Non-noble Metals and Catalysis: Computational Insights

Jeremy N. Harvey

Department of Chemistry, KU Leuven, Celestijnenlaan 200F, Leuven, B-3001 Belgium
jeremy.harvey@kuleuven.be

In my talk I will present insights from computation into the mechanism of catalysis by non-noble metal catalysts. I will also discuss the challenges involved in theoretical modelling of catalysis more generally. One major challenge in non-noble metal catalysis is the wide diversity of ligation and redox states that may be present under catalytic conditions. I will start by presenting the relatively 'simple' case of hydroformylation catalysis by cobalt carbonyl complexes [1,2], in which well-defined molecular catalyst species seem to be present and account well for observed behaviour. Then I will switch to discussing the more complicated case of catalysis by iron and nickel complexes [3,4,5] in the presence of solid zinc reductant.

[1] *Computational Kinetics of Cobalt-Catalyzed Alkene Hydroformylation*, L. E. Rush, P. G. Pringle and J. N. Harvey, *Angew. Chem., Int. Ed.*, **2014**, *53*, 8672 – 8676.
[2] *Computational Modelling of Selectivity in Cobalt-Catalyzed Propene Hydroformylation*, E. N. Szlapa and J. N. Harvey, *Chem. Eur. J.*, **2018**, *24*, 17096 - 17104.
[3] *Z-Selective Olefin Synthesis via Iron-Catalyzed Reductive Coupling of Alkyl Halides with Terminal Arylalkynes,* C. W. Cheung, F. E. Zhurkin and X. Hu, *J. Am. Chem. Soc.* **2015**, *137*, 4932-4935.
[4] *Amide Synthesis via Nickel-Catalysed Reductive Aminocarbonylation of Aryl Halides with Nitroarenes*, C. W. Cheung, M. L. Ploeger, and X. Hu, *Chem. Sci.* **2018**, *9*, 655-659.
[5] A. Daru, X. Hu and J. N. Harvey, to be published.