Molecular understanding and controlled functionalization of surfaces towards single-site catalysts and beyond

Christophe Copéret[a,*]

[a] *Department of Chemistry and Applied Biosciences – ETH Zürich, Zürich, CH-8093, Switzerland*
**Corresponding author: ccoperet@ethz.ch*

Abstract: The rational design and development of catalysts require structure – reactivity relationship approach, hence the need for strategies to obtain well-defined surface sites and their detailed characterization. Here, we first discuss the method to control and understand the chemistry at the surface of materials towards the development of heterogeneous catalysts based on single-site or supported nanoparticles and show how this approach can bring about information about industrial catalysts.[1] In this context, we will show how Dynamic Nuclear Polarization Surface Enhanced NMR spectroscopy can provide insightful information about material active site structures, which are not available by other characterization techniques.

Keywords: Single-site catalysts, Supported Nanoparticles, NMR.

References:

[1] a) Surface Organometallic and Coordination Chemistry towards Single-Site Heterogeneous Catalysts: Strategies, Methods, Structures, and Activities. C. Copéret, A. Comas-Vives, M. P. Conley, D. Estes, A. Fedorov, V. Mougel, H. Nagae, F. Núñez-Zarur, P. A. Zhizhko Chem. Rev. **2016**, *16*, 323-421. b) Bridging the Gap between Industrial and Well-Defined Supported Catalysts. C. Copéret, F. Allouche, K. W. Chan, M. P. Conley, M. F. Delley, A. Fedorov, I. B. Moroz, V. Mougel, M. Pucino, K. Searles, K. Yamamoto, P. A. Zhizhko, *Angew. Chem. Int. Ed.* **2017**, DOI: 10.1002/ange.201702387.