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Catalysis by design: well-defined single-site heterogeneous catalysts

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Heterogeneous catalysis a field important industrially and scientifically is increasingly seeking and refining strategies to render it more predictable. The main issue is due to the nature and the population of catalytically active sites. Their number is generally low to very low, their acid strengths or redox properties are not homogeneous, and the material may display related yet inactive sites on the same material. In many heterogeneous catalysts, the discovery of a structure-activity relationship is at best challenging. One possible solution is to generate single-site catalysts in which most, if not all, of the sites are structurally identical. Within this context and using the right tools, the catalyst structure can be designed and well-defined, to reach a molecular understanding. It is then feasible to understand the structure activity relationship and to develop predictable heterogeneous catalysis. Single-site well-defined heterogeneous catalysts can be prepared using concepts and tools of surface organometallic chemistry (SOMC). This approach operates by reacting organometallic compounds with surfaces of highly divided oxides (or of metal nanoparticles). This strategy has a solid track record to reveal structure-activity relationship to the extent that it is becoming now quite predictable. Almost all elements of the periodical table have been grafted on surfaces of oxides (from simple oxides such as silica or alumina to more sophisticated materials regarding composition or porosity). Considering catalytic hydrocarbon transformations, heterogeneous catalysis outcome may now be predicted based on existing mechanistic proposition and the rules of molecular chemistry (organometallic, organic) associated with some concepts of surface sciences. A thorough characterization of the grafted metal centers must be carried out using tools spanning from molecular organometallic or surface chemistry. By selection of the metal, its ligand set, and the support taken as X, L ligands in the Green formalism, the catalyst can be designed and generated by grafting the organometallic precursor containing the functional group suitable to target a given transformation (surface organometallic fragments (SOMF)). The choice of these SOMF is based on the elementary steps known in molecular chemistry applied to the desired reaction. The coordination sphere necessary for any catalytic reaction involving paraffins, olefins and alkynes also can thus be predicted. Only their most complete understanding can allow development of catalytic reactions with the highest possible selectivity, activity and lifetime. This lecture will examine the results of SOMC for hydrocarbon transformations on oxide surfaces bearing metals of group 4-6. The silica-supported catalysts are exhibiting remarkable performances for Ziegler-Natta polymerization and depolymerization, low temperature hydrogenolysis of alkanes and waxes, metathesis of alkanes and cycloalkanes, olefins metathesis, transformation of propane to aromatics and related reactions. In the case of reactions involving molecules that do not contain carbon (water-gas shift, NH₃ synthesis, oxidations etc.) this single site approach is also valid.

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