

# Computational Catalysis—Trends and Outlook

Christoffer Heath Turner 

Department of Chemical and Biological Engineering, The University of Alabama, Box 870203, Tuscaloosa, AL 35487, USA; hturner@eng.ua.edu; Tel.: +1-205-348-1733

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 Pt<sub>3</sub>M 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 Pt<sub>3</sub>Ni is a superior catalyst due to its ability to lower the adsorption energies of O and



**Citation:** Turner, C.H. Computational Catalysis—Trends and Outlook. *Catalysts* **2021**, *11*, 479. <https://doi.org/10.3390/catal11040479>

Received: 13 March 2021

Accepted: 6 April 2021

Published: 8 April 2021

**Publisher's Note:** MDPI stays neutral with regard to jurisdictional claims in published maps and institutional affiliations.



**Copyright:** © 2021 by the author. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (<https://creativecommons.org/licenses/by/4.0/>).

OH involved in the mechanism. In other energy-related and environmental applications, titanium dioxide (TiO<sub>2</sub>) 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 TiO<sub>2</sub>-based applications.

The impact of computational catalysis is continuing to grow at a very rapid pace, so I would like to thank all of the authors for their timely contributions and support of this Special Issue. I am also grateful to Keith Hohn, Editor-in-Chief of *Catalysts*, and the *Catalysts* Editorial Office for their continued support and encouragement.

**Funding:** This research received no external funding.

**Conflicts of Interest:** The author declares no conflict of interest.

## References

1. Salter, E.A.; Wierzbicki, A.; Honkanen, R.E. Quantum-Based Modeling of Dephosphorylation in the Catalytic Site of Serine/Threonine Protein Phosphatase-5 (PPP5C). *Catalysts* **2020**, *10*, 674. [[CrossRef](#)]
2. Kraka, E.; Zou, W.; Tao, Y.; Freindorf, M. Exploring the Mechanism of Catalysis with the Unified Reaction Valley Approach (URVA)—A Review. *Catalysts* **2020**, *10*, 691. [[CrossRef](#)]
3. Park, J.; Kim, H.S.; Lee, W.B.; Park, M.-J. Trends and Outlook of Computational Chemistry and Microkinetic Modeling for Catalytic Synthesis of Methanol and DME. *Catalysts* **2020**, *10*, 655. [[CrossRef](#)]
4. Li, Y.; Tsang, C.-W.; Chan, E.M.H.; Wong, E.Y.C.; Ho, D.C.K.; Lu, X.-Y.; Liang, C. Sustainable Option for Hydrogen Production: Mechanistic Study of the Interaction between Cobalt Pincer Complexes and Ammonia Borane. *Catalysts* **2020**, *10*, 723. [[CrossRef](#)]
5. Zuo, Z.; Yang, X. Mechanistic Insights into Selective Hydrogenation of C=C Bonds Catalyzed by CCC Cobalt Pincer Complexes: A DFT Study. *Catalysts* **2021**, *11*, 168. [[CrossRef](#)]
6. Liu, X.; Qiu, B.; Yang, X. Bioinspired Design and Computational Prediction of SCS Nickel Pincer Complexes for Hydrogenation of Carbon Dioxide. *Catalysts* **2020**, *10*, 319. [[CrossRef](#)]
7. Elahifard, M.; Sadrian, M.R.; Mirzanejad, A.; Behjatmanesh-Ardakani, R.; Ahmadvand, S. Dispersion of Defects in TiO<sub>2</sub> Semiconductor: Oxygen Vacancies in the Bulk and Surface of Rutile and Anatase. *Catalysts* **2020**, *10*, 397. [[CrossRef](#)]