Samuel R. Powell

Curriculum Vitae

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Education

Ph.D., Chemistry **2020-December 2025 (Anticipated)**
Virginia Polytechnic Institute and State University (VT), Blacksburg, VA GPA: 3.65/4.0
Advisor: Prof. Edward Valeev

B.S., Chemistry (ACS certified) **2020**
Ohio Northern University (ONU), Ada, OH GPA: 4.0/4.0
Minors in Physics, Applied Mathematics; member of Honors Program

A.A., Business Administration **2016**
North Central State College (NCSC), Mansfield, OH GPA: 4.0/4.0
Dual enrollment through Pioneer Career and Technology Center, Shelby, OH

Programming Languages

Basic proficiency in: C++, Python, bash
Basic familiarity with: Javascript, Java, HTML, CSS, SQL

Research Experience

VT, Department of Chemistry August 2020-Present
Ph. D. Research Assistant, Advisor: Prof. Edward Valeev
- Implementation of correlation methods in MPQC4 software.
- Assisted in implementing Selected Configuration Interaction, open-shell F12 explicit correlation, and dual-basis Coupled Cluster methods.

VT, Department of Chemistry June 2020-August 2020
Summer Research Assistant. Advisor: Prof. Nicholas Mayhall
- Studied optimal clustering of Polyaromatic Hydrocarbons with TPSCI (Tensor Product State Configuration Interaction) python code.

ONU, Department of Chemistry and Biochemistry August 2017-May 2020
Student Researcher. Advisor: Prof. Trilisa Perrine
- Computed single-point energies, binding and reaction energies, and searched for transition states using QChem with WebMO for modeling and interfacing. Geometry optimizations, vibrational frequencies, and transition states. Bash commands.
- August 2018-May 2020: Modeled the catalytic cycle for the polymerization of lactide and lactones using substituted anionic urea molecules as catalysts. Optimized multi-molecule ground state and searched for transition states.
- August 2017-May 2018: Computed and compared polypeptide-BPA binding pairs to evaluate as molecular detectors. Bound complex optimization and energies.

University of Minnesota, Chemical Theory Center June 2019-August 2019
Summer Undergraduate Research Fellow. Advisor: Prof. Laura Gagliardi
- Optimized geometries and transition states and computed vibrational frequencies, studying catalytic dimerization of butene in Metal-Organic Frameworks (MOFs).
- Performed active space (LASSCF) computations with $Cu_2O_2^{+2}$ model clusters using PySCF to optimize fragmentation of the active space.

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Research Experience, continued

ONU, Department of Chemistry and Biochemistry — January 2018-May 2019
Student Researcher. Advisor: Prof. Jeffrey Gray

- Synthesized aqueous metal colloids by laser ablation; helped develop method for identification and quantification of trace quantities of narcotics by surface enhanced Raman spectroscopy using the metal colloids.
- Performed Raman spectroscopy studies. Characterized colloid solutions using UV/Vis spectroscopy. Laser operation and safety.

Indiana University Department of Chemistry — May 2018-August 2018
Research Experience for Undergraduates (REU) Student. Advisor: Prof. Xingchen Ye

- Synthesized bimetallic copper-nickel nanoparticles for catalytic reduction of CO_2.
- Schlenk synthesis, purification and isolation by centrifuge, drop casting for electron microscopy studies.
- Best REU Poster award (1 of 2) for presentation at Indiana University's Materials Science Symposium.

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

- Synthesized derivatives of Oleuropein for future oncology testing.
- Shlenk synthesis, reaction monitoring by Thin Layer Chromatograpy, column purification, and analysis by ^{1}H NMR.

Other Experience

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

- 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

The Importance of Diffuse Atomic Orbitals in Correlated Calculations. **S. R. Powell**, E. F. Valeev. Poster presentation, ICTAS Spring Poster Session, March 31, 2022, VT, Blacksburg, VA.

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, CA.

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.

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 $Cu_2O_2^{2+}$: 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/.

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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 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 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 $Cu_2O_2^{2+}$: Bis-μ-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.

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, Nov. 8-10, 2019, Davidson, NC.
2019 Fall Meeting of the Mathematical Association of America Ohio Section, Oct. 25-26, 2019, Portsmouth, OH.
2019 University of Minnesota Materials Research Science and Engineering Center Summer Undergraduate Research Expo, Minneapolis, MN, Aug. 7, 2019.
2019 University of Minnesota Chemical Theory Center Summer Research Fellowship Mini-Symposium, Minneapolis, MN, Aug. 6, 2019.
7th Annual OpenMolcas Developers' Workshop, Minneapolis, MN, Jun. 12-14, 2019.
2019 Ohio Northern University Student Research Colloquium, Ada, OH, Apr. 26, 2019.
2019 National Meeting of the American Chemical Society, Orlando, FL, Mar. 30-Apr. 4, 2019.
2018 Symposium on Materials Research, Indiana University, Bloomington, IN, July 23, 2018.

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Meetings and Conferences Attended

2018 Northwest Ohio Undergraduate Symposium for Research and Scholarship, Ohio Northern University, Ada, OH, Apr. 27, 2018.
2017 National Organic Symposium, University of California Davis, Davis, CA, Jun. 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}H, ^{13}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, ONU — August 2019-April 2020
  - Tutoring for General Chemistry, Organic Chemistry, Chemistry for Engineers, Chemistry for Health Sciences, and Analytical Chemistry. Re-explained and reinforced lecture concepts and assisted with application to homework.
- Physical Chemistry I & II Laboratory TA, ONU — August 2019-March 2020
  - Guided students in completion of experiments and safe operation of instruments. Set-up experiments and instruments. Updated of Physical Chemistry I Lab TA Guide.
- Organic Chemistry I Laboratory TA, ONU — 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 reagents and solvents. Waste disposal.
- General Chemistry I Laboratory TA, ONU — August 2017-December 2017
  - Assisted in instruction of laboratory procedures and techniques. Graded laboratory reports and student laboratory notebooks. Set-up laboratory equipment and reagents
- Writing Center Tutor, ONU — January 2017-December 2017
  - Helped students to revise a variety of writing projects and to improve their writing skills. Made appointments and responded to questions via email.
- English Language Tutor, ONU — September 2016-May 2017
  - Supported international students in learning English. Assisted with English and other classes' homework. Guided exercises to 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)

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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 is 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.
- 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.

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Awards and Honors, continued

- 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 — Jun. 2021-Present
- Lead small discussion groups
- Help organize, coordinate, and staff group activities

Gamma Sigma Epsilon Chemistry Honorary, Pi Gamma Chapter (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, November 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 Apr. 2020
College of Arts and Sciences Student Advisory Board — Mar. 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
Mortar Board (Aurora Chapter) — Feb. 2017-Mar. 2019
- Service activities (Reindeer Run, ONU L.O.V.E. Day)
- New member selection and tapping