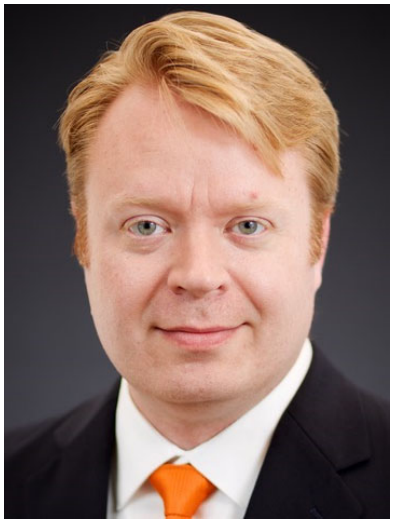
Friday 10 Sep 2021

# ESSENTIALS IN WATER'S WORKINGS SEEN AT SMALL AND LARGE SCALES



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Aqueous environments are central to chemical and biomolecular systems, and the interactions with water govern many of the processes in these system. These environments and the unique properties of water principally build out of its strong and dynamic network of hydrogen bonding interactions. In this virtual seminar, we will discuss distinct ways that we can incorporate hydrogen bonding interactions in both microscopically sized computational and macroscopically sized physical models of water. For the computational models, we will explore how we can treat hydrogen bonding with orientational spherical harmonic functions, this enabling modeling of aqueous environments in a manner upwards of 100 times faster than standard approaches. For the physical models, we will show how to build interactive 3D printed structures that capture how the coupling of geometry and strong interactions in water gives rise to its diversity in microscopic structure.

**6:30-7:00 pm Social time** *Join early to meet Oklahoma chemistry students and professionals from around the state.*

**7:00-8:00 pm Presentation**
**The meeting will be virtual via zoom.**

*This meeting has a waiting room. Please wait for the host to let you in.*

ZOOM LINK Meeting ID: **929 7070 6931** Passcode: **143917**

zoom meeting link

**Christopher Fennell Biographical Sketch**

Dr. Fennell is an Associate Professor in the Chemistry Department at Oklahoma State University that specializes in Theoretical and Computational Chemistry. He received his Ph.D. in Chemistry from the University of Notre Dame, did postdoctoral research in Computational Biophysics at the University of California San Francisco, and was a Junior Research Fellow in the Laufer Center for Physical and Quantitative Biology at Stony Brook University before coming to OSU in 2013. His primary research work is focused on developing computational models for diversity in molecular materials, exploring aqueous solvation processes, and investigating biomolecular dynamics and association. He has developed several chemistry outreach efforts that span from iPhone application development to a science outreach program at OSU called Molecular World Building. Dr. Fennell is a recent recipient of the National Science Foundation CAREER award and has been extensively involved in expanding research computing access in Oklahoma and at High Performance Computing resource sites around the USA.