



Luke Bertels

Eugene P. Wigner Fellow

Where and when did you earn your PhD?

I earned my PhD at University of California–Berkeley in the group of Martin Head-Gordon in 2020.

What was the subject of your dissertation?

My dissertation focused on developing and applying theoretical approaches to studying the electronic structure theory of small molecules to gain insight into chemical reaction paths.

What was your dissertation's major contribution to your field?

My dissertation contributed to the understanding of silicon-carbide formation in the interstellar medium, benchmarking reactive force fields for hydrogen combustion, and developing new zeroth-order representations for correlated wavefunction calculations.

Who is your ORNL mentor and which group and division are you working in?

My ORNL mentor is Ryan Bennink, Quantum Computational Science group leader in the Computational Sciences and Engineering Division. I am in Ryan's group. The goal of the Quantum Computational Science group is to develop the potential of quantum computing to accelerate discovery in domain sciences.

What will your fellowship research focus on?

My fellowship research will focus on combining the novel technologies of artificial intelligence and quantum computing. Specifically, I will develop classical and quantum machine learning approaches using adaptive neural networks to study strongly correlated chemical systems.

What is your project's expected contribution to your field?

The work of my fellowship will provide new, efficient methods to extend the reach of both classical and quantum simulation towards the study of strongly correlated molecules. This work will also inspire further developments combining artificial intelligence and quantum computing to study big problems in domain sciences.

What are your research interests?

My research interests include developing a suite of computational approaches to accurately and efficiently study the quantum many-body problem, specifically the electronic structure theory of molecules and materials. I'm especially excited about the promise of quantum algorithms for physical simulation and the use of artificial intelligence-inspired approaches using neural networks.

What led you to science and your specific discipline?

My mother was a research scientist and would bring my brothers and I to her research lab beginning from a young age. This instilled in me a lifelong love of science. My chemistry, physics, and math teachers in high school focused my interests towards the physical sciences, and early undergraduate research experience cemented my interests in theoretical chemistry.

What did you do before coming to ORNL?

Before coming to ORNL I was a postdoctoral researcher in the group of Nicholas Mayhall at Virginia Tech studying quantum algorithms for chemical applications.

Could you share an interesting fact or two about yourself?

I am both an avid hiker and an amateur cook. I'm also the eldest of four brothers.

What nonscience topic or activity is important to you and why?

My faith is very important to me as a parallel way of understanding the world and a way to answer the questions that science cannot. I enjoy serving in worship services at my church and serving the community through volunteering opportunities.

