Special Issue

15th Anniversary of *Catalysts*: The Development and Future of Computational Catalysis

Message from the Guest Editors

Computational catalysis sits at the intersection of chemistry and physics, harnessing computational power to understand and design catalysts and catalytic processes at the atomic level. Fifteen years ago, this area of physical chemistry was largely unexplored, but today it represents an indispensable component of modern catalysis, driving progress in both academic research and industrial innovation. This success is primarily due to the efforts of a vibrant community of researchers who are driving a shift from trial-and-error experiments to computer-guided design of a new generation of catalysts primed to face global challenges. In particular, recent methodological advances in quantum chemistry as well as in classical simulations—often coupled with machine learning—have empowered researchers to explore reaction mechanisms with unprecedented precision. Computational catalysis has emerged as a robust tool for understanding the interplay between molecular structure and chemical reactivity. The behavior of complex catalytic systems can be rationalized, ranging from transition metal complexes to enzymes and their mimetics, as well as heterogeneous catalytic surfaces.

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