

Editorial

# Editorial: Special Issue on “Advanced Strategies for Catalyst Design”

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The word catalyst comes from the Greek *καταλύσις*, which means dissolution and was introduced in 1836 by the Swedish Berzelius. All chemists know that the availability of an efficient catalyst is extremely valuable to enhance the reaction rate and optimize the regio- and stereoselectivity. The discovery of novel catalysts is based on different approaches, like simulation of different catalyzed reactions, trial and error procedures, screening of existing libraries of catalysts, and last but not least, good chemical intuition and knowledge. More often, a combination of these ways is employed, and serendipity plays an important role too. Anyway, the highly ambitious goal is the control of chemical reactions using accurately designed catalysts (i.e., molecules or materials that not only are efficient but also may have additional important requirements, like low cost and low environmental impact).

To quantify the importance of rationally tailored catalysts, a search in the Scopus database was performed, which returned 43,897 entries associated with the string “Catalyst AND Design” in the period from 1928 to 2021; among these, 20,838 entries belong to the period 2016–2021, clearly suggesting that the interest and the effort in catalyst design have been rapidly increasing in the last 5 years (Figure 1a). When strategy is included in the search by typing the complete string “Catalyst AND Design AND Strategy,” 4087 entries are found in the period 2016–2021 (Figure 1b). Importantly, in both graphs in Figure 1, the number of works is increasing year after year, indicating the interest of the scientific community in the rational and guided search for novel catalytic systems. In this scenario, computational methods represent a valid support for different reasons. First, in the last 2 decades, accurate quantum chemistry protocols have provided mechanistic details of elementary and complex reactions, thus providing quantitative energetic and kinetic insight. Taking advantage of the impressive silicon technology development, chemical reactions involving complex systems can nowadays be investigated using (super)computers. Finally, machine-assisted screening of large datasets of chemical compounds is considered a common good practice to explore *in silico* the potential activity or extract those features that seem relevant to design a functional molecule. All these observations let us foresee that, in the very near future, chemists will be able to design efficient catalysts and then prepare them in the lab, minimizing synthetic effort and costs.

In this Special Issue, 11 contributions dealing with different problems of catalysis are gathered, and the main topics are summarized here.

Lei Ma et al. [1] have reported on a strategy to protect palladium catalysts by sulfur species and have applied it to the catalytic oxidation of methane.

The problem of asymmetric olefin epoxidation has been investigated and thoroughly discussed by Zou et al. [2], who employed salenMn immobilized on graphene oxide as catalyst.



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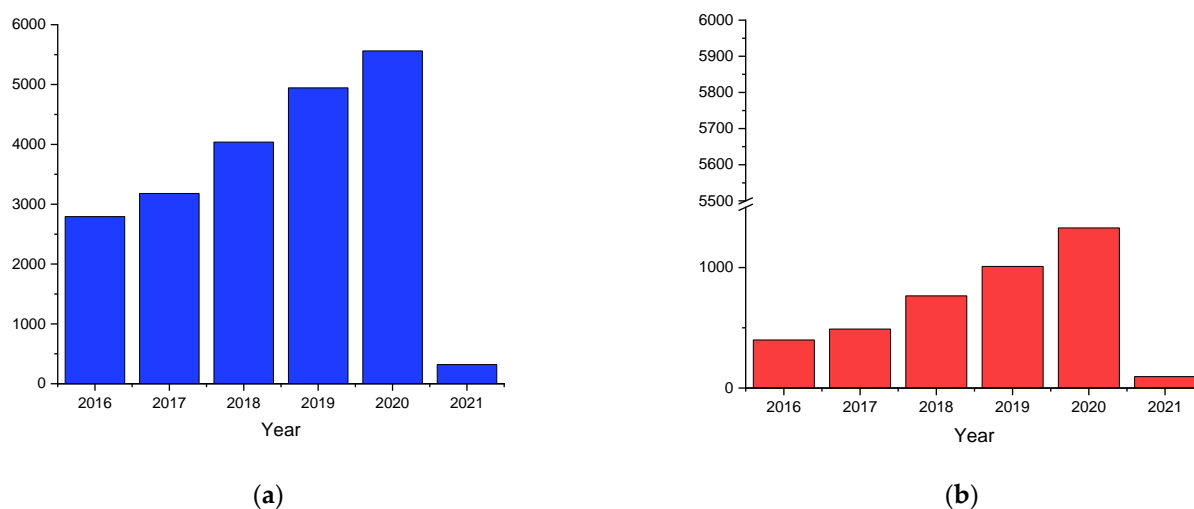
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**Figure 1.** Results of a search in the Scopus database limited to the period 2016–2021: (a) search string “Catalyst AND Design”; (b) Search string “Catalyst AND Design AND Strategy.” Last access to the database on 22 December 2020.

Kobayashi and Sunada have described the synthesis of a four coordinated Fe(II) digermyl complex, inspired by the silicon analog, which is used as catalyst in the dehydrogenation of ammonia borane [3].

Contreras et al. have reported on improvements in the reduction of NO<sub>x</sub> using C<sub>3</sub>H<sub>8</sub> and H<sub>2</sub> by adding Pt to the Ag/Al<sub>2</sub>O<sub>3</sub>-WO<sub>x</sub> catalyst [4].

The work by He et al. [5] deals with the removal of elementary mercury in the presence of SO<sub>2</sub> using Mn/Ti nanorods, showing how the coating with TiO<sub>2</sub> protects Mn by the unwanted deactivation by SO<sub>2</sub>.

The review article by Zhang et al. [6] focuses on acetylene hydrochlorination catalyzed by activated carbon-supported HgCl<sub>2</sub> and the challenge of finding a nontoxic catalyst. Particularly, noble and non-noble metal and nonmetal catalysts are considered alternative candidates, and advantages and issues are critically discussed.

The paper by Zan et al. have reported on their research of substitutes for fossil fuel-based petroleum products [7]. They have presented the synthesis of 22-carbon tricarboxylic acid and its ester via the Diels-Alder reaction starting from PUFAs and their esters and fumaric acid and fumarate, respectively. Iodine has been used as catalyst.

Carlucci et al. have been working on strategies to produce biofuels using as source waste cooking oil, and they succeeded in optimizing the reaction conditions (acid catalysis) to reach high yields, up to 99% [8].

Dini and et al. have carried out a study on the disposal of chemical waste from wastewaters, proposing the technique of contact glow discharge electrolysis (CGDE) with a promising low-cost implication [9].

Finally, Kim et al. and Orian et al. have contributed with two theoretical studies [10,11]. In the former, the asymmetric cyanation of olefins with ethyl cyanofornate catalyzed by Ti(IV) has been explored, while in the latter, the acetylene [2+2+2] cycloaddition to benzene catalyzed by Rh/Cr indenyl fragments has been investigated. The accurate description of the reaction mechanisms combined with the activation strain model nicely demonstrates that times are mature to perform a rigorous and quantitative catalyst design in silico.

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