

Karl Pierce

Research Assistant



297 New Kent Rd Blacksburg, VA 24060



(440)724-1498



LinkedIn GitHub



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 of

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

Education

2016-PhD Theoretical Chemistry

Virginia Tech

2012-2016 B.S. Chemical Physics

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

Blacksburg, VA

Houston, TX

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.

Research Assistant 2015-2016

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 indus-

try 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

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 Colloquim 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

NASA Glenn

Attended a week-long summer school at the Max-Plank 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



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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 Virginia Tech

Award for excellence in research in leadership

2012,2014 C-USA Commissioner's Honor Roll Rice University