

Editorial

Computational Catalysis—Trends and Outlook

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Computational catalysis has been one of the most dynamic research fields over the last decade, and it now represents a critical tool for the analysis of chemical mechanisms and active sites. The growth in this area has been accelerated by steady improvements in computational speed and a maturation of robust software tools, providing opportunities for more realistic models and the application of powerful analysis techniques. As the field of computational catalysis continues to expand, the gap between a model and reality is beginning to narrow. More effort is now focused on capturing secondary effects (structural defects, solvation environment, deactivation events, thermal distortions, etc.), extending the time scales accessible, and incorporating machine learning and descriptor-based methods for catalyst screening.

This Special Issue highlights the diverse impact that computational catalysis investigations can provide, ranging from key reaction systems in the energy sector to complex biological processes [1]. In addition, the rapid evolution of the underlying theoretical methods, such as the unified reaction valley approach highlighted in this Special Issue, provides powerful tools for the broader community.

One of the most critical (and often the most difficult aspect) of any computational catalysis study is the identification of the transition state complex within a reaction mechanism. This can be difficult or impossible to identify experimentally, but several different computational catalysis tools have been recently developed to help provide this information. The unified reaction valley approach (URVA) highlighted here is one such methods [2]. It follows the potential energy surface of a reaction path with a specific focus on the curvature of the reaction path. The normal vibrational modes identified along the path, as well as a decomposition of the path curvature into internal coordinates, provides rich information about the chemical changes taking place (e.g., bond breaking events). The information about a single transition state or a single reaction mechanism is the first step towards developing an understanding of a catalytic system. Other tools are now being developed for combining individual reaction events into a comprehensive reaction network. Park et al. [3] provide a nice overview of the powerful role that microkinetic modeling can play, especially by connecting the dominant reaction pathways to experimental systems (as a function of temperature and pressure), as well as a specific example with the catalytic synthesis of methanol and dimethyl ether.

These computational catalysis tools and others pave the way for complex catalytic systems to be studied on modern computer systems. Of particular recent interest have been metal pincer complexes, which have the potential to provide highly active and selective catalytic sites, and they may provide an economical alternative to traditional precious metal catalysts (Pt, Ru, etc.). These pincer complexes may play a future role in hydrogen production and storage [4] and the hydrogenation of alkenes or carbonyl sites [5,6]. In terms of a hydrogen economy, the development of economic fuel cell designs still presents a challenging bottleneck, and the catalyst cost has been a key focus for many years. Cui et al. have used density-functional theory to examine Pt₃M alloys involving 3d transition metals on oxygen-doped graphene for catalyzing the oxygen reduction reaction (ORR). They are able to identify key sites and intermediates in the ORR mechanism, and they find that Pt₃Ni is a superior catalyst due to its ability to lower the adsorption energies of O and



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OH involved in the mechanism. In other energy-related and environmental applications, titanium dioxide (TiO₂) has played a very important role. Despite its long technological importance, there are still many unanswered questions about its atomistic structure and the impact on performance in photocatalysis, solar cells, etc. To shed more light on the existing controversy, Elahifard et al. [7] have provided a rigorous investigation into the dispersion of oxygen-vacancies in both the bulk phase and at the surfaces of anatase and rutile. This can provide critical information for pushing the performance envelope of many TiO₂-based applications.

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