

# Daniel Devore, Ph.D.

✉ [ddevore@mail.smu.edu](mailto:ddevore@mail.smu.edu) | ✉ [ddevorecollege1@gmail.com](mailto:ddevorecollege1@gmail.com) | 📞 +1 (484) 633-7745 | 📠 0000-0002-5753-4260 |  
🌐 [github.com/daniel-devore](https://github.com/daniel-devore) | 🌐 [linkedin.com/in/daniel-devore](https://www.linkedin.com/in/daniel-devore) | 🌐 [danieldevorebio.godaddysites.com](https://danieldevorebio.godaddysites.com)  
🌐 [credly.com/users/daniel-devore.edb3fcba](https://credly.com/users/daniel-devore.edb3fcba)

## Education

**Baylor University** Defense date: May 7, 2024; Graduation date: Aug. 2024  
Ph.D. Chemistry | PI: Dr. Kevin Shuford **GPA: 3.78/4.00**  
Dissertation: "Leveraging Noncovalent Interactions for  $\sigma$ -hole Mediated Molecular Assembly"  
**Westminster University of Salt Lake City, UT** Graduation date: Jun. 2019  
B.S. Chemistry | Advisor: Dr. Jessica Johnston **GPA: 3.22/4.00**  
Research: "Thermodynamic Dissociation of Protonated Methionine"  
**Westminster University of Salt Lake City, UT** Graduation date: Jun. 2019  
B.S. Mathematics | Advisor: Dr. Sean Raleigh **GPA: 3.22/4.00**

## Professional Awards and Appointments

**Postdoctoral Fellowship, Southern Methodist University** May 2024 – Current  
**Outstanding Graduate Research Productivity Award Recipient, Baylor University** 2024  
• Department of Chemistry and Biochemistry  
**Graduate Fellowship Recipient, Baylor University** 2019 – 2024  
**American Chemical Society Student Chapter: Westminster University** Sept. 2018 – Jun. 2019  
**President** Leadership, Budgeting, Event Planning  
• Lead student chapter board meetings, budget considerations, and event planning.

## Research Experience

**Southern Methodist University** May 2024 – Present  
**Postdoctoral Research Fellow | PI: Dr. Devin Matthews** Linux, Python, Bash, C++, CFOR, SLURM  
• Application of Singular Value Decomposition to reduce tensor dimensions for computational scaling reduction for closed- and Open-shell Coupled Cluster methods (CCSDT-1a/b, CC3, CCSDT-2, CCSDT-3, CCSD(T)).  
• Employment of EOMEE-CCSD methods for the determination of vibrational frequencies in excited states of pyrone.  
**Baylor University** Jul. 2019 – May 2024  
**Graduate Research Assistant | PI: Dr. Kevin Shuford** Mac, Linux, Python, Bash, Gaussian, Psi4, Orca, LModeA, PBS  
• Development and characterization of novel halogen-containing molecular building blocks that exhibit a unique set of tunable electronic properties through  $\sigma$ -hole formation and supramolecular assembly with DFT.  
• Structure elucidation and spectroscopic characterization, using *ab initio* methods, of noncovalently bound clusters relevant to the atmosphere, such as molecular chlorofluorocarbons and their hydrates.  
• Employment of TD-DFT to elicit the photochemical effects that result from the complexation of halogen-containing molecular building blocks through  $\sigma$ -hole interactions.  
**Westminster College of Salt Lake City, UT** Jun. 2016 – May 2019  
**Undergraduate Research Assistant | Advisor: Dr. Jessica Johnston** Gaussian  
• Demonstration and characterization of the thermodynamic dissociation of protonated methionine using DFT to compare to experiment.

## Grant and Fellowship Proposal Experience

**Frontera Computational Science Fellowships** 2023 – 2024  
**Research Development and Computational Resource Fellowship | Baylor University (rejected)**  
• Project Title: "Modulating CO<sub>2</sub> Adsorption on Graphitic Carbon Nitride with Intermolecular Halogen Bonds"

## Publications

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1. K. A. French, **D. P. Devore**, T. L. Ellington, K. L. Shuford, Probing the Hybrid  $\sigma/\pi$ -holes in  $sp^2$ -hybridized Chalcogen Bond Donors and their Complexes with Ammonia. *ChemPhysChem*, 2025, 000, e202500381 [10.1002/cphc.202500381](#)
2. **D. P. Devore**, T. L. Ellington, K. L. Shuford, Investigating Halogen Bonds in Substituted Graphitic Carbon Nitride through Vibrational Spectroscopy. *Phys. Chem. Chem. Phys.*, 2025, 27, 17852 – 17863 [10.1039/D5CP02395E](#)
3. **D. P. Devore**, K. L. Shuford, Data and Molecular Fingerprint Driven Machine Learning Approaches to Halogen Bonding. *J. Chem. Inf. Model.* 2024, 64, 21, 8201 – 8214 [10.1021/acs.jcim.4c01427](#)
4. **D. P. Devore**, T. L. Ellington, K. L. Shuford, Illuminating the Performance of Electron Withdrawing Groups in Halogen Bonding. *ChemPhysChem*, 2024, 25, e202400607 [10.1002/cphc.202400607](#)
5. **D. P. Devore**, T. L. Ellington, K. L. Shuford, Elucidating the Role of Electron Donating Groups in Halogen Bonds. *J. Phys. Chem. A*, 2024, 128, 8, 1477 – 1490 [10.1021/acs.jpca.3c06894](#)
6. T. L. Ellington, **D. P. Devore**, W. M. U. G. De Alwis, K. A. French, K. L. Shuford, Shedding Light on the Vibrational Signatures in Halogen-Bonded Graphitic Carbon Nitride Building Blocks. *ChemPhysChem*, 2023, 24, e202200812, [10.1002/cphc.202200812](#)
7. **D. P. Devore**, T. L. Ellington, K. L. Shuford, Interrogating the Interplay between Hydrogen and Halogen Bonding in Graphitic Carbon Nitride Building Blocks. *J. Phys. Chem. A*, 2020, 124, 51, 10817–10825 [10.1021/acs.jpca.0c09154](#)

## Oral Presentations

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1. **D. P. Devore** and D. A. Matthews, Applying Tensor Decomposition to Open-Shell CCSD(T). *36<sup>th</sup> IUPAP Conference on Computational Physics– CCP2025*, virtual conference, Oak Ridge National Laboratory (ORNL) (November 2025)
2. **D. P. Devore** and D. A. Matthews, Pursuing rank reduced CCSD(T) for open-shell systems. *57<sup>th</sup> ACS Meeting in Miniature – MiM*, Eastern Texas A&M, Commerce, TX (April 2025)
3. **D. P. Devore** and K. L. Shuford, Predicting halogen bond properties through machine learning. *Southwest Regional Meeting – SWRM*, Waco, TX (October 2024)
4. **D. P. Devore**, Leveraging the Noncovalent Interactions for  $\sigma$ -hole Mediated Molecular Assembly. *Dissertation Defense Seminar*, Baylor University, Waco, TX (May 2024)
5. **D. P. Devore**, V. S. K. Choutipalli, and K. L. Shuford, CO<sub>2</sub> esterification through halogen bonding. *American Chemical Society National Meeting and Exposition – ACS*, New Orleans, LA (March 2024)
6. **D. P. Devore**, Bringing Computational Chemistry to the Forefront. *Advanced Instrumentation Workshop – AIW*, Baylor University, Waco, TX (October 2023)
7. **D. P. Devore**, Bringing HTC to Chemistry. *Open Science Grid (OSG) School – Lightning Talk*, University of Wisconsin, Madison, WI (August 2023)
8. **D. P. Devore**, T. L. Ellington, and K. L. Shuford, Halogen Bond Assisted Self-Assembly. *Guest Seminar Coffee Hour*, Baylor University, Waco, TX (April 2023)
9. **D. P. Devore**, T. L. Ellington, and K. L. Shuford, The Positive Side to Halogens: A  $\sigma$ -hole Interaction Study. *Southwest Regional Meeting – SWRM*, Baton Rouge, LA (November 2022)
10. **D. P. Devore**, Introduction to Computational Chemistry in the Shuford Group. *Graduate Recruitment Weekend – Baylor University*, Waco, TX (February 2022)
11. W. M. Uvin De Alwis and **D. P. Devore**, Introduction to Computational Chemistry. *Advanced Instrumental Workshop – AIW*, Baylor University, Waco, TX (October 2021)
12. **D. P. Devore**, A New Way to Think about Halogen Atoms: The Halogen Bond. *Dissertation Prospectus Seminar*, Baylor University, Waco, TX (May 2021)
13. **D. P. Devore**, Halogen Bond Induced Non-covalent Interactions in Graphitic Carbon Nitriles. *Guest Seminar Coffee Hour*, Baylor University, Waco, TX (January 2020)
14. **D. P. Devore**, J. Johnston, and P. B. Armentrout, Mechanism of Decomposition of Protonated Methionine: A Computational Study. *American Chemical Society National Meeting and Exposition – ACS*, Orlando, FL (March 2019)
15. **D. P. Devore**, J. Johnston, and P. B. Armentrout, Mechanism of Decomposition of Protonated Methionine: A Computational Study – Part 3. *Geek Fest (Departmental Seminar)*, Westminster University, Salt Lake City, UT (September 2018)
16. **D. P. Devore**, J. Johnston, and P. B. Armentrout, Mechanism of Decomposition of Protonated Methionine: A Computational Study – Part 2. *Geek Fest (Departmental Seminar)*, Westminster University, Salt Lake City, UT (September 2017)
17. **D. P. Devore**, J. Johnston, and P. B. Armentrout, Mechanism of Decomposition of Protonated Methionine: A Computational Study – Part 1. *Geek Fest (Departmental Seminar)*, Westminster University, Salt Lake City, UT (September 2016)

## Poster Presentations

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1. **D. P. Devore** and D. A. Matthews, Scaling Reduction in Open-Shell CCSD(T) through Tensor Decomposition. *53<sup>rd</sup> Annual Meeting of the Southeast Theoretical Chemistry Association – SETCA*, The University of Memphis, Memphis, TN (May 2025)
2. **D. P. Devore** and D. A. Matthews, Diagrammatic Approach to Rank Reduced CCSD(T) for Open-Shell Systems. *Research and Innovation Week*, Southern Methodist University, Dallas, TX (April 2025)
3. **D. P. Devore** and K. L. Shuford, Data and Molecular Fingerprint Driven Machine Learning for Halogen Bonding QSPR/QSAR. *#RSCPoster – Royal Society of Chemistry, LinkedIn* (March 2024)
4. **D. P. Devore**, T. L. Ellington, and K. L. Shuford, Distance of Detection: A  $\sigma$ -hole Sensing Study. *Southwest Regional Meeting – SWRM*, Oklahoma City, OK (November 2023)
5. **D. P. Devore**, T. L. Ellington, and K. L. Shuford, Bounding onto the Trampoline of Halogen Bonds with Graphitic Carbon Nitride. *#RSCPoster – Royal Society of Chemistry, Twitter* (February 2023)
6. **D. P. Devore**, T. L. Ellington, and K. L. Shuford, Springing into Vibrational Properties of Halogen Bonding Interactions. *Austin Symposium on Molecular Structure and Dynamics at Dallas – ASMD@D*, Dallas, TX (February 2023)
7. **D. P. Devore**, T. L. Ellington, and K. L. Shuford, Guided Exploration of Halogen Bonding Interactions in Doped Graphitic Carbon Nitride Building Blocks with Vibrational Spectroscopy. *10<sup>th</sup> triennial Conference on Molecular Quantum Mechanics – MQM*, Blacksburg, VA (June 2022)
8. **D. P. Devore**, T. L. Ellington, and K. L. Shuford, Fundamental Observations Behind the Effects of Electron Donating and Electron Withdrawing Groups on Halogen Bond Donor  $\sigma$ -holes. *American Chemical Society National Meeting and Exposition – ACS*, San Diego, CA (March 2022)
9. **D. P. Devore**, T. L. Ellington, and K. L. Shuford, Electron Donating Group Effects on Halogen Bond Donor  $\sigma$ -holes. *Southeastern Regional Meeting of the American Chemical Society – SERMACS*, Birmingham, AL (November 2021)
10. Cooperative Hydrogen and Halogen Bonding in Graphitic Carbon Nitride Building Blocks. *International Conference on Electronic Materials (IUMRS-ICEM) and XIX Brazilian Materials Research Society (MRS) Meeting*, Rio de Janeiro, Brazil (August 2021)
11. **D. P. Devore**, T. L. Ellington, and K. L. Shuford, Probing the Electron Withdrawing Effects in the  $\sigma$ -hole of Halogen Bond Donors. *American Chemical Society National Meeting and Exposition – ACS*, Atlanta, GA (August 2021)
12. **D. P. Devore**, T. L. Ellington, and K. L. Shuford, Halogen Bonding in Graphitic Carbon Nitride Building Blocks. *Southwest Theoretical and Computational Chemistry Annual Meeting – SWTCC*, Oklahoma University, Norman, OK (October 2019)
13. **D. P. Devore**, J. Johnston, and P. B. Armentrout, Thermodynamic Mechanism for the loss of CH<sub>3</sub>SH from Protonated Methionine. *255<sup>th</sup> American Chemical Society National Meeting and Exposition – ACS*, New Orleans, LA (March 2018)
14. **D. P. Devore**, J. Johnston, and P. B. Armentrout, Thermodynamic Properties of the loss of CH<sub>3</sub>SH from Protonated Methionine. *253<sup>rd</sup> American Chemical Society National Meeting and Exposition – ACS*, San Francisco, CA (March 2017)

## Skills

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### Programming Languages:

Python, Bash, C++

### Quantum Chemical Software:

Gaussian, Psi4, Orca, CFOUR, Multiwfn, LModeA, NCIPLOT4, QTAIM-based frameworks, DFT and *ab initio* applications

### Quantum Chemical Software Development:

CFOUR

### Molecular Viewers:

Gaussview, VMD, VESTA, Avogadro, XCrysden, JMol, Gabedit.

### High Performance Computing:

PBS, Torque, SLURM, user administration tools for local desktop and remote compute cluster environments

### Operating Systems:

macOS, Windows, Linux

### Office Software:

Microsoft Office Products, LibreOffice products, *LaTeX*

### Reference Managers:

BibTeX, Endnote, Zotero

## Certifications

### Qiskit Global Summer School 2025 – Quantum Excellence

August 2025

#### IBM

Qiskit Summer School

- Skills: Python, Qiskit, Quantum Applications, Quantum Computing

### Machine Learning with Python: Foundations

August 2023

#### LinkedIn

InLearning

- Skills: Python, Machine Learning

## Teaching Experience

### Postdoctoral Mentor for Graduate Students

- Afifa Yousaf 2024 – Current
- Duc Anh Lai 2024 – Current

### Graduate Mentor for Graduate Students

- Uvin de Alwis 2019 – 2024
- Kirk French 2019 – 2024
- Gabriele Pinto 2022
- Michael Brdecka 2022
- Puja Rijal 2023 – 2024

### Graduate Mentor for Undergraduate Students

- Danielle Paraiso 2022

### Class Instructor

#### Teaching Assistant

- General Chemistry I Lab 2019
- General Chemistry II Lab 2020, 2022

#### Teacher Substitute

- General Chemistry I Class – extensive & intensive properties, units, and sig. figs. Jan. 18, 2024

### Workshop Class Instructor

#### Mentor

- Computational Chemistry Mentor 2019, 2021, 2022, 2023
  - Introduce Computational Chemistry to Undergraduates and Professors

## Workshops and Programs Attended

1. Qiskit Global Summer School: The Past, Present and Future of Quantum Computing, IBM Quantum July 2025
2. Project Management Workshop for Graduate Students and Postdocs, Southern Methodist University April 2025
3. Searching Intelligently: Faculty Search Committee Workshop, Southern Methodist University Sept. 2024
4. GPS Workshop: Post-doctoral Positions in Canada, Baylor University April 2024
5. GPS Workshop: ATL Practical Pedagogy: Lecture for Learning, Baylor University Jan. 2024
6. Virtual Winter School on Computational Chemistry, CECAM Jan. 2024
7. Grant Writing Workshop, SWRM ACS, Oklahoma City, OK Nov. 2023
8. Teaching Philosophy Statement Workshop, Baylor University Sept. 2023
9. Open Science Grid (OSG) User School, University of Wisconsin Aug. 2023
10. 4<sup>th</sup> i-CoMSE: Fundamentals and Applications of DFT, Boise State University Jun. 2023
11. Dissertation Writing Lab, Baylor University May 2023
12. Graduate Writing Center: Diversity Statement Workshop, Baylor University April 2023
13. GPS Workshop: CV Speed Dating, Baylor University April 2023
14. GPS Workshop: Developing an Online Presence, Baylor University Mar. 2023
15. Virtual Winter School on Computational Chemistry, CECAM Feb. 2023
16. PsiCon, Atlanta, GA Dec. 2021
17. Quantum Multiscale School, Denton, Tx Oct. 2021
18. Grant Writing Workshop, Baylor University Jan. 2020
19. NASA L'SPACE Academy II - NPWEE Jan. 2019 – May 2019
20. NASA L'SPACE Academy I - Mission Concept Academy Aug. 2018 – Dec 2018

# Leadership, Affiliations, and Volunteering

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## **Memberships**

- National Postdoctoral Association (NPA), Golden Key International Honour Society (GK), American Chemical Society (ACS), Royal Society of Chemistry (RSC), National Society of High School Scholars (NSHSS).

## **Southwest Regional Meeting (SWRM) ACS**

October 2024

### **Presider**

*Computational Chemistry Section*

- Preside over the Morning Computational Chemistry session at SWRM 2024 in Waco, TX.

## **Heart of Texas Undergraduate Research Conference**

April 2024

### **Volunteer Judge**

*Computer Science, Engineering, Mathematics, Statistics, and Chemistry*

- Judge Undergraduate Computer Science, Engineering, Mathematics, Statistics, and Chemistry research projects.

## **Central Texas Science and Engineering Fair (CTSEF)**

Feb. 2022, Feb. 2023, Feb. 2024

### **Volunteer Judge**

*Materials Science, Environmental Science for Sustainable Materials, Physics and Astronomy*

- Judge research projects and presentations for middle school students in Central Texas.

## **Baylor University Undergraduate Research and Scholarly Achievement (URSA)**

April 2023

### **Volunteer Judge**

- Judge Undergraduate Chemistry and Biochemistry research projects.

## **Advanced Instrumentation Workshop, Baylor University**

2019, 2021, 2022, 2023

### **Volunteer**

- Introduced undergraduates and professors to Gaussian and computational chemistry

## **Baylor University Graduate Recruitment Weekend**

Feb. 2020, Feb. 2021, Feb. 2022, Feb. 2023

### **Volunteer**

- Introduced the Shuford Group's research to interest prospective graduate students.

### **Mentor**

Feb. 2020, Feb. 2023

- Kirk French

- Ericsson McDermott

## **Baylor University Research and Internship Day**

Oct. 2022

### **Volunteer Judge**

*Chemistry and Physics*

- Organized by Baylor Undergraduate Research in Science and Technology (BURST) Organization
- Judge Undergraduate Chemistry and Physics research projects.