

# Curriculum Vitae: Samuel Powell

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## Education:

### **Ph.D. Program, Chemistry, August 2020-Present**

Virginia Polytechnic Institute and State University (VT), Blacksburg, Virginia

Advisor: Prof. Edward Valeev

GPA: 3.65/4.0

### **B.S., Chemistry, May 2020 (ACS certified)**

Ohio Northern University (ONU), Ada, Ohio

Minors in Physics, Applied Mathematics; member of Honors Program

GPA: 4.0/4.0

### **A.A., Business Administration, May 2016**

North Central State College (NCSC), Mansfield, Ohio

Dual enrollment through Pioneer Career and Technology Center, Shelby, Ohio

GPA: 4.0/4.0

## Programming Languages:

**Basic proficiency in:** C++, Python, bash, Javascript

**Basic familiarity with:** Java, HTML, CSS

## Research Experience:

Graduate Student Researcher. Advisor: Prof. Edward Valeev      August 2020-Present  
Department of Chemistry, VT

- Development of MPQC quantum chemistry software
- Selected Configuration Interaction

Student Researcher. Advisor: Prof. Nicholas Mayhall      June 2020-August 2020  
Department of Chemistry, VT

- Research with TPSCI (Tensor Product State Configuration Interaction) python code
- Clustering studies of polyaromatic hydrocarbon molecules

Student Researcher. Advisor: Prof. Trilisa Perrine      August 2017-May 2020  
Donald J. Bettinger Dept. of Chemistry and Biochemistry, ONU

- Computational research with QChem 4.3 and 5.2 using WebMO for modeling and interfacing. Geometry optimizations, vibrational frequencies, and transition states. Bash commands.
- August 2018-May 2020: Modeling the catalytic cycle for the polymerization of lactide and lactones using substituted anionic urea molecules as catalysts. Ground state and multi-molecular transition state searching.
- August 2017-May 2018: Modeling of polypeptides binding to BPA as molecular detectors. Modeling peptides, including hydrogen bonding to BPA.

### Research Experience, Continued:

Summer Undergraduate Research Fellowship in Theoretical Chemistry June 2019-August 2019

Chemical Theory Center, University of Minnesota. Advisor: Prof. Laura Gagliardi

- Catalytic dimerization of butene in Metal-Organic Frameworks (MOFs). Computational research with Gaussian 16. Geometry optimization, frequency calculations, energy scans.
- Active space computations with  $\text{Cu}_2\text{O}_2^{+2}$ -type model clusters using PySCF.

Student Researcher. Advisor: Prof. Jeffrey Gray January 2018-May 2019  
Donald J. Bettinger Dept. of Chemistry and Biochemistry, ONU

- Laser ablated aqueous metal colloids for surface enhanced Raman spectroscopy identification and quantitation of trace quantities of narcotics.
- Laser operation and safety. Raman spectroscopy. UV/Vis characterization of colloid solutions.

REU Student Researcher. Advisor: Prof. Xingchen Ye May 2018-August 2018  
Department of Chemistry, Indiana University

- Synthesis of copper-nickel nanoparticles for catalysts for reduction of  $\text{CO}_2$ .
- Schlenk synthesis, purification and isolation by centrifuge, drop casting for TEM and SEM imaging.
- Best REU Poster award (1 of 2) for presentation at Indiana University's Materials Science Symposium. Award included funding to present at Spring 2019 ACS National Conference.

REU Student Researcher. Advisor: Prof. Kristine Nolin May 2017-July 2017  
Department of Chemistry, University of Richmond

- Synthesis of the derivatives of Oleuropein.
- Shlenk synthesis, TLC, column purification, and analysis by  $^1\text{H}$  NMR.

### Other Experience:

Student Co-Op Worker January 2018-March 2020  
Quality Control and Research and Development Labs, American Trim, Lima, Ohio.

- Quality control testing of incoming materials and outgoing products for composition and physical properties.
- Formulation and development of new and improved products.
- Formulation mixing, color comparisons, thermal and UV cure of polymer coatings, abrasion, adhesion, and film strength testing.

### Presentations:

**Title.** Presenting Author.

**A Dual-Basis Approach to Explicitly Correlated Methods.** S. R. Powell, E. F. Valeev. Poster presentation at the WATOC 2020 World Congress, July 3-8, 2022, Vancouver, BC, Canada.

**Improved-Efficiency Selected Configuration Interaction.** S. R. Powell, E. F. Valeev. Poster presentation, ICTAS Spring Poster Session, April 22, 2022, VT, Blacksburg, VA.

**Improved-Efficiency Selected Configuration Interaction.** S. R. Powell, E. F. Valeev. Digital poster presentation, ICTAS Spring Poster Session, May 2021, VT, Blacksburg, VA.

**Presentations, Continued:**

**A Catalytic Cycle of Lactone Polymerization with Anionic Ureas: A**

**Computational Investigation.** S. R. Powell, T. M. Perrine. Virtual poster submitted to the ACS Spring 2020 virtual Expo, April 29, 2020.

<https://doi.org/10.1021/scimeetings.0c04329>.

**Localized Active Space Self-Consistent Field Treatment of  $\text{Cu}_2\text{O}_2^{2+}$ :**

**Accuracy and Affordability.** S. R. Powell, R. U. Pandharkar, L. Gagliardi.

Virtual poster submitted to the ACS Spring 2020 virtual Expo, March 30, 2020. <https://doi.org/10.1021/scimeetings.0c00418>.

**A Catalytic Cycle of Lactone Polymerization with Anionic Ureas: A**

**Computational Investigation.** S. R. Powell, T. M. Perrine. Virtual poster submitted to the Ohio Northern University Digital Student Research Symposium, opened April 24, 2020,

[https://digitalcommons.onu.edu/student\\_research\\_colloquium/2020/posters/13/](https://digitalcommons.onu.edu/student_research_colloquium/2020/posters/13/).

**A Catalytic Cycle of Lactone Polymerization with Anionic Ureas: A**

**Computational Investigation.** S. R. Powell, T. M. Perrine. Virtual poster submitted to the Bowling Green State University Undergraduate Symposium for Research and Scholarship, April 18, 2020.

<https://www.bgsu.edu/2020curs>.

**A Computational Investigation of the Catalytic Cycle of Urea Anions as**

**Catalysts for Ring-opening Polymerization of Lactones.** S. R. Powell, T. M. Perrine. Poster presentation at Gamma Sigma Epsilon Chemistry Honorary Centennial Convention, November 9, 2019, Davidson, NC.

**Applications of Symmetry and Group Theory in Chemistry.** S. R. Powell. Oral presentation at 2019 Fall Meeting of the Mathematical Association of America Ohio Section, October 25, 2019, Portsmouth, OH.

**Localized Active Space Self-Consistent Field Study of  $\text{Cu}_2\text{O}_2^{2+}$ : Bis- $\mu$ -oxo to Peroxo Isomerization.** S. R. Powell, R. U. Pandharkar, L. Gagliardi. Poster presentation at 2019 University of Minnesota Materials Research Science and Engineering Center Summer Undergraduate Research Expo, August 7, 2019, Minneapolis, MN.

**Dimerization of 1-Butene on Nickel Decorated UiO-66 MOF: Zeigler-Natta**

**Metallocycle Mechanism.** S. R. Powell, N. Khetrapal, L. Gagliardi. Oral presentation at the 2019 Chemical Theory Center Summer Research Fellowship Mini-symposium, August 6, 2019, Minneapolis, MN.

**A Computational Investigation of the Catalytic Cycle of Urea Anions as**

**Catalysts for Ring-opening Polymerization of Lactones.** S. R. Powell, T. M. Perrine. Poster presentation at Ohio Northern University's Student Research Colloquium, April 26, 2019, Ada, OH.

**Toward Rapid, Facile Detection of Trace Narcotics Using Laser-ablated**

**Metal Nanoparticles for Surface-Enhanced Raman Spectroscopy.** S. R. Powell, T. F. Dunn, J. A. Gray. Poster presentation at Ohio Northern University's Student Research Colloquium, April 26, 2019, Ada, OH.

**Seed Mediated Synthesis of Bimetallic Copper-Nickel Nanoparticles for**

**Catalysis.** S. R. Powell, S. Jeong, X. Ye. Poster presentation at The Division of Colloids and Surface Chemistry's Fundamental Research in Colloids, Surfaces, and Nanomaterials poster session at the American Chemical Society's 2019 National Meeting, March 31, 2019, Orlando, FL.

### **Presentations, Continued:**

**Seed Mediated Synthesis of Bimetallic Copper-Nickel Nanoparticles for Catalysis.** S. R. Powell, S. Jeong, X. Ye. Poster presentation at Indiana University's Symposium on Materials Research, July 23, 2018, Bloomington, IN.

**Computational Modeling of BPA Detection via BPA-Peptide Interactions.** M. R. Nieszala, S. R. Powell, T. M. Perrine. Poster presentation at the 2018 Northwest Ohio Undergraduate Symposium for Research and Scholarship, April 27, 2018, Ada, OH.

**Synthesis of Derivatives of Oleuropein.** S. R. Powell, K. Nolin. Oral presentation at 2017 TIM (Theoretically Interesting Molecules) REU Consortium End-of-Summer Meeting, July 29, 2017, Grand Valley State University, MI.

### **Meetings and Conferences Attended:**

WATOC 2020 World Congress, July 3-8, 2022, Vancouver, BC, Canada.

Centennial Convention of Gamma Sigma Epsilon Chemistry Honorary Society, November 8-10, 2019, Davidson, NC.

2019 Fall Meeting of the Mathematical Association of America Ohio Section, October 25-26, 2019, Portsmouth, OH.

2019 University of Minnesota Materials Research Science and Engineering Center Summer Undergraduate Research Expo, Minneapolis, MN, August 7, 2019.

2019 University of Minnesota Chemical Theory Center Summer Research Fellowship Mini-Symposium, Minneapolis, MN, August 6, 2019.

7th Annual OpenMolcas Developers' Workshop, Minneapolis, MN, June 12-14, 2019.

2019 Ohio Northern University Student Research Colloquium, Ada, OH, April 26, 2019.

2019 National Meeting of the American Chemical Society, Orlando, FL, March 30-April 4, 2019.

2018 Symposium on Materials Research, Indiana University, Bloomington, IN, July 23, 2018.

2018 Northwest Ohio Undergraduate Symposium for Research and Scholarship, Ohio Northern University, Ada, OH, April 27, 2018.

2017 National Organic Symposium, University of California Davis, Davis, CA, June 25-29, 2017.

### **Instruments, Software, and Techniques:**

Quantum mechanical calculations using QChem 5.2 and 4.3, Gaussian 16, and PySCF • Molecular modeling with WebMO and GaussView •  $^1\text{H}$ ,  $^{13}\text{C}$ , and 2-D NMR • IR Spectroscopy (salt plates and KBr pellet) • Raman spectroscopy (solution phase) • GC & GC-MS • HPLC • Laser safety and operation • Schlenk synthesis • Column purification • Liquid-liquid extraction and separation • Centrifuge purification • Drop-casting • Spectrometry and spectroscopy instrumentation and techniques • Viscosity determination (viscometers and Zahn cup) • Screen printing • UV and thermal cure of polymer coatings • Microsoft Office • ChemDraw • Topspin NMR software • Omnic • Spectra Suite

### Teaching Experience:

- Chemistry Tutor August 2019-April 2020
  - Tutoring for General Chemistry, Organic Chemistry, Chemistry for Engineers, Chemistry for Health Sciences, and Analytical Chemistry. Assisting in reinforcing lecture concepts and applications to homework problems.
- Physical Chemistry I & II Laboratory TA August 2019-March 2020
  - Assisted in completion of experiment and operation of instruments. Set-up of experiments and instruments. Updating of Physical Chemistry I Lab TA Guide.
- Organic Chemistry I Laboratory TA August 2018-December 2018
  - Assisted in instruction of laboratory procedures and techniques. Graded laboratory reports and student laboratory notebooks. Reinforced lecture concepts through application to laboratory exercises. Refilling reagent and solvent containers. Waste disposal.
- General Chemistry I Laboratory TA August 2017-December 2017
  - Assisted in instruction of laboratory procedures and techniques. Graded laboratory reports and student laboratory notebooks. Reinforced lecture concepts through application to laboratory exercises.
- Writing Center Tutor January 2017-December 2017
  - Helped students to revise a variety of writing assignments and to improve their writing skills. Made appointments and responded to writing questions via email.
- English Language Tutor September 2016-May 2017
  - Supported international students in learning English. Assisted with English and other classes' homework. Helped improve pronunciation, vocabulary, writing skills, and cultural fluency.

### Graduate Courses (VT):

**Chemistry:** Electronic Structure Theory, Quantum Chemistry & Spectroscopy, Chemical Thermodynamics

**Mathematics:** Numerical Linear Algebra, Numerical Analysis and Software (audit), Matrix Theory (audit)

### Courses (ONU):

**Chemistry:** Inorganic Chemistry 2, Advanced Physical Chemistry, Physical Organic Chemistry, Physical Chemistry 1 & 2 (with labs), Inorganic Chemistry (with lab), Polymer Chemistry, Analytical Chemistry (with lab), Organic Chemistry 1 & 2 (with labs), General Chemistry 1 & 2 (with labs)

**Mathematics:** Differential Equations, Calculus 1, 2, and 3 (multivariate), Discrete Mathematics, Linear Algebra (independent study)

**Physics:** Mathematical Methods, Modern Physics, Nuclear Physics, Physics 1 and 2 (with labs), Quantum Mechanics (audit)

**Programming:** Programming 1 (C++), Programming 2 (Java)

### **Awards and Honors:**

- Virginia Tech Institute for Critical Technology and Applied Science (ICTAS) Doctoral Scholar Fellowship. One of ten offered across the university each year. Awarded to outstanding incoming graduate students based on demonstrated leadership, outstanding academic accomplishment, and potential for success in their field.
- The American Institute of Chemists Award in Chemistry, 2020. Awarded to outstanding graduating students in chemistry or biochemistry (One chemistry award, one biochemistry) based on demonstrated leadership ability, character, scholastic achievement, and advancement potential in the chemical professions.
- Phi Lambda Upsilon Honorary Chemical Society, 2020. Awarded to graduating seniors with minimum 30 semester hours of chemistry, minimum 3.5/4.0 GPA, and that rank in top 20% of seniors in department or institution.
- De-Lap Holcomb Scholarship, 2020. Awarded by the Gamma Sigma Epsilon Chemistry Honor Society Pi Gamma chapter in recognition of leadership and service to the society as well as personal scholarship and character.
- Chemistry Departmental Honors, 2020. Awarded to one top-achieving senior in both chemistry and biochemistry majors.
- Undergraduate Award in Physical Chemistry, 2020. Awarded by ONU through the ACS Division of Physical Chemistry to recognize an undergraduate student who has demonstrated excellence in physical chemistry and related fields based on research, coursework, and/or dedication. The student should be committed to a career in chemistry, broadly defined.
- John F. Conn Award, Gamma Sigma Epsilon award for student research presentation at 2019 Centennial Convention.
- The Barry Goldwater Scholarship, 2019. National scholarship recognizing Sophomore and Junior undergraduate students in the natural sciences, engineering, and mathematics who have a strong commitment to a career in research, an intellectual intensity in their field, and a potential to contribute to research in their field.
- Roy W. Sonntag Award, 2019. Awarded by the Gamma Sigma Epsilon Chemistry Honor Society (Pi Gamma) in recognition of outstanding service to the society.
- ONU Dean's List, all 8 semesters (FA 2018-SP 2020). Maintain a minimum 3.5 GPA with full-time enrollment and no incomplete grades.
- The Sophia Felker Award, 2019. Awarded to a junior in the Division of Mathematics and Natural Sciences. The candidate must have completed between 80 and 107 semester hours at Ohio Northern University and have the highest GPA.
- The Outstanding Student in Organic Chemistry Award, 2019. Awarded by the ONU Department of Chemistry and Biochemistry to recognize a chemistry or biochemistry major for outstanding performance in sophomore organic chemistry.
- Linda Schultz Scheuerman Scholarship, 2019: Awarded to a senior chemistry major in honor of Byron L. Hawbecker. Recognizes outstanding academic performance and promise of growth in a scientific or medical profession.
- Chemistry Alumni Scholarship, 2019. Presented to a major(s) in the Chemistry Department who are chosen each year by the department faculty.
- Junior Class Scholar, 2018-2019. Awarded to students with the highest GPAs in the Department of Chemistry and Biochemistry.
- Junior Class Honors, 2018-2019. Highest GPA in the College of Arts and Sciences.



### **Awards and Honors, continued:**

- Undergraduate Award in Analytical Chemistry, 2017-2018 Year. Awarded by the American Chemical Society Division of Analytical Chemistry. Awarded to a student who has demonstrated excellence in analytical chemistry, based on any combination of research, interest, coursework, or motivation and dedication.
- Chemistry Alumni Scholarship, 2018. Presented to a major(s) in the Chemistry Department who are chosen each year by the department faculty.
- Sophomore Class Scholar, 2017-2018. Awarded to students with the highest GPAs in the Department of Chemistry and Biochemistry.
- Sophomore Class Honors, 2016-2017. Highest GPA in the College of Arts and Sciences.
- The Chemical Rubber Company Freshman Chemistry Achievement Award, 2016-2017 Year. Presented each year to an outstanding chemistry or biochemistry major who has demonstrated outstanding achievement in General Chemistry.
- Freshman Class Scholar, 2016-2017. Awarded to students with the highest GPAs in the Department of Chemistry and Biochemistry.
- Freshman Class Honors, 2016-2017. Highest GPA in the College of Arts and Sciences.

### **Activities and Involvement**

- Member, Heterodox Academy, August 2022-Present
- Member, Free Software Foundation, Spring 2022-Present
- Volunteer A/V Assistant, Northstar Church, Blacksburg, VA, Fall 2021-Present
  - Managing lighting, projection, or livestream direction, 2 times / month
  - Lighting, projection, and audio services for events held at the church
- Youth Group Volunteer, Northstar Church, Blacksburg, VA, June 2021-Present
  - Lead small discussion groups
  - Help organize, coordinate, and staff group activities
- Gamma Sigma Epsilon Chemistry Honorary Society, Pi Gamma Ch. (ONU), Apr. 2018-May 2020
  - Several outreach and community events each year
  - Grand Alchemist (President), April 2019-April 2020
    - Chapter voting delegate at Centennial Convention, Nov. 8-10, 2019
    - Planning and leading meetings
    - Coordinating outreach events
- Student Members of the American Chemical Society (ONU), Sept. 2016-May 2020
  - Semiweekly meetings, spring and fall picnics, various community events.
  - President, April 2019-April 2020
    - Planning and leading meetings
    - Coordinating outreach events
  - Treasurer, April 2017-April 2019
    - Budgetary and checking account management
    - Issuing reimbursements
- Sigma Pi Sigma Physics Honorary Society (ONU), Inducted April 2020
- Student Advisory Board (SAB), March 2017-May 2019
  - Representative of the Department of Chemistry and Biochemistry
    - Monthly meetings, various outreach events
  - Member of Administrative Assistants' Day Committee
    - Preparation and distribution of gifts and notes

**Activities and Involvement, Continued:**

- Mortar Board (Aurora Chapter), Active member February 2017-March 2019
  - Regular meetings
  - Service activities (Reindeer Run, ONU L.O.V.E. Day)
  - New member selection and tapping