# Chemistry and Biochemistry

# Spring 2022 seminar

Please join us for the following seminar!

## Using Computational Chemistry and Biomimetic Models to Investigate Catalysis at Enzyme Active Sites

**Speaker:**

**Professor**

**Ben Gherman**

**When:**

**Friday, April 15th**
**1:00 pm**

**Where:**

**bit.ly/chicochem**

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Metalloenzymes catalyze a wide range of biologically interesting reactions. Direct computational modeling of these enzymes can be challenging due to, for example, the sheer size of the protein system and the variety of interactions occurring within the enzyme. Biomimetic models of the active site (synthetic ligand systems with a highly similar metal coordination to that found in the enzyme) provide, however, an alternative means of studying the enzyme chemistry. They have the advantage of not only being smaller and more computationally tractable, but also of being readily chemically modifiable. The latter in particular allows for specific effects on the reaction chemistry to be studied, for instance that from altering the electronic characteristics of the active site ligands which coordinate to the metal center. Combined with computational chemistry methods such as density functional theory (DFT), biomimetic models allow for a remarkably effective exploration of metalloenzyme chemistry. Two case studies of metalloenzymes to which this methodology has been applied will be presented – (a) peptide deformylase (PDF), which is involved in protein biosynthesis in eubacteria and is therefore an antibacterial target and (b) non-heme iron halogenases, which use high-valent iron-oxo intermediates to catalyze halogenation of C-H bonds in the biosynthesis of natural products.