

## ABSTRACT

Title: **Chemical Innovation via Computational-Experimental Synergy with Applications in Catalysis**

Presenter: Dr. Travis Dudding, PhD

Research in the Dudding group focuses on the synergistic use of experimental and computational chemistries as an innovative strategy for developing or improving chemical processes. Our group is actively developing new catalysts and catalytic systems, ligands, and molecules with unique physical properties for a range of applications. In this talk recent highlights of our work will be presented, showcasing how this combined experimental and computational approach to tackling chemical problems is allowing for innovation. Of specific focus will be aspects of our successful programs in hydrogen bond and strong Brønsted acid catalysis as well as cyclopropenium-based chemistries providing for the discovery and advancement of broad-spectrum technologies. In terms of the leitmotif of cyclopropenium ions, our group is actively developing new catalysts and catalytic systems, ligands, and molecules with unique (photo)physical properties for a range of applications. This includes the advancement of proton sponges, Au(I)-catalysis leveraged upon cyclopropenium ions and small molecules for task-specific bio-, material-, and medical-driven applications. In addition, in light of the prominent role of fluorine in biology, medicine, and materials, briefly covered in this talk will be recent developments from my group for the chemo- and regioselective fluorination of diverse substrates.

