## Metal-ligand cooperativity and Second-sphere effects in Catalysis : 3 stories based on a joint Experimental and Computational study

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Organometallic catalysis has undergone significant evolution, starting with the exploration of transition metals and progressing towards ligand modifications to tune the properties of the metal center by playing on electronic and steric effects. As the field progressed, attention shifted towards the design of the second-sphere of coordination. For instance, tailoring the nearby ligands to equal the reactivity of noble metals with more abundant alternative, or induce challenging transformation with an improve control on the selectivity is a strategy that has met several successes. In this talk, I will share three stories in which a joint experimental and computational study has highlighted the unique role of the ligand in the Oxygen atom transfer reaction with an iron dipyrrin complex, the CO<sub>2</sub> to CO reduction with iron porphyrins, and selective C-N bond formation with dirhodium-nitrene catalysts.

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