

Brielle Shope

E: bmt5hv@virginia.edu

Education

Ph.D. in Chemistry, University of Virginia, Expected May 2025

Advisor: Prof. Robin T. Garrod

Thesis: "Astrochemical Modeling of High- and Low-mass Star-Forming Regions"

Committee: Prof. Ilse Cleeves (Chair), Prof. Zhi-Yun Li, Prof. Remy Indebetouw

M.S. in Physics, Ball State University, July 2020

Thesis: "Visualization of orbital free models of the kinetic energy density in solids"

Advisory Committee: Prof. Antonio Cancio (Advisor and Chair), Prof. Robert Berrington, and Prof. Mahamud Subir

B.A. in Chemistry, Taylor University, August 2018

minors in Physics and Spanish, cum laude

Advisor: Prof. D. Brandon Magers

Academic Experience Abroad

Trinity Christian College, Semester in Spain Program – Summer 2018

Seville, Spain | Completion of Spanish minor

Taylor University, Footsteps of Paul Program – January 2015

Greece and Italy | Covered core Bible credit

Research Experience

University of Virginia PhD Research

2020 – Present

- Studied the chemical mechanisms and abundances of chemical species in star-forming regions using the three-phase chemical model, MAGICAL (Model for Astrophysical Gas and Ice Chemical Kinetics and Layering)
- Produced a 2D radiation hydrodynamical and chemical model of star-formation chemistry from cloud collapse through protostellar disk formation
- Collaboration with James Webb Space Telescope and Atacama Large Millimeter Array science teams to compare model predictions to observations

Ball State University Masters Research

2018 – 2020

- Modeled kinetic energy density (KED) as functional of particle density using ABINIT density functional theory (DFT) software
- Conducted photometric observations of WASP-52b exoplanet transit via remote controlled 40-in SARA-RM telescope
- Assisted in constructing a dual dipole antenna array for the detection of radio signals from Jupiter, the Galactic Center, and the Sun

NSF REU – Princeton University and Czech Academy of Sciences 2016 – 2018

- NSF training program in which students spend a summer at Princeton and are invited to return for a subsequent year in the Czech Republic, living and working in a renovated château.
- Investigated dibenzo-18-crown-6 through use of NMR techniques, DFT calculations, and molecular dynamic simulations

Taylor University Directed Research 2016 – 2017

- Initiated a continued study at Taylor University between REU travels
- Utilized PSI4 & Gaussian computational chemistry software for conformer optimizations and binding energy calculations

Professional Development**The Astrochemistry Report, LLC, Owner and Editor-in-chief** 2023 – Present

- Founded a digital astrochemistry communications journal that aims to raise awareness on current findings for the general public

University of Virginia, Introduction to Python for PhD+ July 2021, September 2022

- Completed two-day and six-week data literacy python courses
- Skills learned: Utilization of Numpy, Pandas, and Matplotlib

Planetarium Assistant, Charles W. Brown Planetarium 2018 – 2020

- Presented live educational programs to school groups and adults
- Designed K-8th Next Generation Science Standard modules for RSA Cosmos

Publications

Shope, B.M. et al., *CORINOS III. Coupled Chemical and Radiation Hydrodynamical Modeling Comparisons of B335, L483, IRAS 15398, and Ser-emb 7 Column Densities*. In preparation to submit to ApJ.

Rocha, W.R.M. et al., *Ice inventory towards the protostar Ced 110 IRS4 observed with the James Webb Space Telescope. Results from the ERS Ice Age program*. 2025, A&A. **A288**

Shope, B.M. et al., *Coupled Chemical and Radiation Hydrodynamical Modeling of Hot Corinos: Comparison with CORINOS JWST data*. In prep to submit to A&A.

Bonfand, M. et al. *Combined hydrodynamic and gas-grain chemical modeling of hot cores. II. Two-dimensional simulations and synthetic observations (in prep)*

Shope, B.M. et al., *Interstellar Glycolaldehyde, Methyl Formate, and Acetic Acid II. Chemical Modeling of the Bimodal Abundance Pattern in NGC 6334I*. 2024, ApJ. **972** 146

Shope, B.M., Akinola, A., Cancio, A. *Visualization of orbital free models of kinetic energy density in solids*. In preparation to submit to Mol. Phys.

Yang, Y. et al., *CORINOS. I. JWST/MIRI Spectroscopy and Imaging of a Class 0 Protostar IRAS 15398-3359*. 2022, ApJL. **941** L13

Shope, B., Magers, D.B., Pelczer, I. et al. *NMR and computational studies of ammonium ion binding to dibenzo-18-crown-6*. 2023, Struct Chem. **34** 713-722

Research Presentations

Invited Colloquium

NASA Goddard	May 2023
Ball State University, Department of Physics & Astronomy	September 2022
University of California – Irvine, Density Functional Theory (DFT) group, virtual	July 2020

Oral Contributions

UVA Chemistry Department Fall Retreat	October 2024
VICO-CICO Fall 2023 Workshop	December 2023
4th Year Seminar (PhD Requirement)	December 2023
American Chemical Society Fall 2023 National Meeting	August 2023
VICO-CICO Fall 2022 Workshop	December 2022
COSPAR 44 th Scientific Assembly, Virtual	July 2022

Teaching Experience

University of Virginia Graduate Teaching Assistant	2020-2022
<i>Introduction to Radio Astronomy, General Chemistry Laboratory</i>	
Ball State University Graduate Teaching Assistant	2018-2020
<i>Introduction to Physics, Physics for Teachers, Introduction to Astronomy</i>	
Ball State Institute for Gifted in Mathematics (BIG M) Student Assistant	Summer 2019
<i>Assisted summer residential mathematics program for 5th & 6th grade students</i>	

Scientific Outreach

Dark Skies Bright Kids Star Party (September 2021, 2022) • Alexandria – Monroe Public Library Astronomy Presentation (June 2019) • Center Grove Elementary Science Day Experiments (May 2019) • Afterschool *Lift* Program Experiments (April 2018)

Scholarships & Awards

Virginia Space Grant Consortium Fellowship	2023 – Present
Chemistry Travel Award	Summer 2023
Kavli-IAU Astrochemistry VIII Symposium Travel Grant	Spring 2023
Graduate School of Arts & Sciences Research Grant	Spring 2023
PUI Visit Fund Travel Award	Fall 2022
Graduate Merit Fellowship, Ball State University	2018 – 2020
Outstanding Chemistry Research Award, Taylor University	2017
NSF REU Travel Grant, Gibbs Biothermodynamic Conference	2016
Dean Scholarship	2014 – 2018
Community Life Scholarship	2014 – 2018
Chemistry Departmental Scholarship	2014 – 2018

Leadership Experience

The Astrochemistry Report, LLC Owner & Editor-in-chief	2023 – Present
University of Virginia Astrochemistry Discussions, Co-Organizer	2023
Graduate School of Arts and Sciences Council, Social Chair	2022 – 2023
ACS Student Chapter, President	2017 – 2018
ACS Student Chapter, Event Coordinator	2016 – 2017

Professional Societies

American Chemical Society (2016 – 2018, 2022 – Present) • Sigma Pi Sigma American Institute of Physics Honors Society (2020 – Present) • Indiana Academy of Science (2020 – 2021) • American Physical Society (APS) (2019-2020)

Research Poster Presentations

“Chemical Modeling of Methyl Formate, Glycolaldehyde, and Acetic Acid Bimodal Abundance Ratios in NGC 6334I”, **Brielle Shope**, Robin T. Garrod, Kavli-IAU Astrochemistry VIII Symposium, Traverse City, MI, July 10-14, 2023.

“Chemical Modeling of Methyl Formate, Glycolaldehyde, and Acetic Acid Bimodal Abundance Ratios in NGC 6334I”, **Brielle Shope**, Robin T. Garrod, 3rd Year Poster Session (PhD Requirement), April 6, 2023

“Methyl Formate, Glycolaldehyde, and Acetic Acid Abundance Ratios in NGC 6334I”, **Brielle Shope**, Robin T. Garrod, 2022 Chemistry Department Open House & Graham Lecture, October 2022

“Methyl Formate, Glycolaldehyde, and Acetic Acid Abundance Ratios in NGC 6334I”, **Brielle Shope**, Robin T. Garrod, 2021 UVA Chemistry Department Retreat, King Family Vineyards, October 2021

“Visualization of orbital free models of kinetic energy density in solids”, **Brielle Tilson**¹, Antonio Cancio, 2020 Virtual Student Symposium at Ball State University, April 2020

“DFT Study of Ligand Binding”, **Brielle Tilson**, D. Brandon Magers, David Řeha, Babak Minofar, István Pelczer, Jannette Carey, Ball State Physics Department Colloquium, Muncie, IN, April 2019

“Ammonium Ligand Binding to dibenzo-18-crown-6 in Solvent”, **Brielle Tilson**, Brandon Magers, David Řeha, Babak Minofar, István Pelczer & Jannette Carey, Taylor University Celebration of Scholarship, Upland, IN, April 2018

“Ammonium ligand binding to dibenzo-18-crown-6 in solvent”, **B.M. Tilson**, D.B. Magers, B. Minofar, D. Řeha, J. Carey, ACS National Meeting, New Orleans, LA, March 2018

“Ammonium Ligand Binding to dibenzo-18-crown-6 via Density Functional Theory”, **Brielle Tilson**, D. Brandon Magers, David Řeha, Babak Minofar, 7th Visegrad Symposium on Structural Systems Biology, Nové Hrady, Czech Republic, June 2017

“Ammonium Ligand Binding to dibenzo-18-crown-6 via Density Functional Theory”, **Brielle Tilson**, D. Brandon Magers, Taylor University Celebration of Scholarship, Upland, IN, May 2017

¹ Last name changed from Tilson to Shope in 2021

“Ammonium Ligand Binding to dibenzo-18-crown-6 via Density Functional Theory”, **Brielle Tilson**, D. Brandon Magers, 29th Annual Butler Undergraduate Research Conference, Indianapolis, IN, April 2017

“NMR Experiments and Molecular Dynamics Simulations on a Model Host-Guest Complex”, **Brielle Tilson**, Rebecca Katz, Babak Minofar, David Řeha, Jannette Carey, 30th Annual Gibbs Biothermodynamic Conference | Carbondale, IL | September 2016