

DISTINGUISHED
STAFF FELLOWS
AT ORNL



Victor Fung

Eugene P. Wigner Fellow

Where and when did you earn your PhD?

I received my PhD in chemistry from the University of California–Riverside in 2019.

What was the subject of your dissertation?

My doctoral research focused on using first-principles computational chemistry to study alkane conversion on heterogeneous catalysis.

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

My work provided mechanistic insights and chemical descriptors that can be used for discovering and designing better catalysts to break C–H bonds.

Who is your ORNL mentor and where are you working on campus?

My mentor is Bobby Sumpter, Theory and Computation section head in the Center for Nanophase Materials Sciences (CNMS). I am working in the Nanomaterials Theory Institute at CNMS.

What will your fellowship research focus on?

My fellowship research involves obtaining fundamental physicochemical descriptors of chemical properties, conducting high-throughput materials screening, and developing machine learning methods for materials discovery and design. Specific topics of my research include methane capture and conversion, heterogeneous C–N functionalization, and prediction of nanomaterial structure and properties.

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

My work will help accelerate the discovery and design of new functional materials to solve important issues facing our society today.

What are your research interests?

My research interests lie at the intersection of probing physical and chemical phenomena such as chemical bonding and developing computational tools that guide scientists to the most promising materials for physical study.

What led you to science and your specific discipline?

For as long as I can remember, my father would take me to bookstores to buy books, and when I was young, I was really interested in astronomy, so we bought small telescopes to look at the moon and stars. My love of science started with astronomy and biology, but I found my way to chemistry in college. I was not familiar with the field of computational chemistry until I got a job in a lab as an undergraduate research assistant. I had such an enjoyable experience that I knew I wanted to focus my career on using computational tools to understand the world and advance scientific progress.

What did you do before coming to ORNL?

I interned as an Office of Science Graduate Student Research fellow in ORNL's Chemical Sciences Division during my PhD. After that fellowship, I became a Eugene P. Wigner Fellow in ORNL's Distinguished Staff Fellowship program.

Could you share an interesting fact or two about yourself?

I like cooking because it draws on hands-on chemistry and the experimental process—something I don't usually encounter as a theoretical chemist. I find the process of trying to develop recipes and understanding the role of each ingredient for a particular dish to be very enjoyable.

I also like to think about how computational science might impact the development of solutions for global warming. Computational chemistry will show us better ways to remove greenhouse gases from the atmosphere or convert them and will help us find more sustainable and renewable sources of energy. I am also excited by how open science techniques—citizen science and pooling computer resources—will move society toward a more sustainable future.

