UNIVERSITY OF LOUISVILLE

COLLEGE OF ARTS & SCIENCES

Department of Chemistry

Brown and Williamson Series
September 16, 2022
@4:00 pm
CB LL16

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Adventures in the Spatial Extremes of Electronic Structure Theory

ABSTRACT:

The DeYonker laboratory uses quantum chemistry to study two very different types of problems. First, we are developing software to automate, simplify, standardize, and validate the construction of atomic-level enzyme models. Enzyme simulations are notoriously challenging as their large size prevents modeling the whole enzyme with highly accurate but computationally expensive quantum mechanical (QM) methods. Determining which biological sub-units necessarily should be included in the QM-model remains ambiguous, and current practices for model construction typically suffer from human bias and unclear methodology. Our software, RINRUS (Residue Interaction Network ResidUe Selector), uses protein topology to construct residue interaction networks for the prediction of appropriate QM-only models of enzyme active sites. By embedding reproducibility into an enzyme model construction workflow, mechanistic hypotheses can, for the first time, be rigorously tested on a large scale with tens to tens of thousands of different protein models. The second major research thread is to increase our understanding of small inorganic molecules in the gas phase interstellar medium. While the electronic structure of organic molecules implicated in pre-biotic chemistry and origin-of-life reactions are a substantial focus of the astrochemistry community, the interactions of these molecules with metals that hold a crucial role in biology (such as Group IA/IIA atoms, Mn, Fe, and Zn) have scarcely been investigated. We explore the precise electronic and rovibrational spectroscopy of diatomics, triatomics, and tetraatomics with novel metal-carbon bonds.

BIO:

Nathan J. DeYonker is from Troy, Michigan. He received a B.Sc. in chemistry from the University of Michigan-Ann Arbor and did his Ph.D. work at the University of Georgia under the direction of Henry F. Schaefer III. After graduating in 2005, he worked with Professors Angela K. Wilson and Thomas R. Cundari at the University of North Texas. From 2009 to 2015 he was a research scientist at the University of Memphis, working with Charles Edwin Webster, before being rehired into a tenure-track position. He is now an Associate Professor of Chemistry at the University of Memphis. Research in the DeYonker laboratory at the University of Memphis is generally focused on two fronts of computational chemistry. We use quantum chemistry to model spectroscopy of molecules that are proposed to exist in space but have not yet been isolated or characterized on Earth. Studying these new molecules improves our knowledge of stellar formation and proto-biological reactions. On a rather different molecular size scale, Dr. DeYonker was awarded a prestigious NSF Early Faculty CAREER award through the Infrastructure Innovation for Biological Research program to develop an automated, rules-based software toolkit for the computational study of enzymes at the atomic-level using reproducible and rationally created models. When not working, reading, or writing, he enjoys tinkering with modular synthesizers and hanging out with his daughter Patti and his wife April.