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Computational Chemistry on Predicting Catalytic Reactions

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Deadline for manuscript submissions:
30 October 2024

Message from the Guest Editors

It is our pleasure to invite you to participate in a Special Issue dedicated to the discovery of the fundamental events in catalytic processes: elementary steps, their energy requirements and the driving forces allowing for otherwise unlikely chemical transformations towards often precious reaction products. This part of chemistry lies in the interface between synthesis, kinetics and simulation, and the fact that it deals with chemical transformations at the microscopic level implies that it is a challenging area, where a mechanistic confirmation is a rare event. In this scenario, the contribution of sensibly designed computational simulations may be key to help understand the evidence gathered from experimental probes, like reaction rate determination, kinetic isotopic effects, solvent effects, labeling experiments, etc.

We hope that this Special Issue will be an excellent venue to gather research advances in the field of catalytic reaction mechanisms in which the above synergistic communion between simulation and experiment is portrayed.