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Editorial

Computational Chemistry and Catalysis: Prediction and Design

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The combination of computational chemistry and catalysis is an insightful approach that can be utilized to predict and design a catalyst, its function and the outcome of the catalytic chemical reaction that this catalyst activates in terms of activity, selectivity and applications. In recent decades, the progress achieved within the applied theoretical framework concerning density functional theory (DFT) and solvation models has substantially permitted the explanation of the activity and selectivity of the catalyst function and of the related reaction mechanisms, either at the molecular or bulk levels, under homogeneous and heterogeneous conditions by using transition metal, organo-, photoredox and surface catalysis.

This Special Issue of *Catalysts* contains eight research articles that deal with different aspects of combining experimental and computational methods and are aimed at predicting chemical reactions and explaining and rationalizing the catalytic activity of catalytically active species or materials. The interested reader will find a new strategy that was developed by Pan et al. for the design of highly efficient metal catalysts, such as Pt(111), for selective nitroarene hydrogenation via the modulation of the d-band center position using DFT-type calculations. Their experimental work validates their prediction [1]. Ferrante et al. provide a contribution that covers the performance of a Pd/graphene system for hydrogen storage by using DFT-based molecular dynamic simulations to study the fate of a hydrogen molecule shot at different kinetic energies toward a hydrogenated palladium cluster, which is anchored on the vacant site of a defective graphene sheet [2]. Theoretical guidance to design catalysts for propane aromatization based on experimental findings and DFT calculations is also provided by Fan et al. in his study [3]. A further step in the modeling and prediction of a catalyst and its catalytic activity is carried out by Ren et al., who successfully use data mining technology for the modeling and screening of methanation catalysts [4]. Bizon et al.'s contribution revolves around the use of mathematical and numerical simulation to evaluate the potential of extending the multifunctionality of catalytic heterogenous chemical reactors down to the single-pellet level [5].

Since the production of biofuels under catalytic conditions has become one of the most key sustainable technologies, catalyst design and prediction of the chemical process are highly required. In this respect, Ramli et al. address the catalytic production of biodiesel fuel through the conversion of *Phoenix dactylifera* L. seed oil to fatty acid methyl ester via a transesterification reaction using Ce-Zr/Al-MCM-41 mono- and bimetallic catalysts. The reaction conditions were optimized by using a response surface methodology based on the central composite design [6].

The final two contributions of this Special Issue are by Ben El Ayouchia and Domingo et al. They combine an experimental study and molecular electron density theory to investigate, on one hand, the click of 1,2,3-triazole derivatives by a Ag(I)-catalyzed azide–alkyne cycloaddition (AgAAC) reaction as well as its mechanistic pathway, and, on the other hand, the use of copper(I)-catalyzed azide–alkyne cycloaddition (CuAAC) to accomplish the regioselective formation of the 1,2,3-triazole function by using well-defined discrete copper catalysts [7,8].

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