“Fluorinated Alkoxide Complexes for Unusual Reactivity and Electronic Structure”

The increase in global energy demands, coupled with growing environmental concerns, necessitates the development of viable technologies to store solar energy. Towards this end, my group is focused on developing efficient catalysts that convert CO$_2$ to CO, methanol or formic acid. My talk will first describe our mechanistic studies on known CO$_2$ hydrogenation catalysts, whereby mechanistic insight is gleaned through thermochemical studies and allows for tuning the product selectivity. We also have uncovered a unique mechanism for CO$_2$ hydrogenation, whereby CO$_2$ must first bind to the ligand before subsequent reduction occurs. I will then discuss how we have used the same thermochemical approach to study the mechanism of electrocatalytic CO$_2$ reduction in a combined carbon capture & reduction system. Finally, I will present a novel ligand scaffold that, when put on Co, allows for both the hydrogenation of CO$_2$ to formate and the electrochemical reduction of CO$_2$ to formate; this is unique in that no H$_2$ is produced electrocatalytically. The collective work underscores the importance of the effective hydricity as a parameter of interest and in using thermochemical parameters to rationalize and uncover alternative mechanisms. The studies presented are contextualized in developing an understanding of how to rationally design energy-efficient CO$_2$ reduction catalysts.