

# **SMALL MOLECULE ACTIVATION AT TRANSITION METAL CENTERS: STRUCTURE-FUNCTION CORRELATIONS**

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Small molecule activation constitutes one of the main frontiers of inorganic and organometallic chemistry, with much effort directed towards the development of new processes for the selective and sustainable transformation of abundant small molecules such as dioxygen (O<sub>2</sub>), water (H<sub>2</sub>O), hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>) or protons (H<sup>+</sup>) into high-value chemical feedstocks and energy resources. Because nature mostly uses metal ions to activate these relatively inert molecules and modulate their reactivity, much inspiration for the field has come from bioinorganic chemistry. This talk will focus on some of the recent highlights from our group on homogeneously catalyzed bioinspired activation of small molecules, as well as stoichiometric reactions that further our understanding towards such ends. It will cover many aspects of small molecule activation including: organometallic chemistry, spectroscopy, synthesis, and detailed mechanistic studies involving trapping of reactive intermediates. The demonstrated examples will help to emphasize the continuous effort of our group in uncovering the structure-reactivity relationships of biomimetic model complexes, which may allow vital insights into the prerequisites necessary for the design of efficient catalysts for the selective functionalization of unactivated C–H bonds, O<sub>2</sub>/H<sub>2</sub>O/H<sub>2</sub>O<sub>2</sub> activations, or H<sup>+</sup> reductions by using cheap and readily available first-row transition metals under ambient conditions.