Computational methods are increasingly applied to investigate reaction pathways. However, the proposed mechanisms are not always sufficiently validated. I will discuss the state-of-the-art in DFT modelling of metal-catalyzed reactions and show approaches to validate computationally proposed pathways,\cite{1, 2} Examples from two areas of organometallic catalysis are included: 1) **Hydrogenation**. In particular, recent insights into Co-catalyzed hydrogenation are discussed, where a mechanism proposed by us explains the experimental substrate preferences,\cite{2} and 2) **CO$_2$ incorporation**. C-CO$_2$ bond formations with late transition metal complexes (e.g. Rh, Ni, Pd, and Cu) are discussed,\cite{3, 5} alongside a novel base-mediated reaction developed in our laboratory.\cite{4} Based on our computational work, we propose trends as to when metal-CO$_2$ interactions should be expected during C-CO$_2$ bond formation.

![Figure 1](image)

**Figure 1. To bind or not to bind:** we present trends as to when metal-CO$_2$ interactions should be expected for C-CO$_2$ bond formation.\cite{3-5}


