

# Inorganic Chemistry Seminar

## Prof. Diaconescu Group



### Ruxi Dai

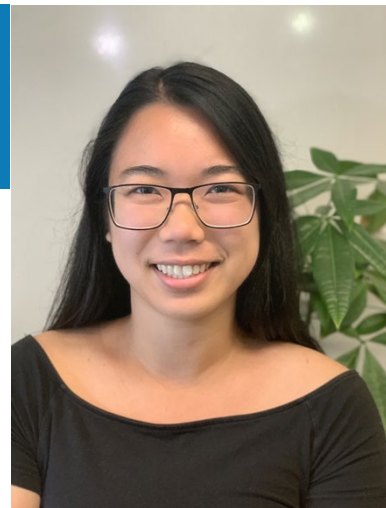
“Redox switchable catalysts for the preparation of biodegradable copolymers with novel properties”

**Abstract:** Biodegradable polymers are a potential solution for the worldwide "white pollution" issue. Lactones and epoxides are promising monomers to construct such polymers, and, when copolymerized together, allow for tuning of copolymer properties. A zirconium catalyst, bearing a ferrocene unit at the ligand backbone as the redox center, was used to perform the copolymerization of lactones and epoxides in a redox switchable manner. Multiblock copolymers can be prepared using this method; their characterization shows that the self-assembly and mechanical properties can be modified as the number of blocks is changed.

### Amy Lai

“Predicting redox-switchable reactivity for the ring opening polymerization of lactones and epoxides”

**Abstract:** Redox-switchable catalysis is an atom economical method, where multiple catalytically active species can be generated from a single precursor. Our group has employed several redox-active ferrocene-supported metal complexes to ring open polymerize cyclic esters, ethers, and carbonates and have found unique reactivities between its neutral and oxidized states. As there are many more variations of metal complexes to investigate, here we explore rational methods to prioritize synthesis of new compounds and predict their orthogonal monomer selectivity. First, we used principle component analysis to chemically map 64 variations of the metal complex, based on their subtle electronic and steric properties. This chemical map was used as an experimental guide to diversify and evenly sample the chemical space. In particular, an aluminum compound, (salfen)Al(OiPr) (salfen = ,1'-di(2,4-bis-*tert*-butyl-salicylimino)ferrocene) was suggested because of its distinct ligand framework and was promptly investigated. Now with a total of 11 redox-switchable ferrocene-based metal complexes in our experimental database, we surveyed several machine learning algorithms to predict the orthogonal reactivity for caprolactone and found that an accuracy up to 75% can be achieved by using the random forest classifier. This exemplifies that catalyst design of intricate organometallic complexes and reactivity prediction is feasible through *in silico* characterization.



Wednesday, May 19<sup>th</sup> 2021