TOWARDS NEW CONCEPTS IN THE DESIGN OF HETEROGENEOUS CATALYSTS

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ABSTRACT

In its classical definition, a catalyst is a substance that increases the rate of a reaction without being consumed considerably. The active site in the catalyst and its interaction with reactant(s), transition state(s), and product(s) define whether the desired reaction will proceed with a higher rate and selectivity at relatively mild conditions compared to the noncatalysed reaction. It is not surprising that the design of such active sites is one of the main targets of catalyst engineering. However, the nature of the active site is not always clear. In the case of homogeneous catalysts and enzymes, they can be easily identified, however, the description of active sites in the case of heterogeneous catalysts may become more controversial. A typical example is a metal nanoparticle, where the active sites – the metal atoms – may be located at the steps, kinks, terraces, etc., each one of these sites bearing different properties. In this sense, one could easily argue that homogeneous catalysis is a much more powerful approach towards the design of better catalysts given the rather high level of predictability, design, and engineering of these systems, especially when compared to heterogeneous catalysts. Yet, issues related not only to the obvious challenge of recyclability but also to deactivation and the use of low concentrations of homogenous catalysts have placed heterogeneous catalysts at the forefront of chemical industry.

The problems presented by both homogeneous and heterogeneous catalysts have triggered intense research over the last few decades in the quest for alternative systems that, ideally, would bridge the gap between these two subdisciplines of catalysis by implementing truly single catalytic sites at the surface of a solid catalyst. The challenge at hand is certainly not trivial: progress in this direction requires the discovery of new materials able to offer sufficient design possibilities as to allow for an exquisite control in the implementation of catalytic functions. This colloquium will focus on, and stress the advantages of, three classes of materials that have the potential to become the ideal homo-hetero bridge: zeolites, metal-organic frameworks (MOFs) and porous organic frameworks (POFs).

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