories*	$100,964
09/09–08/16	NSF EPS-0903787 (CompChem Focus Area Leader) *Modeling and Simulation of Complex Systems*	Award total: $23,000,000 PI total: $950,338
07/10–06/13	NSF CHE-0957317 (PI) *Development and Application of Multicentered Integrated Methods for Weakly Bound Clusters*	$363,173
09/10–08/12	NSF EPS-1006983 (co-PI) *Broadening Workstation Connectivity to Enhance Research Productivity and Student Preparation in Computational Sciences*	Award total: $1,176,470 PI total: $256,591
08/12–07/16	NSF CHE-1256713 (co-PI) *REU Site: Ole Miss Physical Chemistry Summer Research Program*	$300,000
09/13–10/17	NSF CHE-1338056 (PI) *MRI: Acquisition of a GPU Cluster for Computational Science in Mississippi*	$300,000
08/14–07/17	NSF IIA-1430364 (Senior Personnel, UM lead investigator) *Track-2: The Smart MATerial Design, Analysis, and Processing (SMATDAP) consortium*	Award total: $2,699,753 PI total: $320,428
08/15–07/18	NSF CHE-1460568 (co-PI) *REU Site: Ole Miss Physical Chemistry Summer Research Program*	$270,000
08/17–07/22	NSF CHE-1664998 (PI) *Computational Characterization of Non-covalent Clusters with New & Existing Methods*	$374,939
09/18–08/22	NSF CHE-1757888 (co-PI) *REU Site: Ole Miss Physical Chemistry Summer Research Program*	$299,682
08/22–07/25	NSF CHE-2154403 (PI) *Computational Characterization of Inter and Intramolecular NonCovalent Interactions*	$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 Oxaspirocycle 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 π-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 π-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 Bondng 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}C and ^{19}F Hyperfine Coupling Constants

Macey L. Renault May 2008
Examination of Cooperative Effects in π–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
Conformational Analysis of a Furan, Thiophene Alternating π System

Suhwan Paul Lee May 2018
Energetics and Vibrational Signatures of Nucleobase Argyrophilic Interactions

Katarina M. Pittman May 2018
Computational Investigation on Electronic Structures and Properties of 4,6-bis(nitroimino)-1,3,5-triazinan-2-one: An Insensitive Munitions Compound

Hailey B. Reed May 2018
Investigations of Vibrational Signatures of Nitrobenzenes Enhanced by Argyrophillic Interactions

Yasmeen Abdo May 2019
Structures, Energetics, and Vibrational Frequencies of Microhydrated Hexafluorophosphate, $PF_6^-(H_2O)_{n=1,2}$ from DFT and Ab Initio Computations

Caroline A. Rader May 2019
Benchmark Structures and Harmonic Vibrational Frequencies of Hydrated Halide Ions: $X^-(H_2O)_n$, X = F, Cl, Br, and I (where n = 1–4)

Carly A. Rock May 2019
Solvation of Isoelectronic Halide and Alkali Metal Ions by Noble Gas Atoms

Johnny Yang May 2021
A Theoretical Study of Concerted Proton Transfer in $(HF)_n$, $(H_2O)_n$, and $(HCl)_n$ where $n = 3, 4, 5$

Rachel Huynh May 2022
Microhydration of the Superhalogen Beryllium Trifluoride Anion, $BeF_3^-(H_2O)_{n=1-3}$

Qihang (Jeffrey) Wang May 2022
Relative Energy Comparison for Water Clusters using MP2, df-MP2, and CCSD(T):MP2 Methods

Anna Robertson May 2023
Microhydration of Hexachlorophosphate Anion

XII. Publications (128 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_2" 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/pub011HCAredirect.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_{16} and C_{17} 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

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

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 π 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}C and ^{19}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

36 J.A. Anderson, B.W. Hopkins, J.L. Chapman*, and G.S. Tschumper, *J. Mol. Struct.* (THEOCHEM), **771**, 65–71 (2006). "A systematic assessment of density functionals and ONIOM schemes for the study of hydrogen bonding between water and the side chains of serine, threonine, asparagine, and glutamine" http://doi.org/10.1016/j.theochem.2006.03.042

37 A. Jones Weldon and G.S. Tschumper, *J. Org. Chem.*, **71**, 9212–9216 (2006). "Energetics of Oxaspirocycle Prototypes: 1,7-Dioxaspiro[5.5]undecane and 1,7,9-Trioxadispiro[5.1.5.3]hexadecane" http://doi.org/10.1021/jo061689e

38 B.W. Hopkins, A.M. ElSohly*, and G.S. Tschumper, *Phys. Chem. Chem. Phys.*, **9**, 1550–1558 (2007). "Reliable structures and energetics for two new delocalized $\pi \ldots \pi$ prototypes: cyanogen dimer and diacetylene dimer" http://doi.org/10.1039/b616878g

39 A. Jones Weldon and G. S. Tschumper, *Int. J. Quantum Chem.*, **107**, 2261–2265 (2007). "Intrinsic conformational preferences of and an anomeric-like effect in 1-substituted silacyclohexanes" http://doi.org/10.1002/qua.21336

40 A.M. ElSohly*, C.L. Shaw*, M.E. Guice*, B.D. Smith*, and G.S. Tschumper, *Mol. Phys.*, **105**, 2777–2782 (2007). "Analytic gradients for the multicentred integrated QM:QM method for weakly bound clusters: efficient and accurate 2-body:many-body geometry optimizations" http://doi.org/10.1080/00268970701633126

41 D.M. Bates, J.A. Anderson, P. Oloyede, and G.S. Tschumper, *Phys. Chem. Chem. Phys.*, **10**, 2775–2779 (2008). "Probing the effects of heterogeneity on delocalized $\pi \cdots \pi$ interaction energies" http://doi.org/10.1039/b718720c

42 A.M. ElSohly* and G.S. Tschumper, *Int. J. Quantum Chem.*, **109**, 91–96 (2009). "Comparison of polarization consistent and correlation consistent basis sets for noncovalent interactions" http://doi.org/10.1002/qua.21876

43 K.L. Copeland, J.A. Anderson, A.R. Farley*, J.R. Cox, and G.S. Tschumper, *J. Phys. Chem. B*, **112**, 14291–14295 (2008). "Probing Phenylalanine/Adenine π-Stacking Interactions in Protein Complexes with Explicitly Correlated and CCSD(T) Computations" http://doi.org/10.1021/jp805528v

44 A.M. ElSohly*, B.W. Hopkins, K.L. Copeland, and G.S. Tschumper, *Mol. Phys.*, **107**, 923–928 (2009). "Anchoring the potential energy surface of the diacetylene dimer" http://doi.org/10.1080/00268970802695404

45 D.M. Bates and G.S. Tschumper, *J. Phys. Chem. A*, **113**, 3555–3559 (2009). "CCSD(T) Complete Basis Set Limit Relative Energies for Low-Lying Water Hexamer Structures" http://doi.org/10.1021/jp8105919

46 A.A. Howard*, G.S. Tschumper, and N.I. Hammer, *J. Chem. Phys. A*, **114**, 6803–6810 (2010). "Effects of Hydrogen Bonding on Vibrational Normal Modes of Pyrimidine" http://doi.org/10.1021/jp101267w

47 A.M. Wright, L.V. Joe*, A.A. Howard*, G.S. Tschumper, and N.I. Hammer, *Chem. Phys. Lett.*, **501**, 319–323 (2011). "Spectroscopic and computational insight into weak noncovalent interactions in crystalline pyrimidine" http://doi.org/10.1016/j.cplett.2010.11.046

48 D.N. Reinemann*, A.M. Wright, J.D. Wolfe*, G.S. Tschumper, and N.I. Hammer, *J. Phys. Chem. A*, **115**, 6426–6431 (2011). "Vibrational Spectroscopy of N-Methyliminodiacetic Acid (MIDA)-Protected Boronate Ester: Examination of the B–N Dative Bond" http://doi.org/10.1021/jp112016j

49 D.M. Bates, J.R. Smith*, T. Janowski, and G.S. Tschumper, *J. Chem. Phys.*, **135**, 044123 (2011). "Development of a 3-body:many-body integrated fragmentation method for weakly bound clusters and application to water clusters $(H_2O)_{n=3-10,16,17}$" http://.doi.org/10.1063/1.3609922

50 E.G. Hohenstein, H.M. Jaeger, E.J. Carrell, G.S. Tschumper, and C.D. Sherrill, *J. Chem. Theory Comput.*, **7**, 2842–2851 (2011). "Accurate Interaction Energies for Problematic Dispersion-Bound Complexes: Homogeneous Dimers of NCCN, P_2 and PCCP" http://.doi.org/10.1021/ct200374m

51 D.M. Bates, J.R. Smith*, and G.S. Tschumper, *J. Chem. Theory Comput.*, **7**, 2753–2760 (2011). "Efficient and Accurate Methods for the Geometry Optimization of Water Clusters: Application of Analytic Gradients for the 2-body:Many-Body QM:QM Fragmentation Method to $(H_2O)_n$, $n = 3 - 10$" http://.doi.org/10.1021/ct200176t

52 J.C. Howard*, N.I. Hammer, and G.S. Tschumper, *ChemPhysChem*, **12**, 3262–3273 (2011). "Structures, Energetics and Vibrational Frequency Shifts of Hydrated Pyrimidine" http://.doi.org/10.1002/cphc.201100457

53 V.R. Jupally, R. Kota, E.V. Dornshuld, D.L. Mattern, G.S. Tschumper, D. Jiang, and A. Dass, *J. Am. Chem. Soc.*, **133**, 20258–20266 (2011). "Interstaple Dithiol Cross-Linking in $Au_{25}(SR)_{18}$ Nanomolecules: A Combined Mass Spectrometric and Computational Study" http://.doi.org/10.1021/ja206436x

54 E.J. Carrell, C.M. Thorne*, and G.S. Tschumper, *J. Chem. Phys.*, **136**, 014103 (2012). "Basis set dependence of higher-order correlation effects in π-type interactions" http://.doi.org/10.1063/1.3671950

55 K.L. Copeland and G.S. Tschumper, *J. Chem. Theory Comput.*, **8**, 1646–1656 (2012). "Hydrocarbon/Water Interactions: Encouraging Energetics and Structures from DFT but Disconcerting Discrepancies for Hessian Indices" http://.doi.org/10.1021/ct300132e

56 K.L. Copeland and G.S. Tschumper, *J. Chem. Theory Comput.*, **8**, 4279–4284 (2012). "Effects of Heterogeneity in Small π-Type Dimers: Homogeneous and Mixed Dimers of Diacetylene and Cyanogen" http://.doi.org/10.1021/ct300644a

57 A.M. Wright, A.A. Howard*, J.C. Howard*, G.S. Tschumper, and N.I. Hammer, *J. Phys. Chem. A*, **117**, 5435–5446 (2013). "Charge Transfer and Blue Shifting of Vibrational Frequencies in a Hydrogen Bond Acceptor" http://.doi.org/10.1021/jp401642b

58 T.L. Ellington and G.S. Tschumper, *Comput. Theor. Chem.*, **1021**, 109–113 (2013). "Anchoring the potential energy surface of the nitrogen/water dimer, $N_2 \cdots H_2O$, with explicitly correlated coupled-cluster computations" http://.doi.org/10.1016/j.comptc.2013.06.035

59 K.L. Copeland, S.J. Pellock*, J.R. Cox, M.L. Cafiero, and G.S. Tschumper, *J. Phys. Chem. B*, **117**, 14001–14008 (2013). "Examination of Tyrosine/Adenine Stacking Interactions in Protein Complexes" http://.doi.org/10.1021/jp408027j

60 J.C. Howard and G.S. Tschumper, *J. Chem. Phys.*, **139**, 184113 (2013). "*N*-body:Many-body QM:QM vibrational frequencies: Application to small hydrogen-bonded clusters" http://.doi.org/10.1063/1.4829463

61 E.V. Dornshuld and G.S. Tschumper, *J. Comput. Chem.*, **35**, 479–487 (2014). "Characterization of the potential energy surfaces of two small but challenging noncovalent dimers: $(P_2)_2$ and $(PCCP)_2$" http://.doi.org/10.1002/jcc.23522

62 Y.P. Bhavsar-Jog, E.V. Dornshuld, T.A. Brooks, G.S. Tschumper, and R.M. Wadkins, *Biochemistry*, **53**, 1586–1594 (2014). "Epigenetic Modification, Dehydration, and Molecular Crowding Effects on the Thermodynamics of i-Motif Structure Formation from C-Rich DNA" http://.doi.org/10.1021/bi401523b

63 D.N. Reinemann*, G.S. Tschumper, and N.I. Hammer, *ChemPhysChem*, **15**, 1867–1871 (2014). "Characterizing the B–P Stretching Vibration in Phosphorus-Substituted Phosphine Boranes" http://.doi.org/10.1002/cphc.201400036

64 E.V. Dornshuld, C.M. Holy*, and G.S. Tschumper, *J. Phys. Chem. A*, **118**, 3376–3385 (2014). "Homogeneous and Heterogeneous Noncovalent Dimers of Formaldehyde and Thioformaldehyde: Structures, Energetics, and Vibrational Frequencies" http://.doi.org/10.1021/jp502588h

65 J.T. Kelly, S. Xu, J. Graham, J.M. Nilles, D. Radisic, A.M. Buonaugurio, K.H. Bowen, N.I. Hammer, and G.S. Tschumper, *J. Phys. Chem. A*, **118**, 11901–11907 (2014). "Photoelectron Spectroscopic and Computational Study of Hydrated Pyrimidine Anions" http://.doi.org/10.1021/jp504724v

66 E.V. Dornshuld, R.A. Vergenz, and G.S. Tschumper, *J. Phys. Chem. B*, **118**, 8583–8590 (2014). "Peptide Bond Formation via Glycine Condensation in the Gas Phase" http://.doi.org/10.1021/jp504924c

67 J.C. Howard, J.L. Gray*, A.J. Hardwick*, L.T. Nguyen*, and G.S. Tschumper, *J. Chem. Theory Comput.*, **10**, 5426–5435 (2014). "Getting down to the Fundamentals of Hydrogen Bonding: Anharmonic Vibrational Frequencies of $(HF)_2$ and $(H_2O)_2$ from Ab Initio Electronic Structure Computations" http://.doi.org/10.1021/ct500860v

68 A.J. Huckaba, F. Giordano, L.E. McNamara, K.M. Dreux, N.I. Hammer, G.S. Tschumper, S.M. Zakeeruddin, M. Grätzel, M.K. Nazeeruddin, and J.H. Delcamp, *Adv. Energy Mater.*, **5**, 1401629 (2015). "Indolizine-Based Donors as Organic Sensitizer Components for Dye-Sensitized Solar Cells" http://.doi.org/10.1002/aenm.201401629

69 J.M. Carr, G.S. Tschumper, and A.P. Lathem*, *Helv. Chim. Acta*, **98**, 582–588 (2015). "*Boyd* Group Electronegativity Influence on the *Parr* Global Electrophilicity of *Vilsmeier* Reagent-Derived Imidates: New Insights toward Improving *Mitsunobu* Chemistry" http://.doi.org/10.1002/hlca.201400340

70 J.C. Howard and G.S. Tschumper, *J. Chem. Theory Comput.*, **11**, 2126–2136 (2015). "Benchmark Structures and Harmonic Vibrational Frequencies Near the CCSD(T) Complete Basis Set Limit for Small Water Clusters: $(H_2O)_{n=2,3,4,5,6}$" http://.doi.org/10.1021/acs.jctc.5b00225

71 Y. Wang, X. Zhang, S. Lyapustina, M.M. Nilles, S. Xu, J.D. Graham, K.H. Bowen, J.T. Kelly, G.S. Tschumper, and N. I. Hammer, *Phys. Chem. Chem. Phys.*, **18**, 704–712 (2016). "The onset of electron-induced proton-transfer in hydrated azabenzene cluster anions" http://.doi.org/10.1039/C5CP02746B

72 K.M. Dreux and G.S. Tschumper, *Comput. Theor. Chem.*, **1072**, 21–27 (2015). "Anchoring the potential energy surface of an important atmospheric van der Waals dimer, the $H_2O\cdots O_2$ complex" http://.doi.org/10.1016/j.comptc.2015.08.022

73 J. Wilson*, J.S.D. Williams, C. Petkovsek*, P. Reves*, J.W. Jurss, N.I. Hammer, G.S. Tschumper, and D.L. Watkins, *RSC Adv.*, **5**, 82544–82548 (2015). "Synergistic effects of halogen bond and $\pi-\pi$ interactions in thiophene-based building blocks" http://.doi.org/10.1039/c5ra16680b

74 A.F. DeBlase, C.T. Wolke, G.H. Weddle, K.A. Archer, K.D. Jordan, J.T. Kelly, G.S. Tschumper, N.I. Hammer, and M.A. Johnson, *J. Chem. Phys.*, **143**, 144305 (2015). "Water network-mediated, electron-induced proton transfer in anionic $[C_5H_5N\cdot(H_2O)_n]^-$ clusters" http://.doi.org/10.1063/1.4931928

75 J.C. Howard, J.D. Enyard, and G.S. Tschumper, *J. Chem. Phys.*, **143**, 214103 (2015). "Assessing the accuracy of some popular DFT methods for computing harmonic vibrational frequencies of water clusters" http://.doi.org/10.1063/1.4936654

76 P. Brogdon, F. Giordano, G.A. Puneky*, A. Dass, S.M. Zakeeruddin, M.K. Nazeeruddin, M. Grätzel, G.S. Tschumper, and J.H. Delcamp, *Chem. Eur. J.*, **22**, 694–703 (2016). "A Computational and Experimental Study of Thieno[3,4-b]thiophene as a Proaromatic π-Bridge in Dye-Sensitized Solar Cells" http://.doi.org/10.1002/chem.201503187

77 E.V. Dornshuld and G.S. Tschumper, *J. Chem. Theory Comput.*, **12**, 1534–1541 (2016). "Big Changes for Small Noncovalent Dimers: Revisiting the Potential Energy Surfaces of $(P_2)_2$ and $(PCCP)_2$ with CCSD(T) Optimizations and Vibrational Frequencies" http://.doi.org/10.1021/acs.jctc.5b01105

78 J.T. Kelly, A.K. McClellan*, L.V. Joe*, A.M. Wright, L.T. Lloyd*, G.S. Tschumper, and N.I. Hammer, *ChemPhysChem*, **17**, 2782–2786 (2016). "Competition between Hydrophilic and Argyrophilic Interactions in Surface Enhanced Raman Spectroscopy" http://.doi.org/10.1002/cphc.201600678

79 S.T. Nguyen*, A.L. Rheingold, G.S. Tschumper, and D.L. Watkins, *Cryst. Growth Des.*, **16**, 6648–6653 (2016). "Elucidating the Effects of Fluoro and Nitro Substituents on Halogen Bond Driven Assemblies of Pyridyl-Capped π-Conjugated Molecules" http://.doi.org/10.1021/acs.cgd.6b01321

80 T.L. Ellington, P.L. Reves*, B.L. Simms, J.L. Wilson*, D.L. Watkins, G.S. Tschumper, and N.I. Hammer, *ChemPhysChem*, **18**, 1267–1273 (2017). "Quantifying the Effects of Halogen Bonding by Haloaromatic Donors on the Acceptor Pyrimidine" http://.doi.org/10.1002/cphc.201700114

81 K.M. Dreux, L.E. McNamara, J.T. Kelly, A.M. Wright, N.I. Hammer, and G.S. Tschumper, *J. Phys. Chem. A*, **121**, 5884–5893 (2017). "Probing Dative and Dihydrogen Bonding in Ammonia Borane with Electronic Structure Computations and Raman under Nitrogen Spectroscopy" http://.doi.org/10.1021/acs.jpca.7b03509

82 G.S. Tschumper, T.L. Ellington and S.N. Johnson, *Ann. Rep. Comput. Chem.*, **13**, 93–115, (2017). "Dissociation in Binary Acid/Base Clusters: An Examination of Inconsistencies Introduced Into the Many-Body Expansion by Naïve Fragmentation Schemes" http://.doi.org/10.1016/bs.arcc.2017.06.003

83 Y.A. Abdo*, J.W. Weeks*, W. Layfield*, W.M. Tremlett*, J.W. Graham*, M.E. Tabor*, S.E. Causey*, J.M. Carr, and G.S. Tschumper, *Chem. Lett.*, **47**, 156–159 (2018). "Intramolecular Hydrogen Bonding in α-Epoxy Alcohols: A Conformational Analysis of 1,2-Dialkyl-2,3-epoxycyclopentanol Diastereomers" http://.doi.org/10.1246/cl.170932

84 S.N. Johnson and G.S. Tschumper, *J. Comput. Chem.*, **39**, 839–843 (2018). "Hydrogen bonding in the mixed HF/HCl dimer: Is it better to give or receive?" http://.doi.org/10.1002/jcc.25157

85 C.A. Carpenter*, P. Brogdon, L.E. McNamara, G.S. Tschumper, N.I. Hammer, and J.H. Delcamp, *Inorganics*, **6**, 22 (2018). "A Robust Pyridyl-NHC-Ligated Rhenium Photocatalyst for CO_2 Reduction in the Presence of Water and Oxygen" http://.doi.org/10.3390/inorganics6010022

86 S.T. Nguyen*, T.L. Ellington, K.E. Allen, J.D. Gorden, A.L. Rheingold, G.S. Tschumper, N.I. Hammer, and D.L. Watkins, *Cryst. Growth Des.*, **18**, 3244–3254 (2018). "Systematic Experimental and Computational Studies of Substitution and Hybridization Effects in Solid-State Halogen Bonded Assemblies" http://.doi.org/10.1021/acs.cgd.8b00398

87 T.M. Sexton, J.C. Howard, and G.S. Tschumper, *J. Phys. Chem. A*, **122**, 4902–4908 (2018). "Dissociation Energy of the $H_2O\cdots HF$ Dimer" http://.doi.org/10.1021/acs.jpca.8b03397

88 N.I. Hammer and G.S. Tschumper, *ACS Symposium Series*, **1295**, 157–175 (2018). "Importance of a Truly Cohesive Theme in a REU Program" in Best Practices for Chemistry REU Programs, edited by M. Griep and L. Watkins http://.doi.org/10.1021/bk-2018-1295.ch011

89 S.N. Johnson, C.R. Hutchison†, C.M. Williams*, C.L. Hussey, G.S. Tschumper, and N.I. Hammer, *J. Phys. Chem. C*, **122**, 27673–27680 (2018). "Intermolecular Interactions and Vibrational Perturbations within Mixtures of 1-Ethyl-3-methylimidazolium Thiocyanate and Water" http://.doi.org/10.1021/acs.jpcc.8b07114

90 B.R. Westbrook*, K.M. Dreux, G.S. Tschumper, J.S. Francisco, and R.C. Fortenberry, *Phys. Chem. Chem. Phys.*, **20**, 25967–25973 (2018). "Binding of the atomic cations hydrogen through argon to water and hydrogen sulfide" http://.doi.org/10.1039/C8CP05378B

91 S.P. Lee*, S.N. Johnson, T.L. Ellington, N. Mirsaleh-Kohan, and G.S. Tschumper, *ACS Omega*, **3**, 12936–12943 (2018). "Energetics and Vibrational Signatures of Nucleobase Argyrophilic Interactions", http://.doi.org/10.1021/acsomega.8b01895

92 K.M. Dreux and G.S. Tschumper, *J. Comput. Chem.*, **40**, 229–236 (2019). "Examination of the structures, energetics, and vibrational frequencies of small sulfur-containing prototypical dimers, $(H_2S)_2$ and H_2O/H_2S", http://.doi.org/10.1002/jcc.25578

93 J.T. Kelly, T.L. Ellington, T.M. Sexton, R.C. Fortenberry, G.S. Tschumper, and K.R. Asmis, *J. Chem. Phys.*, **149**, 191101 (2018). "Communication: Gas phase vibrational spectroscopy of the azide-water complex" http://.doi.org/10.1063/1.5053671

94 T.M. Sexton and G.S. Tschumper, *Mol. Phys.*, **117**, 1413–1420 (2019). "2-body:Many-body QM:QM study of structures, energetics, and vibrational frequencies for microhydrated halide ions" http://.doi.org/10.1080/00268976.2018.1554827

95 S.N. Johnson, T.L. Ellington, D.T. Ngo*, J.L. Nevarez*, N. Sparks, A.L. Rheingold, D.L. Watkins, and G.S. Tschumper, *CrystEngComm*, **21**, 3151–3157 (2019). "Probing non-covalent interactions driving molecular assembly in organo-electronic building blocks" http://.doi.org/10.1039/C9CE00219G

96 K.M. Pittman*, H.R. McAlexander, G.S. Tschumper, and M.K. Shukla, *J. Phys. Chem. A*, **123**, 3504–3509 (2019). "Computational Investigation on Electronic Structures and Properties of 4,6-Bis(nitroimino)-1,3,5-triazinan-2-one: An Insensitive Munition Compound" http://.doi.org/10.1021/acs.jpca.9b00736

97 A.E. Steen, T.L. Ellington, S.T. Nguyen*, S. Balasubramaniam, I. Chandrasiri, J.H. Delcamp, G.S. Tschumper, N.I. Hammer, and D.L. Watkins, *J. Phys. Chem. C*, **123**, 15176–15185 (2019). "Characterization of Furan- and Thiophene-Containing Bispyridyl Oligomers via Spectroscopic, Electrochemical, and TD-DFT Methods" http://.doi.org/10.1021/acs.jpcc.9b01510

98 B.E. Smith, J.M. Carr, and G.S. Tschumper, *Molecules*, **24**, 2523 (2019). "*Cis/Trans* Energetics in Epoxide, Thiirane, Aziridine and Phosphirane Containing Cyclopentanols: Effects of Intramolecular OH$\cdots$O, S, N and P Contacts" http://.doi.org/10.3390/molecules24142523

99 A.E.S. Hardin, T.L. Ellington, S.T. Nguyen*, A.L. Rheingold, G.S. Tschumper, D.L. Watkins, and N.I. Hammer, *Inorganics*, **7**, 119 (2019). "A Raman Spectroscopic and Computational Study of New Aromatic Pyrimidine-Based Halogen Bond Acceptors" http://.doi.org/10.3390/inorganics7100119

100 Y.P. Bhavsar-Jog, E.V. Dornshuld, T.A. Brooks, G.S. Tschumper, and R.M. Wadkins, *Molecules*, **24**, 3619 (2019). "Co-Localization of DNA i-Motif-Forming Sequences and 5-Hydroxymethylcytosines in Human Embryonic Stem Cells" http://.doi.org/10.3390/molecules24193619

101 T.M. Sexton, W.Z. Van Benschoten*, and G.S. Tschumper, *Chem. Phys. Lett.*, **748**, 137382 (2020). "Dissociation energy of the HCN$\cdots$HF dimer" http://.doi.org/10.1016/j.cplett.2020.137382

102 H. Shirley, T.M. Sexton, N.P. Liyanage, C.Z. Palmer*, L.E. McNamara, N.I. Hammer, G.S. Tschumper, and J.H. Delcamp, *Eur. J. Inorg. Chem.*, **2020**, 1844–1851 (2020). "Effect of "X" Ligands on the Photocatalytic Reduction of CO_2 to CO with Re(pyridylNHC-CF_3)$(CO)_3$X Complexes" http://.doi.org/10.1002/ejic.202000283

103 R. Schwan, C. Qu, D. Mani, N. Pal, G. Schwaab, J.M. Bowman, G.S. Tschumper, and M. Havenith, *Angew. Chem. Int. Ed. Engl.*, **59**, 11399 (2020). "Observation of the Low-Frequency Spectrum of the Water Trimer as a Sensitive Test of the Water-Trimer Potential and the Dipole-Moment Surface" http://.doi.org/10.1002/anie.202003851

104 M.A. Perkins, K.R. Barlow, K.M. Dreux, and G.S. Tschumper, *J. Chem. Phys.*, **152**, 214306 (2020). "Anchoring the hydrogen sulfide dimer potential energy surface to juxtapose $(H_2S)_2$ with $(H_2O)_2$" http://.doi.org/10.1063/5.0008929

105 E.J. Carrell, C.M. Thorne*, and G.S. Tschumper, *J. Chem. Phys.*, **153**, 069901 (2020). "Erratum: "Basis Set Dependence of Higher-Order Correlation Effects in π-Type Interactions" [J. Chem. Phys. 136, 014103 (2012)]" http://.doi.org/10.1063/5.0021960

106 Y.A. Abdo* and G.S. Tschumper, *J. Phys. Chem. A*, **124**, 8744–8752 (2020). "Competition Between Solvent-Solvent and Solvent-Solute Interactions in the Microhydration of the Hexafluorophosphate Anion, $PF_6{}^-(H_2O)_{n=1,2}$" http://.doi.org/10.1021/acs.jpca.0c06466

107 H.P. Shirley, T.M. Sexton, N.P. Liyanage, M.A. Perkins, S.A. Autry, L.E. McNamara, N.I. Hammer, S. Parkin, G.S. Tschumper and J.H. Delcamp, *ChemPhotoChem*, **5**, 353–361 (2021). "Probing the Effects of Electron Deficient Aryl Substituents and a π-System Extended NHC Ring on the Photocatalytic CO2 Reduction Reaction with Re-pyNHC-aryl Complexes" http://.doi.org/10.1002/cptc.202000296

108 B.R. Westbrook, E.M. Valencia*, S.C. Rushing*, G.S. Tschumper and R.C. Fortenberry, *J. Chem. Phys.*, **154**, 041104 (2021). "Anharmonic vibrational frequencies of ammonia borane (BH_3NH_3)" http://.doi.org/10.1063/5.0040050

109 M.A. Webb, L.M. Cline* and G.S. Tschumper, *J. Phys. Chem. A*, **125**, 6228–6237 (2021). "Torsional Profiles of Thiophene and Furan Oligomers: Probing the Effects of Heterogeneity and Chain Length" http://.doi.org/10.1021/acs.jpca.1c04714

110 K.R. Barlow, S.M. Goodlett*, S.N. Arradondo and G.S. Tschumper, *Mol. Phys.*, **116**, e1967495 (2021). "Fundamental vibrational frequencies of isolated 2-phosphaethynolate and 2-phosphaethynthiolate anions: OCP^- and SCP^-" http://doi.org/10.1080/00268976.2021.1967495

111 A.E. Williams, N.I. Hammer and G.S. Tschumper, *J. Chem. Phys.*, **155**, 114306 (2021). "Relative energetics of CH_3CH_2O, CH_3CHOH, and CH_2CH_2OH radical products from ethanol dehydrogenation" http://doi.org/10.1063/5.0062809

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

113 D. Karunathilaka, R.M.G. Rajapakse, A.E. Hardin, T.M. Sexton, N.E. Sparks, J.J. Mosely, A.L. Rheingold, N.I. Hammer, G.S. Tschumper and D.L. Watkins, *CrystEngComm*, **24**, 4564–4572 (2022). "Correlation of solid-state order to optoelectronic behavior in heterocyclic oligomers" http://dx.doi.org/10.1039/D2CE00560C

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_9" 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_2" 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_9" 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 fluorenium-indolizine chromophores" https://doi.org/10.1039/D4SC00733F

127 S. Jäger, J. Khatri, P. Meyer, S. Henkel, G. Schwaab, A. Nandi, P. Pandey, K.R. Barlow, M.A. Perkins, G.S. Tschumper, J.M. Bowman, A. van der Avoird and M. Havenith, *Nat. Commun.* **15**, 9540 (2024). "On the nature of hydrogen bonding in the H2S dimer" https://doi.org/10.1038/s41467-024-53444-6

128 Y. Xue and G.S. Tschumper, *J. Chem. Phys.*, **162**, 144305 (2025). "Systematic characterization of the homogeneous and heterogeneous hydrogen halide dimers" https://doi.org/10.1063/5.0267887

C. Publications not Refereed/Peer-Reviewed

129 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

130 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

118 2024 Southwest Regional Meeting (SWRM) of the American Chemical Society Waco, TX, 20–23 Oct. 2024

119 10th SeedMol (Symposium on Electronic Structure and Molecular Dynamics) Piren'opolis, Brazil, 4–8 Nov. 2024

120 Department of Physical Sciences, Truman State University, Kirksville, MO, 24 Jan. 2025

121 Department of Chemical and Biochemical Engineering, Missouri University of Science and Technology, Rolla, MO, 10 March 2025

122 Department of Physics, Missouri University of Science and Technology, Rolla, MO, 20 March 2025

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 Occassion of His 80th Birthday, Atlanta, GA, 7 June 2024

24 77th International Symposium on Molecular Spectroscopy, Urbana-Champaign, IL, 17–21 June, 2024

25 2025 Annual Meeting of the Southeast Theoretical Chemistry Association (SETCA), Memphis, TN, 8–10 May 2025

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.

19 WATOC 2025: 13th Triennial Congress of the World Association of Theoretical and Computational Chemists, Oslo, Norway, 22–27 June 2025.

XIV. Current Research Assistants

Thufail Ismail	Postdoctoral Research Associate
Zach Palmer	Postdoctoral Research Associate
Max Tucker	Ph.D. Student
Molly Austell	Undergraduate Chemistry Major