



Karl Pierce

Research Assistant

297 New Kent Rd
Blacksburg, VA 24060

(440)724-1498

LinkedIn
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@ karl.m.pierce@gmail.com

About Me

Results-driven, adaptable scientist with experience in both laboratory and theoretical research. Thrives in independent and group settings with ambitions to collaborate and improve interdisciplinary research.

Skills

Electronic Structure Theory

C++

Parallel Programming

Mathematics

Quantum Mechanics

LaTeX

Python

SLURM

Independent Research★
Communication★ Experimental
Design★

Objective

Passionate about the application of novel mathematics to problems in physics, chemistry and computational modeling.

Education

2016- PhD Theoretical Chemistry Blacksburg, VA
Virginia Tech

2012-2016 B.S. Chemical Physics Houston, TX
Rice University

Publications

Approximation of Tensor Networks : Application to Grid-Free Tensor Factorization of the Coulomb Interaction
Pierce, K.; Rishi, V.; Valeev, E. F. Robust . 2021, 17 (4), 2217-2230.
<https://doi.org/10.1021/acs.jctc.0c01310>.

Professional Experience

2016- Graduate Research Assistant Virginia Tech

PhD supervised under Dr. Edward Valeev
Studying electronic structure theory, higher-order tensor algebra, and advanced data compression and algorithmic optimization schemes. Developed production level tools in the software packages **BTAS**, a higher-order tensor algebra library, **TiledArray**, a scalable tensor framework for high-performance tensor arithmetic, and **MPQC**, a platform for ab initio electronic structure methods simulation.

2015-2016 Research Assistant Rice University

Supervised under Dr. Gustavo Scuseria
Completed a senior chemistry research project using the Gaussian software package. Using the Generalized Hartree-Fock (GHF) method, I benchmarked the disassociation behavior of diatomic transition metal complexes with the goal of demonstrating the utility of GHF over more expensive electronic structure theory approaches.

2014-2015 Research Assistant Rice University

Supervised under Dr. Emilia Morosan
Created novel metallic single and multi-crystals with exotic magnetic properties utilizing techniques such as liquid flux growth, vapor deposition and arc melting. Studied the structure of such metallic crystals using small angle X-Ray Diffractometry. Studied ternary phase diagrams and the underlying physics of superconductivity. Loaded samples onto and probed magnetic properties using a superconducting quantum interference device (SQUID) magnetometer. Mentored younger students on laboratory safety and laboratory methods.

2013 Visiting Scientist University of Akron

Supervised under Dr. Shing-Chung "Josh" Wong
Studied polymer development techniques, designed mechanical testing for biomedical devices based on IEEE and FDA testing requirements and built testing apparatus and benchmarked approved industry devices.

2012 Research Assistant University of Akron

8 weeks part time under Dr. Shing-Chung "Josh" Wong
Lead design project to study polymer microfibers produced using a dry-jet wet spinning technique. Built a device to create polymers using the dry-jet wet spinning technique.



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2011

Research Assistant

NASA Glenn

Supervised under Dennis Stocker

Assisted in NASA's advanced combustion via microgravity (ACME) experiments. Generated Volumetric measurements for ignition fuel required on the international space station.

Posters and Presentations

2021

Colloquium at Vienna University of Technology

Seminar

Utility of the Canonical Polyadic Decomposition and Robust Tensor Network Approximations

2019

Virginia Tech Department of Chemistry Internal Seminar

Seminar

Reduced Cost Electronic Structure Theory via the Canonical Polyadic Decomposition

2019

American Chemical Society National Meeting

Poster

Towards Reduced Scaling Higher Order Coupled Cluster Methods via Tensor Decomposition.

2018

Modern Wavefunction Methods in Electronic Structure Theory

Poster

Reducing Complexity and Cost of High-Order Coupled-Cluster Method via Canonical Polyadic Decomposition of Hamiltonian

2018

Penn Conference in Theoretical Chemistry and Electronic Structure Workshop

Poster

Reducing Complexity and Cost of High-Order Coupled-Cluster Method via Canonical Polyadic Decomposition of Hamiltonian.

2018

Virginia Tech Department of Chemistry Preliminary Exam

Seminar

Reduced Scaling of Accurate Electronic Structure Methods using Tensor Decompositions

2017

Southeast Theoretical Chemistry Association Meeting

Poster

Toward Efficient Canonical Product Decomposition in TiledArray Framework

Summer School

2018

MolSSI Summer School and Workshop Parallel Computing in Molecular Sciences

Berkely, CA

Participated in a three-day lecture series where researchers in academia and from Berkeley national lab. Discussed computational parallelism and communication on homogenous and heterogeneous CPU/GPU computer systems.

2018

Modern Wavefunction Methods in Electronic Structure Theory

Gelsenkirchen, Germany

Attended a week-long summer school at the Max-Planck institute in Germany directed towards Ph.D. students and postdocs with aims to teach advanced topics in the field of ab initio electronic structure theory, reduced scaling algorithms, and software implementations on modern hardware.

Teaching Experience

Fall 2016

General Chemistry Lab

Spring 2017

Physical Chemistry Lab

Fall 2017

General Chemistry Lab

Spring 2018

Physical Chemistry: Thermodynamics

Professional Affiliations

The American Chemical Society



Karl Pierce

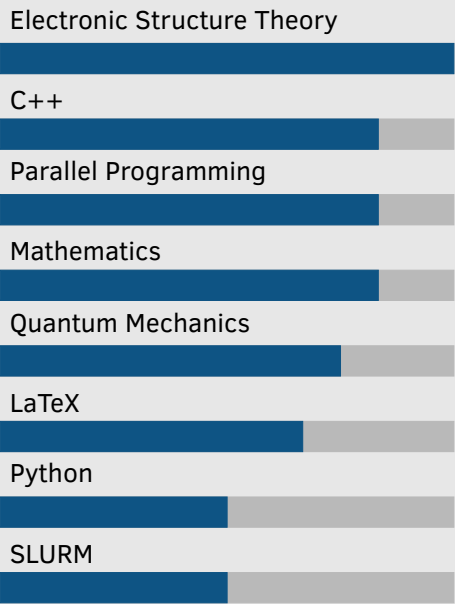
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Skills



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Relevant Coursework

- Electronic Structure Theory
- Group Theory
- Matrix Theory
- Abstract Algebra
- Partial Differential Equations
- Quantum Chemistry
- Quantum Physics 1 and 2
- Advanced Inorganic Chemistry

Extra-curricular Activities

- | | | |
|-------|---|------------------------|
| 2017- | Pole Vault Coach | Blacksburg High School |
| | Designed individualized athletic training and programming as a head coach for youth athletes. | |

Awards

- | | | |
|-----------|---|-----------------|
| 2021 | Graduate School Doctoral Assistanship Award
Award for excellence in research in leadership | Virginia Tech |
| 2012,2014 | C-USA Commissioner's Honor Roll | Rice University |