HIGHLANDS IN CHEMISTRY SEMINAR SERIES

NICK MAYHALL

VIRGINIA TECH

"Using quantum computers to solve quantum chemistry problems"

Quantum mechanical simulations of molecules provides a sub-atomic understanding of chemical reactions and properties. Due to the exponential scaling of the simulation of many-body systems, these simulations are obtained only as approximations to the electronic Schrödinger equation. Although, in principle one can increase the sophistication of an approximation arbitrarily until a desired accuracy is reached, more sophisticated calculations rapidly become intractable for even the largest supercomputers. Quantum computers provide a promising route to bypass these limitations in molecular simulation. Our efforts in this space are divided into two channels: 1) modeling systems with potential for use as quantum platforms and 2) improving quantum algorithms for molecular simulation. In this talk, I will discuss some of the basic ideas underlying the use of quantum computation for the purpose of molecular simulation and describe some of the recent work from our group.

SEPTEMBER 4, 2020

2:30PM

ZOOM

FACULTY HOST:
ALAN ESKER

COLLEGE OF SCIENCE
CHEMISTRY
VIRGINIA TECH