Strategies for Hydrogen Transformation: From Classical Catalysis to Radical Chemistry

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Abstract

The talk will be divided into two main topics that reflect the research focus of Cristina Yebra Garcia's group.

Topic 1: Hydrogen Storage. The first part will cover the latest findings on iridium-catalyzed formic acid dehydrogenation. It highlights the use of [CpIr(κ²-NN)(Cl)][OTf] complexes—featuring κ²-NN pyridyl-triazole ligands—as catalysts under neat conditions (i.e., in the absence of an external solvent). These systems exhibit excellent performance, achieving turnover frequencies (TOF_max) of up to 10,703 h^{-1}, and selectively produce a 1:1 mixture of hydrogen and carbon dioxide, with no detectable carbon monoxide. Kinetic studies and ^{1}H NMR spectroscopy confirm that the active species is [CpIr(CO)H_2].

Topic 2: Palladium(I)-NHC Metalloradicals – Reactivity Towards Small Molecules. This section will focus on the synthesis, characterization, and reactivity of mononuclear Pd(I)-NHC metalloradicals. The speaker will discuss their reactions with O_2, which result in the formation of radical superoxide species, and with H_2, which proceed via a radical pathway to yield Pd(II) monohydride complexes.