Molecular Understanding and Controlled Functionalization of Surfaces Towards Single-Site Catalysts and Beyond

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The rational design and development of catalysts require structure – reactivity relationship approach, hence the need for strategies and methodologies to obtain tailored surface sites with molecular-level characterization.

Here, we first discuss the method to control and understand the chemistry at the surface of materials towards the development of well-defined – so-called single-site – heterogeneous catalysts and show how this approach can bring about information about industrial catalysts. 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. We will also show that single-sites can be used to tailor supported nanoparticles with controlled interfaces and catalytic properties and illustrate this approach towards the development of efficient catalysts for the conversion of hydrocarbons and CO_2.

[1] 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.* **2018**, *57*, 6398-644 – DOI: 10.1002/anie.201702387

[2] 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.