“Molecular Catalysts for Water Oxidation and Oxygen Reduction”

Water oxidation (WO) to molecular dioxygen and its inverse reaction oxygen reduction (OR) to water, are the two key reactions involved in water splitting and hydrogen fuel cells respectively. The mastering of both reactions WO and OR catalyzed by Transition Complexes (TMC) is an essential requirement for their potential applications in widespread energy applications. In both cases the O-O bond formation and breakage step is crucial and needs to be fully understood as well as all the previous activation pathways. Additionally the oxidation of water to molecular oxygen is also a reaction of interest from a biological perspective since it is the main reaction occurring at the Oxygen Evolving Center of Photosystem II (OEC-PSII). A few Ru and Co complexes will be presented that are capable of catalyzing the water oxidation and the oxygen reduction reactions. Additionally their performance and mechanistic pathways will be disclosed based on electrochemical, kinetics, oxygen labeling experiments and DFT calculations.