# Karl Pierce, PhD

Postdoctoral Research Scientist


(440)724-1498

LinkedIn
GitHub

kpierce@flatironinstitute.org


## 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
- Tensor algebra
- C++
- Distributed Programming
- Mathematics
- Quantum Mechanics
- LaTeX
- Julia
- CMake

Independent Research⋆ Communication⋆ Experimental Design⋆

## Objective

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

## Education

**2016-2021** PhD Theoretical Chemistry — Blacksburg, VA
*Virginia Tech*

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

## Publications

**2022** Efficient construction of canonical polyadic approximations of tensor networks
Pierce, K.; Valeev, E. 2023, 19 (1), 71–81

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

**2021** Breaking the curse of dimensionality in electronic structure methods: towards optimal utilization of the canonical polyadic decomposition
Pierce, K. (2021) [Doctoral dissertation, Virginia Tech, Blacksburg]. http://hdl.handle.net/10919/107964

## Professional Experience

**Sept 2022-** Flatiron Software Research Fellow — The Flatiron Institute
Postdoctoral researcher at the Center for Computational Quantum Physics. Working with faculty researchers on developing and advancing theories in computational quantum physic and developing distributed functionality and maintaining the ITensors software package.

**2022** Research Scientist — Virginia Tech
Developing efficient electronic structure methods for large molecules and condensed phase. Building parallel implementations of these methods using the standard C++ language for standard and heterogeneous massively parallel computer systems. In this role I plan and conduct research projects requiring independent evaluation, selection, and substantial adaptation or modification of standard techniques and procedures. Additionally, I devise new approaches to problems, plan, conduct and coordinate all phases of scientific research. Furthermore, I mentor graduate students and postdocs.

**2016-2021** Graduate Research Assistant — Virginia Tech
PhD supervised under Dr. Edward Valeev
Studied 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.

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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.

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

2023 SIAM Conference on Computational Science and Engineering — Seminar
Introduction to the ITensor Software Library for Tensor Network Calculations

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*

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## Summer School

**2022** — Argonne Training Program on Extreme-scale Computing — Chicago, IL
Participated in an intensive two week summer school learning modern key skills, approaches, and about tools to design, implement and execute scientific applications on state of the art, leadership-class computing systems of today and the future.

**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-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.

## Certificates

**2022** — NVIDIA Certificate in Scaling CUDA C++ Applications to Multiple Nodes

**2022** — NVIDIA Certificate in Fundamentals of Accelerated Computing with CUDA C/C++

## Teaching Experience

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|---|---|
| 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

## Extra-curricular Activities

**2017-2022** — Pole Vault Coach — Blacksburg High School
Designed individualized athletic training and programming as a head coach for youth athletes.

**2012-2016** — Division 1 Athlete — Rice University
Participated in Division 1 athletics at Rice University as a pole vaulter on the track and field team.

## 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