

Nathan J. DeYonker

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Current Employment

Associate Professor, September 2021 – Present
Department of Chemistry, The University of Memphis, Memphis, TN

Assistant Professor, August 2016 – August 2021
Department of Chemistry, The University of Memphis, Memphis, TN

Research Scientist, July 2009 – August 2016
Department of Chemistry, The University of Memphis, Memphis, TN

Director, Computational Research on Materials Institute at the University of Memphis (CROMIUM),
August 2014 – Present

Previous Employment

Postdoctoral Fellow, July 2005 – July 2009
University of North Texas, Denton, TX, advisors: Profs. Angela K. Wilson and Thomas R. Cundari

Education

Ph. D. Chemistry, 2005
Dissertation: “Transition Metals and Excited States: Challenging Applications of *ab initio* Chemistry”
University of Georgia, Athens, GA, advisor: Prof. Henry F. Schaefer III

B. Sc. Chemistry, Minor in Astrophysics, May 2001
University of Michigan, Ann Arbor, MI

Awards / Honors

Finalist for the “Emerging Technology Award” by the American Chemical Society COMP division,
Boston, MA, August 2007.

National Natural Science Foundation of China “Research Fellowship for International Young Scientists”,
September 2009.

The University of Warwick IAS Residential Fellowship, June 2017.

University of Memphis CAS Travel Enrichment Fund, June 2017.

University of Memphis Research Foundation Ventures Professorship, August 2019. Named professorship created to support research and sponsored programs activities.

University of Memphis Michael K. Harless Faculty Excellence Award, August 2019. The award is given to an outstanding junior faculty member.

Scialog: Chemical Machinery of the Cell 2020/2021 Fellow, July 2020. One of thirteen early career scientists selected for the 2020-2021 Scialog conference, cosponsored by the Research Corporation for Scientific Advancement and the Gordon and Betty Moore Foundation.

Current Support

09/01/2019 – 08/31/2024 NSF CAREER ABI, \$790,231

PI (20% effort) on “A Model-Building Platform for Rational, Rigorous, and Reproducible Computational Enzymology”

09/01/2022 – 08/31/2025 NSF CSDM-A, \$168,321

Co-I (16.7% effort) on “Advancing Our Knowledge of the Transition Metal-Carbon Bond: Integrating Spectroscopy and Theory”

Past Support

02/22/2021 – 12/31/2021 DOE BES SBIR, \$249,415 (subcontract amount to UM/NJD: \$79,837)

Co-I on “New Theory and Ontologies for Quantum Mechanical Cluster Modeling of Proteins and Enzymes”

02/1/2021 – 12/31/2021 University of Memphis Gap Funding award \$7,300

“Catalytic “chemical defects” contributing to Origin of Life Chemistry”

09/01/2019 – 08/31/2021 University of Memphis Research Foundation \$12,000

UMRF Ventures Professorship Award

11/01/2018 – 12/31/2019 University of Memphis Office of Sponsored Programs – Community of Research Scholars, \$2,500

PI on “Synthesis of Research and Teaching Practices with the University of Memphis High Performance Computer”

07/01/2017 – 06/30/2018 University of Memphis CAS Faculty Research Grant, \$9,650

PI (15% effort) on “Rigorous, Rational, and Reproducible Computational Enzyme Models”

04/2014 - 03/2016 National Science Foundation, CBET-1435289, \$35,420

co-PI (14% effort) on “RAPID: Computation of Accurate Binding Energies of Emerging Organic Contaminants on Environmental and Infrastructural Interfaces”. PI was William Alexander (U. of Memphis).

09/26/2012 - 09/26/2013 XSEDE Startup Allocation, 30,000 CPU hours on TeraGrid resources

PI on “In Silico Support of Astrobiology: Using the TeraGrid to Validate and Assist Rotational and Electronic Spectroscopy”.

Publications

Highlights: 86 peer-reviewed publications with 3 submitted, including 6 featured cover articles (#32, #33, #53, #58, #65, and #74) and 1 peer-reviewed book chapter (#22). Corresponding or co-corresponding author of 31 publications (#7, #8, #15, #17, #24, #32, #42, #43, #50, #51, #52, #54, #55, #56, #57, #58, #60, #61, #63, #65, #66, #67, #68, #69, #72, #74, #77, #82, #83, #84, #85, #86). As of October 7, 2021: over 2500 citations total (according to Scopus on 6/23/2022), 2 publications with over 200 citations (#7, #37), 7 publications with over 100 citations (#7, #8, #12, #15, #32, #33, and #37), 12 publications with over 50 citations (#7, #8, #12, #15, #20, #24, #25, #27, #32, #33, #35, #37) and an h-index of 25.

University of Georgia

- 1) B. N. Papas, S. Y. Wang, N. J. DeYonker, H. F. Schaefer, "Naphthalenyl, Anthracenyl, Tetracenyl, and Pentacenyl Radicals and their Anions", *J. Phys. Chem. A* **107**, 6311 (2003).
- 2) N. J. DeYonker, Y. Yamaguchi, W. D. Allen, C. Pak, H. F. Schaefer, K. A. Peterson, "Low-Lying Electronic States of FeCN and FeNC: A Theoretical Journey into Isomerization and Quartet/Sextet Competition", *J. Chem. Phys.* **120**, 4726 (2004).
- 3) S. Kim, S. E. Wheeler, N. J. DeYonker, H. F. Schaefer, "Potential Energy Surface of Oxalyl Chloride", *J. Chem. Phys.* **122**, 234313 (2005).
- 4) N. J. DeYonker, S. Li, Y. Yamaguchi, H. F. Schaefer, T. D. Crawford, R. A. King, K. A. Peterson, "Application of Equation-of-Motion Coupled Cluster Methods to Singlet and Triplet Electronic States of HBO and BOH", *J. Chem. Phys.* **122**, 234316 (2005).
- 5) S. Y. Wang, A. Paul, N. J. DeYonker, Y. Yamaguchi, H. F. Schaefer, "The Ground and Two Lowest-Lying Singlet Excited Electronic States of Copper Hydroxide (CuOH)", *J. Chem. Phys.* **123**, 014313 (2005). Erratum: *J. Chem. Phys.* **124**, 019901.

University of North Texas

- 6) J. P. Lee, K. A. Pittard, N. J. DeYonker, T. R. Cundari, T. B. Gunnoe, and J. L. Petersen, "Reactions of a Ru(II) Phenyl Complex with Substrates that Possess C-N or C-O Multiple Bonds: C-C Bond Formation, N-H Bond Cleavage and Decarbonylation Reactions", *Organometallics*, **25**, 1500 (2006).
- 7) N. J. DeYonker, T. R. Cundari, A. K. Wilson, "The Correlation-Consistent Composite Approach (ccCA): An Alternative to the Gaussian-*n* Methods", *J. Chem. Phys.*, **124**, 114104 (2006).
- 8) N. J. DeYonker, T. Grimes, S. Yockel, A. Dinescu, B. J. Mintz, T. R. Cundari, A. K. Wilson, "The correlation-consistent Composite Approach (ccCA): Application to the G3/99 test set", *J. Chem. Phys.*, **125**, 104111 (2006).
- 9) D. S. Ho, N. J. DeYonker, A. K. Wilson, T. R. Cundari "Accurate Enthalpies of Formation of Alkali and Alkaline Earth Metal Oxides and Hydroxides: An Assessment of the correlation consistent Composite Approach (ccCA)", *J. Phys. Chem. A* **110**, 9767 (2006).
- 10) N. J. DeYonker, T. R. Cundari, A. K. Wilson, C. Sood, D. H. Magers, "Calculation of Gas-Phase Enthalpies of Formation with Chemical Accuracy: The Curious Case of 3-Nitroaniline", *THEOCHEM.*, **775**, 77 (2006).

- 11) A. B. Kazi, T. R. Cundari, E. Baba, N. J. DeYonker, A. Dinescu, A. Kazi, L. Spaine, "Catalytic Synthesis of Arylisocyanates from Nitroaromatics. A Computational Study", *Organometallics*, **26**, 910 (2007).
- 12) N. J. DeYonker, K. A. Peterson, G. Steyl, A. K. Wilson, T. R. Cundari, "Quantitative Computational Thermochemistry of Transition Metal Complexes", *J. Phys. Chem. A*, **111**, 11269 (2007), part of the "Thom H. Dunning, Jr., Festschrift".
- 13) T. V. Grimes, A. K. Wilson, N. J. DeYonker, T. R. Cundari, "Performance of the correlation-consistent Composite Approach for kinetics: A comparison to G3B theory", *J. Chem. Phys.*, **127**, 154117 (2007).
- 14) N. J. DeYonker, D. S. Ho, A. K. Wilson, T. R. Cundari, "Computational s-block Thermochemistry with the correlation consistent Composite Approach and G3", *J. Phys. Chem. A*, **111**, 10776 (2007).
- 15) N. J. DeYonker, A. K. Wilson, K. A. Peterson, "Systematically Convergent Correlation Consistent Basis Sets for Molecular Core-valence Correlation Effects: The third-row atoms Gallium through Krypton", *J. Phys. Chem. A*, **111**, 11383 (2007), part of the "Thom H. Dunning, Jr., Festschrift".
- 16) N. J. DeYonker, N. A. Foley, T. R. Cundari, T. B. Gunnoe, J. L. Petersen, "Combined Experimental and Computational Studies on the Nature of Aromatic C-H Activation by Octahedral Ru(II) Complexes: Evidence for σ -Bond Metathesis from Hammett Studies", *Organometallics*, **26**, 6604 (2007).
- 17) N. J. DeYonker, B. J. Mintz, T. R. Cundari, A. K. Wilson, "Application of the correlation consistent Composite Approach (ccCA) to Third-Row (Ga – Kr) Molecules", *J. Chem. Theory Comput.*, **4**, 328 (2008).
- 18) T. G. Williams, N. J. DeYonker, A. K. Wilson, "Hartree-Fock Complete Basis Set Limit Extrapolations for Transition Metal Diatomics", *J. Chem. Phys.*, **128**, 044101 (2008).
- 19) J. L. Boyer, T. R. Cundari, N. J. DeYonker, T. B. Rauchfuss, S. R. Wilson, "Redox-Activation of Alkene Ligands in Platinum Complexes with Noninnocent Ligands", *Inorg. Chem.*, **48**, 638 (2009).
- 20) N. J. DeYonker, B. R. Wilson, A. W. Pierpont, T. R. Cundari, A. K. Wilson, "Towards the Intrinsic Error of the correlation consistent Composite Approach (ccCA)", *Mol. Phys.*, **107**, 1107 (2009), part of the "Henry F. Schaefer III, Festschrift".
- 21) M. Fianchini, T. R. Cundari, N. J. DeYonker, H. V. R. Dias, "A Non-Classical Copper Carbonyl on a Tri-alkene Hydrocarbon Support", *Dalton Trans.*, **2009**, 2085 (2009).
- 22) N. J. DeYonker, T. R. Cundari, A. K. Wilson, "The correlation consistent Composite Approach (ccCA): Efficient and Pan-periodic Kinetics and Thermodynamics", in: "Progress in Theoretical Chemistry and Physics", J. Maruani, S. Wilson, W. N. Lipscomb, ed., Springer, **19**, 197 (2009).
- 23) Y. Gao, N. J. DeYonker, E. C. Garrett III, A. K. Wilson, T. R. Cundari, P. Marshall, "The Enthalpy of Formation of the Cyclohexadienyl Radical and the C-H Bond Enthalpy of 1,4-Cyclohexadiene: An Experimental and Computational Re-evaluation", *J. Phys. Chem. A*, **113**, 6955 (2009).

- 24) N. J. DeYonker, T. G. Williams, A. K. Imel, T. R. Cundari, A. K. Wilson, "Accurate Thermochemistry for Transition Metal Complexes from First-Principles Calculations", *J. Chem. Phys.*, **131**, 024106 (2009).
- 25) R. E. Cowley, N. J. DeYonker, N. A. Eckert, T. R. Cundari, S. DeBeer George, E. Bill, X. Ottenwaelder, C. Flaschenreim, P. L. Holland, "Three-Coordinate Terminal Imidoiron(III) Complexes: Structure, Spectroscopy, and Mechanism of Formation", *Inorg. Chem.*, **49**, 6172 (2010).
- 26) T. G. Williams, N. J. DeYonker, B. S. Ho, A. K. Wilson, "The correlation consistent Composite Approach: The spin contamination effect on an MP2-based composite methodology", *Chem. Phys. Lett.*, **504**, 88 (2011).

University of Memphis

- 27) H. Gao, Z. Ke, N. J. DeYonker, J. Wang, H. Xu, Z.-W. Mao, D. L. Phillips, C. Zhao, "Dinuclear Zn(II) Complex Catalyzed Phosphodiester Cleavage Proceeds Via a Concerted Mechanism: A Density Functional Theory Study", *J. Am. Chem. Soc.*, **133**, 2904 (2011).
- 28) B. H. G. Swennenhuis, R. Poland, N. J. DeYonker, C. E. Webster, D. J. Darensbourg, A. A. Bengali, "Ligand displacement from $\text{TpMn}(\text{CO})_2\text{L}$ Complexes: A Large Rate Enhancement in Comparison to the $\text{CpMn}(\text{CO})_2\text{L}$ Analogues", *Organometallics*, **30**, 3054 (2011).
- 29) S. M. Gittermann, R. G. Letterman, T. Jiao, G.-L. Leu, N. J. DeYonker, C. E. Webster, T. J. Burkey, "Bond Energies, Reaction Volumes, and Kinetics for σ and π Complexes of $\text{Mo}(\text{CO})_5\text{L}$ ", *J. Phys. Chem. A*, **115**, 9004 (2011).
- 30) M. L. Laury, N. J. DeYonker, W. Jiang, A. K. Wilson, "A Pseudopotential-based Composite Method: The Relativistic Pseudopotential Correlation Consistent Composite Approach (rp-ccCA) for Molecules Containing 4d Transition Metals (Y–Cd)", *J. Chem. Phys.*, **135**, 214103 (2011).
- 31) H.-L. Wang, N. J. DeYonker, H. Gao, C. Tan, X. Zhang, L. Ji, C. Zhao, Z.-W. Mao, "Aquation and Dimerization of Osmium(II) Anticancer Complexes: A Density Functional Theory Study", *RSC Adv.*, **2**, 436 (2012).
- 32) W. Jiang, N. J. DeYonker, A. K. Wilson, "Multireference Character for 3d Transition Metal-Containing Molecules", *J. Chem. Theory Comput.*, **8**, 460 (2012), *featured cover article, February 2012 issue*.
- 33) W. Jiang, N. J. DeYonker, J. J. Determan, A. K. Wilson, "Toward Accurate Theoretical Thermochemistry of First Row Transition Metal Complexes", *J. Phys. Chem. A*, **116**, 870 (2012), *featured cover article, 01/19/2012 issue*.
- 34) H.-L. Wang, N. J. DeYonker, H. Gao, L. Ji, C. Zhao, Z.-W. Mao, "Mechanism of Aquation and Nucleobase Binding of Ruthenium (II) and Osmium (II) Arene Complexes: A Systematic Comparison DFT Study", *J. Organomet. Chem.*, **704**, 17 (2012).
- 35) X. Zhang, A. M. Wright, N. J. DeYonker, T. K. Hollis, N. I. Hammer, C. E. Webster, E. J. Valente, "Synthesis, Air-stability, Photo-bleaching and DFT Modeling of Blue Light-Emitting Platinum CCC-N-Heterocyclic Carbene Pincer Complexes", *Organometallics*, **31**, 1664 (2012).

- 36) S. A. Nedd, N. J. DeYonker, A. K. Wilson, P. Piecuch, M. S. Gordon, "Incorporating a Completely Renormalized Coupled Cluster Approach into a Composite Method for Thermodynamic Properties and Reaction Paths", *J. Chem. Phys.*, **136**, 144109 (2012).
- 37) W. M. Singh, T. Baine, S. Kudo, S. L. Tian, X. A. N. Ma, H. Y. Zhou, N. J. DeYonker, T. C. Pham, J. C. Bollinger, D. L. Baker, B. Yan, C. E. Webster, X. Zhao "Electrocatalytic and Photocatalytic Hydrogen Production in Aqueous Solution by a Molecular Cobalt Complex", *Angew. Chem., Int. Ed.*, **51**, 5941 (2012).
- 38) B. R. Wilson, N. J. DeYonker, A. K. Wilson, "Prediction of Hydrocarbon Enthalpies of Formation by Various Thermochemical Schemes", *J. Comp. Chem.*, **33**, 2032 (2012).
- 39) H.-L. Wang, N. J. DeYonker, X. Zhang, C. Zhao, L. Ji, Z.-W. Mao, "Photodissociation of a Ruthenium(II) Arene Complex and its Subsequent Interactions with Biomolecules: A Density Functional Theory Study", *J. Mol. Modeling*, **18**, 4675 (2012).
- 40) H.-L. Wang, N. J. DeYonker, H. Gao, D. L. Phillips, C. Zhao, L. Ji and Z.-W. Mao "Predicting the Interactions of Organometallic Ruthenium Ethylenediamine Complexes with Mononucleotides: Insights from Density Functional Theory", *RSC Adv.*, **2**, 7849 (2012).
- 41) Z.-F. Li, Y. Fan, N. J. DeYonker, X. Zhang, C.-Y. Su, C. Zhao, "Platinum(II)-catalyzed Cyclization Sequence of Aryl alkynes via C(sp³)-H activation: A DFT study", *J. Org. Chem.*, **77**, 6017 (2012).
- 42) N. J. DeYonker, W. D. Allen, "Taming the Low-Lying Electronic States of FeH", *J. Chem. Phys.*, **137**, 234303 (2012).
- 43) N. J. DeYonker, K. A. Peterson, "Is Near-'Spectroscopic Accuracy' Possible for Heavy Atoms and Coupled Cluster Theory?" An Investigation of the First Ionization Potentials of the Atoms Ga – Kr", *J. Chem. Phys.*, **138**, 164312 (2013).
- 44) K. R. Jorgensen, V. V. Ramasesh, S. Hannibal, N. J. DeYonker, A. K. Wilson, "Complete Basis Set Limits of Local Second-Order Møller-Plesset Perturbation Theory", *Mol. Phys.*, **111**, 1178 (2013), part of the "Trygve Helgaker, Festschrift".
- 45) N. J. DeYonker, C. E. Webster, "Phosphoryl Transfers of the Phospholipase D Superfamily: A Quantum Mechanical Theoretical Study", *J. Am. Chem. Soc.*, **135**, 13764 (2013).
- 46) D. Isrow, N. J. DeYonker, A. Koppaka, P. J. Pellechia, C. E. Webster, B. Captain, "Metal-Ligand Synergistic Effects in the Complex Ni(η^2 -TEMPO)₂. Synthesis, Structures, and Reactivity", *Inorg. Chem.*, **52**, 13882 (2013).
- 47) X. Zhang, Z. Ke, N. J. DeYonker, H. Xu, Z.-F. Li, X. Xu, X. Zhang, C.-Y. Su, D. L. Phillips, C. Zhao, "Mechanism and Enantioselectivity of Dirhodium-Catalyzed Intramolecular C–H Amination of Sulfamate", *J. Org. Chem.*, **78**, 12460 (2013).
- 48) Z.-F. Li, X. Yang, N. J. DeYonker, X. Xu, Z. Ghao, C. Zhao, "Binding Energies and Interaction Origins Between Nonclassical Single-electron Hydrogen, Sodium, and Lithium Bonds and Neutral Boron-containing Radicals: A Theoretical Investigation", *Chinese Sci. Bull.*, **59**, 2597 (2014).

- 49) X. Zeng, H. Wang, N. J. DeYonker, G. Mo, R. Zhou, C. Zhao, "Reaction Mechanism of Oxidative Desulfurization of Heterocyclic Organic Sulfides: A Computational Study", *Theor. Chem. Acc.*, **133**, 1498 (2014).
- 50) N. J. DeYonker and S. A. Shah, "The Role of Core/Valence Electron Correlation in Gallium Halides: A Comparison of Composite Methods", *Theor. Chem. Acc.*, **133**, 1518 (2014).
- 51) N. J. DeYonker, D. T. Halfen, W. D. Allen, L. M. Ziurys, "The Electronic Structure of Vanadium Monochloride Cation (VCl⁺): Tackling the Complexities of Transition Metal Species", *J. Chem. Phys.*, **141**, 204302 (2014).
- 52) N. J. DeYonker, "What a Difference a Decade Hasn't Made: The Murky Electronic Structure of Iron Monocyanide (FeCN) and Iron Monoisocyanide (FeNC)", *J. Phys. Chem. A*, **119**, 215 (2015).
- 53) A. M. Dietrich, A. Thomas, Y. Zhao, E. Smiley, N. Shanaiah, M. Ahart, K. A. Charbonnet, N. J. DeYonker, W. A. Alexander, D. L. Gallagher, "Partitioning, Aqueous Solubility, and Dipole Moment Data for cis- and trans-(4-methylcyclohexyl)methanol, Principle Contaminants of the West Virginia Chemical Spill", *Environ. Sci. Technol. Lett.*, **2**, 127 (2015), *featured cover article, 04/14/2015 issue*.
- 54) N. J. DeYonker, C. E. Webster, "A Theoretical Study of Phosphoryl Transfers of Tyrosyl DNA-phosphodiesterase (Tdp1) and the Possibility of a "Dead-End" Phosphohistidine Intermediate", *Biochemistry*, **54**, 4236 (2015).
- 55) N. J. DeYonker, C. E. Webster, "The *trans-cis* Isomerization of Ni(η^2 -TEMPO)₂: Interconnections and Conformational Complexity", *Inorg. Chim. Acta.*, **436**, 220 (2015).
- 56) A. Osmont, K. Chetehouna, N. Chaumeix, N. J. DeYonker, L. Catoire, "Thermodynamic data of known volatile organic compounds (VOCs) in *Rosmarinus officinalis*: implications for forest fire modeling", *Comput. Theor. Chem.*, **1073**, 27 (2015).
- 57) N. J. DeYonker, K. A. Charbonnet, W. A. Alexander, "Dipole Moments of *trans*- and *cis*-(4-methylcyclohexyl)methanol (4-MCHM): Obtaining the Right Conformer for the Right Reason", *Phys. Chem. Chem. Phys.*, **18**, 17865 (2016).
- 58) S. D. Dickerson, N. J. DeYonker, "Gas Phase Electronic Structure of the 3d Metal Monoacetylides (MCCH, M = Sc .. Zn)", *Int. J. Quantum. Chem.*, **117**, 104 (2017), *featured cover article, 01/15/2017 issue*.
- 59) J. L. Weidhaas, A. M. Dietrich, N. J. DeYonker, R. R. Dupont, W. T. Foreman, D. Gallagher, J. E. Gallagher, A. J. Whelton, W. A. Alexander, "Enabling Science Support During Incident Response for Better Decision Making", *J. Environ. Qual.*, **45**, 1490 (2016).
- 60) M. Fioroni, N. J. DeYonker, "H₂ Formation on Cosmic Grain Siliceous Surfaces Grafted with Fe⁺: A Silsesquioxanes-based Computational Model", *ChemPhysChem*, **17**, 3390 (2016).
- 61) R. G. Letterman, N. J. DeYonker, T. J. Burkey, C. E. Webster, "Calibrating Reaction Enthalpies: The Use of Density Functional Theory and the correlation consistent Composite Approach in the Design of Photochromic Materials", *J. Phys. Chem. A*, **120**, 9982 (2016).
- 62) G. Liang, N. J. DeYonker, X. Zhao, C. E. Webster, "Reduction Potential in Transition Metal Containing Complexes: How expensive? For what accuracy", *J. Comp. Chem.*, **38**, 2430 (2017).

- 63) Q. Cheng, R. C. Fortenberry, N. J. DeYonker, "Towards a Quantum Chemical Protocol for the Prediction of Rovibrational Spectroscopic Data for Transition Metal Molecules: Exploration of CuCN, CuOH, and CuCCH", *J. Chem. Phys.*, **147**, 234104 (2017).
- 64) T. P. Brewster, T. H. Nguyen, W. T. Eckenhoff, N. D. Schley, N. J. DeYonker, "Synthesis and Characterization of Heterobimetallic Iridium-Aluminum and Rhodium-Aluminum Complexes", *Inorg. Chem.*, **57**, 1148 (2018).
- 65) T. J. Summers, Q. Cheng, N. J. DeYonker, "A Transition State 'Trapped'? Modeling Biphenyl Torsional Rotation with a QM-cluster Model of Engineered Threonyl-tRNA Synthetase", *Org. Biomol. Chem.*, **16**, 4090, (2018), *featured cover article, 06/14/2018 issue*.
- 66) M. Torres, S. Khan, M. Duplanty, H. C. Lozano, T. J. Morris, T. Nguyen, Y. V. Rostovtsev, N. J. DeYonker, N. Mirsaleh-Kohan, "Raman and Infrared Studies of Platinum-Based Drugs: Cisplatin, Carboplatin, Oxaliplatin, Nedaplatin and Heptaplatin", *J. Phys. Chem. A*, **122**, 6934 (2018).
- 67) M. Fioroni, A. K. Tartera, N. J. DeYonker, "Propylene oxide formation on a silica surface with peroxo defects: implications in astrochemistry", *J. Phys. Chem. A*, **122**, 9100 (2018).
- 68) M. Fioroni, R. E. Savage, N. J. DeYonker, "On the Formation of Phosphorous Polycyclic Aromatics Hydrocarbons (PPAHs) in Astrophysical Environments", *Phys. Chem. Chem. Phys.*, **21**, 8015 (2019).
- 69) Q. Cheng, N. J. DeYonker, "Theoretical Study of the Low-lying Electronic States of Iron Hydride Cation", *J. Chem. Phys.*, **150**, 234304 (2019).
- 70) W. Thornley, S. A. Wirick, M. Riedel-Topper, N. J. DeYonker, T. E. Bitterwolf, C. J. Stromberg, E. J. Heilweil, "Photodynamics of [FeFe]-Hydrogenase Model Compounds with Bidentate Heterocyclic Ligands", *J. Phys. Chem. A*, **123**, 7137 (2019).
- 71) R. M. Charles III, T. W. Yokley, N. J. DeYonker, T. P. Brewster, "Bimetallic Hydrogen Activation and Hydrogenolysis Facilitated By Late Transition Metal-Aluminum Heterobimetallic Complexes", *Inorg. Chem.*, **58**, 12635 (2019).
- 72) T. J. Summers, B. P. Daniel, Q. Cheng, N. J. DeYonker, "Quantifying Protein Contact Networks through Interaction Energies", *J. Chem. Inf. Model.*, **59**, 5034 (2019).
- 73) R. M. Charles III, H. Tupkar, S. D. Helland, A. Mercado, W. T. Eckenhoff, N. D. Schley, N. J. DeYonker, T. P. Brewster, "Synthesis and Electronic Characterization of Iridium-Aluminum and Rhodium-Aluminum Heterobimetallic Complexes Bridged by 3-Hydroxypyridine and 4-Hydroxypyridine", *Eur. J. Inorg. Chem.*, **2020**, 1192 (2020).
- 74) Q. Cheng, N. J. DeYonker, "Acylation and Deacylation Mechanism and Kinetics of Penicillin G Reaction with Streptomyces R61 DD-peptidase", *J. Comp. Chem.*, **41**, 1685 (2020), *featured cover article 7/5/2020 issue*.
- 75) T. W. Yokley, H. Tupkar, N. D. Schley, N. J. DeYonker, T. P. Brewster, "CO₂ Capture by 2-(Methylamino)pyridine Ligated Aluminum Alkyl Complexes", *Eur. J. Inorg. Chem.*, **2020**, 2958 (2020).
- 76) M. A. Burton, Q. Cheng, D. T. Halfen, J. H. Lane, N. J. DeYonker, L. M. Ziurys. "The Structure of ScC₂ (\tilde{X}^2A_1): A Combined Fourier Transform Microwave/Millimeter-wave Spectroscopy and Computational Study", *J. Chem. Phys.*, **153**, 034304 (2020).

- 77) Q. Cheng, M. C. Washington, J. E. Burns, R. C. Fortenberry, N. J. DeYonker, "Spectroscopic Study of Magnesium Dinitrogen and Sodium Dinitrogen Cation", *Mon. Not. R. Astron. Soc.*, **498**, 5417 (2020).
- 78) R. M. Charles III, N. S. Taylor, A. A. Mercado, C. E. Frost, T. W. Yokley, W. T. Eckenhoff, N. D. Schley, N. J. DeYonker, T. P. Brewster, "Systematic Evaluation of the Electronic Effect of Aluminum-Containing Ligands in Iridium-Aluminum and Rhodium-Aluminum Bimetallic Complexes", *Dalton Trans.*, **49**, 13029 (2020).
- 79) R. C. Fortenberry, N. J. DeYonker "Rovibrational Quantum Chemical Treatment of Inorganic and Organometallic Astrochemicals", *Acc. Chem. Res.*, **54**, 271 (2021).
- 80) M. Fioroni, N. J. DeYonker "Complex Organic Matter Synthesis on Siloxyl Radicals in the Presence of CO", *Front. Chem.*, 621898 (2021), part of special issue on "Refractory Astrochemistry".
- 81) Q. Cheng, N. J. DeYonker, "QM-Cluster Model Study of Guaiacol O-demethylation by P450 Enzyme GcoA", *J. Phys. Chem. B*, **125**, 3296 (2021).
- 82) T. J. Summers, Q. Cheng, M. A. Palma, D.-T. Pham, D. K. Kelso III, C. E. Webster, and N. J. DeYonker, "Cheminformatic quantum mechanical enzyme model design: A catechol-O-methyltransferase case study", *Biophys. J.*, **120**, 3577 (2021).
- 83) T. J. Summers, H. Tupkar, T. M. Ozvat, Z. Tregillus, K. A. Miller, N. J. DeYonker, "Computational Insight into the Rope-skipping Isomerization of Diarylether Cyclophanes", *Symmetry*, **13**, 2127 (2021).
- 84) M. Fioroni, N. J. DeYonker, "Siloxyl radical initiated HCN polymerization: Computation of N-heterocycles formation and surface passivation", *Mon. Not. R. Astron. Soc.*, **512**, 1629 (2022).
- 85) Q. Cheng, N. J. DeYonker, "A Case Study of the Glycoside Hydrolase Enzyme Mechanism Using an Automated QM-cluster Model Building Toolkit", *Front. Chem.*, 854318 (2022), part of special issue "Editors' Showcase: Theoretical & Computational Chemistry"
- 86) D. A. Agbaglo, Q. Cheng, R. C. Fortenberry, J. F. Stanton, N. J. DeYonker, "Theoretical Rovibrational Spectroscopy of Magnesium Tricarbide - Multireference Character Thwarts a Full Analysis of All Isomers", *J. Phys. Chem. A*, **126**, 4132 (2022).
- C. Bell, N. J. DeYonker, C. E. Moore, K. M. Clark, "Unusually Strong Long-range Electronic Coupling Across Redox-Active Bridges in M³⁺/M⁴⁺ Mixed-Valence Complexes of Group 4 Congeners", *J. Am. Chem. Soc.*, *submitted*.
- T. J. Summers, R. Hemmati, J. E. Miller, D. A. Agbaglo, Q. Cheng, N. J. DeYonker, "Evaluating the Active Site-Substrate Interplay Between X-ray Crystal Structure and Molecular Dynamics in Chorismate Mutase", *J. Chem. Inf. Model.*, *submitted*.
- M. Fioroni, N. J. DeYonker, "Fine Astrochemicals: Regioselective Hydrocyanation of Unsaturated Carbon-carbon Bonds", *Chem. Comm.*, *submitted*.

Advising at The University of Memphis

Graduate student awards and fellowships

Thomas Summers - NSF Graduate Research Fellowship Program Award 2018-2021; Outstanding graduate student poster presentation at the 2019 SETCA conference; 1st Place in Physical and Applied Sciences Poster Award at the 31st Annual Student Research Forum at the University of Memphis, March 2019

Joseph Burns - NASA TN Space Grant Fellowship Summer 2019

Undergraduate student awards and fellowships

Justin Miller – J. C. Williams Memorial Scholarship, 2022-2023

Khloe Scott – University of Memphis College of Arts & Sciences Experiential Learning Fellowship, Spring 2022

Manuel Palma – J. C. Williams Memorial Scholarship, 2019-2020

Maura Washington - NASA TN Space Grant Fellowship, Summer 2019

Former postdoctoral researchers:

Dr. Reza Hemmati (PhD, Auburn University, 2021)

Current graduate students (anticipated year of graduation in parenthesis); names of students from underrepresented groups are italicized.

Tejaskumar Suhagia (anticipated PhD, 2024)

Donatus Agbaglo (anticipated PhD, 2024)

Current undergraduates

Justin Miller (anticipated 2024, University of Memphis)

Christopher Barksdale (anticipated 2022, University of Memphis)

Khloe Scott (anticipated 2023, University of Memphis)

Kaustubh Koya (graduated 2022, Collierville High School, attending Vanderbilt University in Fall 2022)

Grace Ward (post-bacc researcher, BS earned Spring 2022 at The University of the South)

Sydney Kong (anticipated 2023, Germantown Houston High School)

Former graduate students mentored

Sarah Pak (co-mentored with Prof. Daniel Nascimento, MS, 2022; anticipated PhD 2026)

Thomas Summers (MS, 2017; PhD earned Summer 2021, now postdoc at University of Nevada-Reno)

Davis Dahlberg (2019 – 2021, MS earned Spring 2021)

Connor Frost (2019 – 2021, MS earned Spring 2021)

Joseph Burns (2018 - 2020)

Roger Letterman (2015 - 2019)

Hannah Lozano (2016 – 2018, MS earned Spring 2018)

Diem-Trang Pham (2017, PhD in Computer Science earned Spring 2022)

Matthew Bassett (2017-2018)

Robert Nathan Waltman (2016-2017)

Fengshan Jiang (2013-2014)

Former undergraduates mentored

Taylor Christian (anticipated 2024, University of Memphis)

Manuel Palma (2021, University of Memphis)

Rebekah Lassiter (2020, Collierville High School)

Maura Washington (2022, University of Memphis)

Baty Daniel (2019, University of North Carolina - Chapel Hill)

Hrishikesh Tupkar (2021, University of Alabama - Tuscaloosa)

Robert Savage (2020, University of Memphis)

Ethan Watson (2021, Northeastern University)

Josh Porter (2019, Mississippi State University)

Chandler Klemm (2018, University of Memphis)

Tyree Morris, joint w/ William Alexander (2018, University of Memphis, *participant in NSF-funded TLSAMP program - Tennessee's Louis Stokes Alliance for Minority Participation*)

Chloe Baker (2018, University of Memphis)

Uday Patel (2018, University of Memphis)

Kelly Tartera, joint w/ Timothy Brewster (2017, University of Memphis)

Taylor Brown, joint w/ William Alexander – REU (2017, University of Memphis)

Katherine Charbonnet (2016, University of Memphis)

Shelby Dickerson – REU (2016, Southern Mississippi University)

Ava Conner, joint w/ C. Edwin Webster - REU (2015, Sewanee: The University of the South)

Linh Nguyen – REU (2015, Austin Peay State University)

Shesha Shah – REU (2014, Christian Brothers University)

Alexander Bernal, joint w/ C. Edwin Webster (2014, University of Memphis)

Service

Related to the American Chemical Society governance:

Memphis Local ACS Chapter Councilor since February 2021.

Panelist for regional Memphis ACS Chapter committee to select ACS Southern Chemist Award recipient for 2021, September – October 2020.

Reviewer for ACS undergraduate Student Chapter yearly reports, June 2019, June 2021, and June 2022.

Member of Decision Committee for ACS undergraduate Student Chapter awards, July – August 2021.

Related to professional organizations:

Member of American Biophysical Society since July 2020.

Member of United Campus Workers (UCW) since February 2017.

Member of Editorial Board for *Frontiers in Theoretical and Computational Chemistry* since April 2014.

Member of American Chemical Society (ACS) and American Association for the Advancement of Science (AAAS) since 2005.

Recent peer reviewer for *ACS Books*, *ACS Catalysis*, *Astrophysical Journal*, *Chemical Physics*, *Chirality*, *Computational and Theoretical Chemistry*, *Dalton Transactions*, *Inorganic Chemistry*, *International Journal of Quantum Chemistry*, *Journal of Chemical and Engineering Data*, *Journal of Chemical Physics*, *Journal of Computational and Theoretical Chemistry*, *Journal of Computational Chemistry*, *Journal of Physical Chemistry A*, *Journal of Quantitative Spectroscopy and Radiative Transfer*, *Monthly Notices of the Royal Astronomical Society*, *Polymer Degradation*, *RSC Advances*, *Scientific Reports*, *Spectrochimica Acta Part A*, and *Theoretical Chemistry Accounts*.

Standing committees/advising @ University of Memphis:

Member of Department of Chemistry Undergraduate Studies Committee, August 2016 – present.

Member of University of Memphis Web Development Team, March 2015 – present.

Director, Computational Research on Materials Institute at the University of Memphis (CROMIUM), August 2014 – present.

Faculty Advisor of the University of Memphis Chapter of the Student Members of the American Chemical Society (SM-ACS), January 2011 – present.

Duties include facilitating meetings with club officers and committees, planning social activities, assisting with budgeting, website design and updates, drafting of a STEM Club Mini-Grant proposal, outreach planning, and career counseling for undergraduates.

Temporary/Ad hoc committees/advising @ University of Memphis:

Committee member of Instructor Coordinator search for The University of Memphis Department of Chemistry, May 2022.

Committee member of Instructor search for The University of Memphis Department of Chemistry, June 2022.

Presenter for Interdisciplinary Team Building Networking Session, organized by Cody Behles and the UM Division of Research and Innovation, September 2020.

Reviewer of Faculty Research Grants for The University of Memphis College of Arts & Sciences, February 2020 – April 2020.

Chair of tenure-track Faculty Search for The University of Memphis Department of Chemistry, October 2019 – April 2020.

Committee member of STEM Pre-Award Staff Member search for The University of Memphis College of Arts and Sciences, December 2019 – January 2020.

Committee member of permanent General Chemistry Instructor search for The University of Memphis Department of Chemistry, August 2018.

Member of Information Technology Services/Faculty Senate Oversight Committee, October 2017 – May 2018.

Ad hoc Evaluation Committee member for the University of Memphis “HPC System for Research” RFP-96622288, December 2017 – March 2018.

Committee member of tenure-track Faculty Search for The University of Memphis Department of Chemistry, December 2016 – April 2017.

Ad hoc Evaluation Committee member for The University of Memphis Department of Chemistry's adoption of a new General Chemistry textbook for August 2015.

Ad hoc Evaluation Committee member for the University of Memphis "HPC System for Research" RFP-54057734, November 2014 – January 2015.

Conference organization and Chairing:

Symposium Co-organizer (with Prof. Leah Dodson, The University of Maryland – Baltimore) – PHYS "Inorganic and Organometallic Astrochemistry" for the Fall National American Chemical Society Meeting in Chicago, IL, August 2022.

Session Chair for COMP symposium "From Homogeneous to Heterogeneous Catalysis: A Computational Perspective" and PHYS symposium "Misconceptions in Astrochemistry: A Chemist's Guide" at the virtual Pacificchem meeting, December 2021.

Symposium Organizer – BIOL "Ground truth: bridging knowledge gaps between computational and experimental enzymology" for the SERMACS Regional Meeting, Birmingham, AL, November 2021.

Regional conference Co-organizer (with Prof. Greg Tschumper, The University of Mississippi) – 2017 meeting of the Southeast Theoretical Chemistry Association (SETCA), hosted by The University of Mississippi, Oxford, MS, May 2017.

Symposium Organizer – INOR General Oral for the SE/SW ACS Regional Meeting, Memphis, TN, May 2015 – November 2015

Session Chair for COMP (General Quantum Chemistry) and INOR (Organometallics – Catalysis) Oral sessions at the 253rd ACS National Meeting and Exposition, San Francisco, CA, April 2017.

Session Chair for PHYS division Oral session at Pacificchem, Honolulu, HI, December 2015.

Session Chair at the 2014 Annual Meeting of the Southeast Theoretical Chemistry Association (SETCA) at Emory University, Atlanta, GA, May 2014.

Session chair for COMP division Oral session at the 247th ACS National Meeting and Exposition, Dallas TX, March 2014.

STEM outreach/service participation:

Volunteered as a Faculty Mentor at the 66th Biophysical Society Annual Meeting, San Francisco, CA, February 2022.

Presenter for University of Memphis Campus School STEAM Day 2021, September 2021.

Judge – Germantown High School "Battle of the Brains" science fair, Germantown, TN, February 2017 & February 2020.

Served on NSF BIO advisory panel, Fall 2020

Served on NSF CHE fellowship panel, Spring 2017 & Spring 2020.

Judge for undergraduate and graduate student posters at various conferences – the 32nd and 33rd Annual Undergraduate Research Conference hosted by The University of Memphis (Feb. 2012 and 2013, respectively), the 53rd Sanibel Symposium, hosted by The University of Florida on St. Simons Island, GA, (Feb. 2013), the 25th and 34th annual Student Research Forum hosted by The University of Memphis (Apr. 2013 and Mar. 2022, respectively), the SERMACS 2016 COMP poster session hosted by University of South Carolina, the 2019 Fall ACS COMP poster session at the National Meeting in San Diego, CA, the 2022 Spring ACS COMP poster session at the National Meeting in San Diego, CA.

Participant/demonstrator – Pink Palace Museum 3rd annual Science of Beer event, Memphis, TN, January 2017.

Presenter – University of Memphis Math Boot Camp 2016, Memphis, TN, August 2016.

Invited participant in EPSCoR Workshop “Fostering Advances in Water Resource Protection and Crisis Communications, Lessons Learned from Recent Disasters” at the US Fish and Wildlife Service’s National Conservation Training Center, near Shepherdstown, WV, June 2015.

Invited participant to the 2010 CENTC Summer School 2010 focusing on “Emerging Perspectives in Catalysis,” hosted by the University of Washington, Seattle, WA, July, 2010.

Teaching Experience

As instructor of record

Fall 2019

“Approximate Molecular Modeling” – University of Memphis graduate level course CHEM 7711/8711

Spring 2015, Spring 2016, Fall 2016, Fall 2017, Fall 2018, Fall 2020, Spring 2021, Fall 2021

“General Chemistry II” – University of Memphis undergraduate level course CHEM 1120

Spring 2017, Spring 2019, Spring 2022

“Foundations of Inorganic Chemistry” – University of Memphis undergraduate level course CHEM 3111

Fall 2014, Spring 2018, Spring 2020

“Systematic Inorganic Chemistry” – University of Memphis graduate level course CHEM 7111/8111

Fall 2015

“Structural Inorganic Chemistry” – University of Memphis graduate level course CHEM 8112

As teaching assistant

Fall 2001 – Fall 2002

“Freshman Chemistry Laboratory I and II” Lab instructor - University of Georgia under the direction of Prof. Bobby J. Stanton.

Spring 2005

“Advanced Quantum Chemistry II” Instructor Assistant - University of Georgia under the direction of Dr. Yukio Yamaguchi and Prof. Henry F. Schaefer III.

Contributed Scientific Lectures and Posters

- 1) "Ab Initio Study of Ground and Excited States of FeCN and FeNC" Poster presented at WATOC-2002 in Lugano, Switzerland, August 2002.
- 2) "Ground and Excited States of FeCN / FeNC: A Theoretical Journey" A contributed talk, presented at the Ohio State University International Symposium on Molecular Spectroscopy at the Ohio State University, Columbus, OH, July 2003.
- 3) "Potential Energy Curves and Linear Excited States of HBO and BOH" A contributed talk, presented at the 2004 Annual Meeting of the Southeast Theoretical Chemistry Association (SETCA) at the University of Mississippi, University, MS, May 2004.
- 4) "Multireference Configuration Interaction and Equation-of-Motion Coupled Cluster Study of Linear HBO and BOH Singlet Electronic States" Poster presented at "Molecular Quantum Mechanics, an International Conference in Honour of Professor Nicholas C. Handy", St. John's College, Cambridge University, England, August 2004.
- 5) "The Correlation Consistent Composite Approach (ccCA)" Poster presented at "Quantitative Quantum Chemistry: An international workshop in honor of Prof. Thom Dunning", Santa Fe, NM, March 2006.
- 6) "The Correlation Consistent Composite Approach" A contributed talk presented at the National American Chemical Society Meeting in Atlanta, GA, March 2006.
- 7) "Recent Developments with the Correlation Consistent Composite Approach" A contributed talk presented at the National American Chemical Society Meeting in Chicago, IL, March 2007.
- 8) "The correlation consistent Composite Approach (ccCA): Efficient Thermochemistry Across the Periodic Table" Poster presented as part of the Academic Employment Initiative at the National American Chemical Society Meeting in Boston, MA, August 2007.
- 9) "The correlation consistent Composite Approach (ccCA): Efficient Thermochemistry Across the Periodic Table" Poster presented at the 16th Conference on Current Trends in Computational Chemistry in Jackson, MS, October 2007.
- 10) "Accurate and 'Pan-periodic' Thermodynamics and Kinetics" An invited talk, presented at Brandeis University, Waltham, MA, February 2008.
- 11) "The correlation consistent Composite Approach (ccCA): Efficient Thermochemistry Across the Periodic Table" Poster presented at the 22nd Austin Symposium on Molecular Structure in Austin, TX, March 2008.
- 12) "The correlation consistent Composite Approach: A Pan-Periodic Model Chemistry" Poster presented at the American Conference on Theoretical Chemistry in Evanston, IL, July 2008.
- 13) "The Continuing Saga of the correlation consistent Composite Approach" An invited talk, presented at the University of Georgia, Athens, GA, August 2008.
- 14) "Accurate and Pan-periodic Energies" An invited talk, presented at Texas Christian University, Fort Worth, TX, January 2009.

- 15) "Accurate and Pan-periodic Energies" An invited talk, presented at the University of Massachusetts – Boston, Boston, MA, February 2009.
- 16) "Accurate and Pan-periodic Energies" An invited talk, presented at the University of Nebraska-Omaha, Omaha, NE, March 2009.
- 17) "Accurate and Pan-periodic Energies" An invited talk, presented at the Sun Yat-Sen University, Guangzhou, Guangdong, China, July 2010.
- 18) "The Many Phosphoryl Transfers of Phospholipase D" An invited talk, presented at The University of Mississippi (Ole Miss), Oxford, MS, March 2012.
- 19) "Focal Point Study of Gas Phase Iron Monohydride" A contributed talk, presented at the Astrobiology Science Conference in Atlanta, GA, April 2012.
- 20) "Focal Point Study of Gas Phase Iron Monohydride" A contributed talk, presented at the 2012 Annual Meeting of the Southeast Theoretical Chemistry Association (SETCA) at the University of Georgia, Athens, GA, May 2012.
- 21) "A Tale of Two Molecules: FeH and PLD" An invited talk presented at Austin Peay State University, Clarksville, TN, February 2013.
- 22) "Is Near-'Spectroscopic Accuracy' Possible For Heavy Atoms and Coupled Cluster Theory?" An invited talk presented at the 53rd Sanibel Symposium, St. Simons Island, GA, February 2013.
- 23) "Metal-ligand Synergistic Effects in Ni(η^2 -TEMPO)₂: Structures and Reactivity" A contributed talk presented at the 245th American Chemical Society National Meeting, New Orleans, LA, April 2013.
- 24) "Taming the Electronic Structure of FeH" A contributed talk presented at the 245th American Chemical Society National Meeting, New Orleans, LA, April 2013.
- 25) "Metal-ligand Synergistic Effects in Ni(η^2 -TEMPO)₂: Structures and Reactivity" An invited talk presented at The University of Georgia, Athens, GA, October 2013.
- 26) "Metal-ligand Synergistic Effects in Ni(η^2 -TEMPO)₂: Structures and Reactivity" An invited talk presented at Mississippi State University, Starkville, MS, November 2013.
- 27) "Phosphoryl Transfers of Tyrosyl DNA-phosphodiesterase: Is Tdp1 a PLD?" A contributed talk presented at the 247th ACS National Meeting and Exposition, Dallas TX, March 2014.
- 28) "The Electronic Structure of Vanadium Monochloride Cation (VCl⁺): At the Crossroads of Experimental and Computational Astrochemistry" Poster presented at the 247th ACS National Meeting and Exposition, Dallas TX, March 2014.
- 29) "The Electronic Structure of Vanadium Monochloride Cation (VCl⁺): At the Crossroads of Experimental and Computational Astrochemistry" Poster presented at the 2014 Annual Meeting of the Southeast Theoretical Chemistry Association (SETCA) at Emory University, Atlanta, GA, May 2014.
- 30) "The Murky Electronic Structure of Iron Monocyanide" Invited talk presented at Rhodes College, Memphis, TN, September 2014.

- 31) "The Murky Electronic Structure of Iron Monocyanide" A contributed talk presented at the 66th Southeastern Regional Meeting of the American Chemical Society, Nashville, TN, October 2014.
- 32) "The Role of Quantum Chemistry in Environmental Contaminant Modeling and Response" Poster presented at the EPSCoR Workshop entitled "Fostering Advances in Water Resource Protection and Crisis Communications, Lessons Learned from Recent Disasters" Shepherdstown, WV, June 2015.
- 33) "Transition metals in astrochemistry: Which roads leading to a better understanding of astrobiology?" Invited talk presented at PHYS special symposium entitled "Bringing Astrochemicals Back to Earth: Formation, Mechanisms, Stability, and Spectroscopic Signatures", 250th American Chemical Society National Meeting, Boston, MA, September 2015.
- 34) "The Role of Quantum Chemistry in Environmental Contaminant Modeling and Response" Poster presented at the 250th American Chemical Society National Meeting, Boston, MA, September 2015.
- 35) "Environmental Fate in Organic Contaminants: The Role of Quantum Chemistry" A contributed talk presented at the 250th American Chemical Society National Meeting, Boston, MA, September 2015.
- 36) "Transition metals in astrochemistry: Which roads leading to a better understanding of astrobiology?" Contributed talk presented at the 71st SWRM/67th SERMACS meeting, Memphis, TN, November 2015.
- 37) "Small and medium fries: Adventures in Computational Chemistry" Invited talk at the College of Charleston, Charleston, SC, November 2015.
- 38) "Transition metals in astrochemistry: Which roads leading to a better understanding of astrobiology?" Invited talk presented at PHYS special symposium entitled "Computational Modeling of d- and f-Block Chemistry: Challenges and Opportunities" at the Pacificchem 2015 meeting in Honolulu, HI, December 2015.
- 39) "Transition metals in astrochemistry: Which roads leading to a better understanding of astrobiology?" Invited talk presented at University of Alabama in Huntsville, Huntsville, AL, March 2016.
- 40) "Transition metals in astrochemistry: Which roads leading to a better understanding of astrobiology?" Invited talk presented at University of Memphis, Memphis, TN, March 2016.
- 41) "Transition metals in astrochemistry: Which roads leading to a better understanding of astrobiology?" Invited talk presented for the Department of Physics, University of Memphis, Memphis, TN, September 2016.
- 42) "Transition metals in astrochemistry: Which roads leading to a better understanding of astrobiology?" Invited talk presented at Millsaps College, Jackson, MS, September 2016.
- 43) "Transition metals in astrochemistry: Which roads leading to a better understanding of astrobiology?" Invited talk presented at Belhaven University, Jackson, MS, September 2016.
- 44) "A transition state 'Trapped': Using the QM cluster model to examine the energetics of constrained biphenyl dihedral rotation within a modified threonyl transfer RNA synthetase", contributed talk presented at the 2016 Southeastern Meeting of the American Chemical Society, Columbia, SC, October 2016.

- 45) “Inorganic computational astrochemistry: Electronic structure of metal monoacetylides and other stories”, an invited talk presented at the COMP special symposium “Electronic Structure: Concepts & Applications” at the 2016 Southeastern Meeting of the American Chemical Society, Columbia, SC, October 2016.
- 46) “Electronic structure and reactivity of astrochemically relevant inorganic hydrides”, a contributed poster presented at the Hydride Toolbox conference hosted by University Pierre and Marie Curie, Paris, France, December 2016.
- 47) “QM cluster model examination of constrained biphenyl dihedral rotation within a modified threonyl-tRNA synthetase: A transition state trapped?”, an invited talk presented at the 253rd American Chemical Society National Meeting, San Francisco, CA, April 2017.
- 48) “Is an exhaustive conformational search necessary for proposing catalytic mechanisms? An investigation of intramolecular Heck catalysis in the formation of colletoic acid derivatives”, a contributed talk presented at the 253rd American Chemical Society National Meeting, San Francisco, CA, April 2017.
- 49) “Astrochemistry: origin of life and origin of my career”, an invited talk presented at the Ned R. McWherter Library 1st annual NEDtalks as part of the McWherter Library Faculty Scholarship Week Exhibition, University of Memphis, April 2017.
- 50) “The role of transition metals in the structure and reactivity of astrochemicals” an invited talk presented at The University of Warwick Centre for Scientific Computing, Coventry, United Kingdom, June 2017.
- 51) “The role of transition metals in the structure and reactivity of astrochemicals” an invited talk presented at University College London, London, United Kingdom, June 2017.
- 52) “Inorganic computational astrochemistry: Rovibrational quartic force fields for copper-containing molecules”, an invited talk presented at COMP special symposium entitled “Contemporary Computational Chemistry” at the 2017 Southeastern Meeting of the American Chemical Society, Charlotte, NC, November 2017.
- 53) “Quantum Chemistry: From the Sagittarius B2 Cloud to Human Saliva” an invited talk presented at Middle Tennessee State University, Murfreesboro, TN, February 2018.
- 54) “New Adventures in Gas Phase Iron Diatomic Electronic Spectroscopy”, a contributed poster presented at the 255th American Chemical Society Meeting, New Orleans, LA, April 2018.
- 55) “Inorganic Computational Astrochemistry: Rovibrational Quartic Force Fields”, a contributed talk presented at the 255th American Chemical Society Meeting, New Orleans, LA, April 2018.
- 56) “Quantum Chemistry: From the Sagittarius B2 Cloud to Protein Bottles”, an invited talk presented at Union University, Jackson, TN, April 2018.
- 57) “Inorganic Computational Astrochemistry: Rovibrational Spectroscopy and Heterogenous Catalysis”, an invited talk presented at the 2018 Annual Meeting of the Southeast Theoretical Chemistry Association (SETCA) at Louisiana State University, Baton Rouge, LA, May 2018.

- 58) “Computational Inorganic Astrochemistry”, an invited talk presented at Mississippi College, Clinton, MS, September 2018.
- 59) “Quantum Chemistry: From the Sagittarius B2 Cloud to Protein Bottles”, an invited talk presented at Texas Woman’s University, Denton, TX, October 2018.
- 60) “Quantum Chemistry: From the Sagittarius B2 Cloud to Protein Bottles”, an invited talk presented at University of North Texas, Denton, TX, October 2018.
- 61) “High Performance Computing at UM”, an invited lightning talk presented at University of Memphis for the Office of Sponsored Programs Research Resources and Labs Lightning Talks meeting, December 2018.
- 62) “Quantum Chemistry: From the Sagittarius B2 Cloud to Protein Bottles”, an invited talk presented at Mississippi University for Women, Columbus, MS, January 2019.
- 63) “Quantum Chemistry: From the Sagittarius B2 Cloud to Protein Bottles”, an invited talk presented at University of Alabama, Tuscaloosa, AL, January 2019.
- 64) “Exploring Convergence of Thermodynamic and Kinetic Properties of QM-cluster Enzyme Models”, a contributed talk presented at the 257th American Chemical Society Meeting, Orlando, FL, April 2019.
- 65) “Rovibrational Quartic Force Fields of Scandium and Titanium Dicarbides” a contributed talk presented at the 257th American Chemical Society Meeting, Orlando, FL, April 2019.
- 66) “Reproducible, Rational, and Rigorous QM-cluster Enzyme Models”, a contributed poster presented at the 2019 Annual Meeting of the Southeast Theoretical Chemistry Association (SETCA) at University of Tennessee-Knoxville, Knoxville, TN, May 2019.
- 67) “Exploring Convergence of Thermodynamic and Kinetic Properties of QM-cluster Enzyme Models”, an invited talk presented at the NIH NHLBI Laboratory of Computational Biophysics, Bethesda, MD, June 2019.
- 68) “Exploring Convergence of Thermodynamic and Kinetic Properties of QM-cluster Enzyme Models”, an invited talk presented at the NREL, Golden, CO, August 2019.
- 69) “Reproducible, Rational, and Rigorous QM-cluster Enzyme Models”, a contributed talk presented at PHYS: Computational Quantum Chemistry: From Promise to Prominence: A Symposium in Honor of Henry F. Schaefer during the 258th American Chemical Society Meeting, San Diego, CA, September 2019.
- 70) “Reproducible, Rational, and Rigorous QM-cluster Enzyme Models”, an invited talk at the University of Tennessee-Knoxville, Knoxville, TN, October 2019.
- 71) “Reproducible, Rational, and Rigorous QM-cluster Enzyme Models”, a contributed talk presented at COMP: Computational Chemistry Applied to Interesting Problems during the Southeastern Meeting of the American Chemical Society, Savannah, GA, October 2019.
- 72) “Rovibrational spectroscopy of magnesium acetylide (MgCCH) and its detection in the interstellar medium”, an invited talk presented at PHYS: Astrochemistry in the Southeast and Beyond during the Southeastern Meeting of the American Chemical Society, Savannah, GA, October 2019.

- 73) “Reproducible, Rational, and Rigorous QM-cluster Enzyme Models”, an invited talk at the University of Memphis Department of Physics, February 2020.
- 74) “Reproducible, Rational, and Rigorous QM-cluster Enzyme Models”, an invited virtual talk at the Auburn University Department of Chemistry and Biochemistry, October 2020.
- 75) “Automating, Analyzing, and Databasing Quantum Mechanical Enzyme Simulations”, an invited virtual talk at the University of Memphis Department of Chemistry, October 2020.
- 76) “Automating, Analyzing, and Databasing Quantum Mechanical Enzyme Simulations”, a contributed poster at the 2021 Annual Meeting of the Biophysical Society, held virtually, March 2021.
- 77) “Rovibrational Quartic Force Fields of Metal Dicarbides and Tricarbides”, an invited symposium talk at the American Physical Society March 2021 meeting: The Chemical Physics of Molecules in Space, held virtually, March 2021.
- 78) “Residue interaction network-based enzyme modeling”, a contributed talk at the Spring 2021 National meeting of the American Chemical Society, April 2021.
- 79) “Residue interaction network-based enzyme modeling”, an invited talk presented at The University of Oklahoma, April 2021.
- 80) “Reproducible, rational, and rigorous QM-cluster enzyme models”, an invited virtual talk presented at a symposium in honor of H. Fritz Schaefer III, entitled “Computational Quantum Chemistry: Synergism Between Theory and Experiment” at the Pacificchem 2021 meeting, December 2021.
- 81) “Rovibrational Quartic Force Fields of Metal Dicarbides and Tricarbides”, an invited virtual talk presented at the symposium “Misconceptions in Astrochemistry” at the Pacificchem 2021 meeting, December 2021.
- 82) “QM-cluster modeling of enzymes used in biofuel valorization”, an invited virtual talk presented at the symposium “From Homogeneous to Heterogeneous Catalysis: A Computational Perspective” at the Pacificchem 2021 meeting, December 2021.
- 83) “Bio/Cheminformation Within Quantum Mechanical Enzyme Simulations”, a contributed poster presented at the 66th Biophysical Society Annual Meeting, San Francisco, CA, February 2022.
- 84) “Challenge accepted: Rovibrational quartic force fields of metal dicarbides and tricarbides”, a contributed talk presented at a symposium in honor of John Stanton, entitled “The Synergy of Theory and Experiment” at the Spring 2022 National meeting of the American Chemical Society, San Diego, CA, March 2022.
- 85) “Residue interaction networks and the cheminformatics of atomic-level enzyme models”, an invited talk presented at a symposium entitled “New Developments in Hybrid QM/QM, QM/MM, and Fragmentation Methods”, at the Spring 2022 National meeting of the American Chemical Society, San Diego, CA, March 2022.
- 86) “Residue interaction networks and the cheminformatics of atomic-level enzyme models”, a contributed talk presented at the Southeastern Theoretical Chemistry Association (SETCA) at Georgia Tech University, Atlanta, GA, May 2022.

87) “Residue interaction networks and the cheminformatics of atomic-level enzyme models”, a contributed poster presented at the 2022 Metallocofactors Gordon Research Conference, at Salve Regina University, Newport, RI, June 2022.

88) “Residue interaction networks and the cheminformatics of atomic-level enzyme models”, an invited oral communication presented at the 12th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2020), Vancouver, British Columbia, Canada, July 2022.