

## Special Issue

# Feature Papers to Celebrate "Computational Catalysis"— Trends and Outlook

### Message from the Guest Editor

As section editor-in-chief of Computational Catalysis in *Catalysts*, to celebrate the establishment of this new section, I am pleased to announce a Special Issue entitled "Feature Papers to Celebrate 'Computational Catalysis'—Trends and Outlooks". This Special Issue will collect both original research articles and reviews on various aspects of the computational methods and applications for predicting and understanding catalytic processes. Potential topics include, but are not limited to, the following items:

- Electronic structure calculations for analyzing reaction mechanisms
- Hybrid and multi-scale simulation methods for extending computational time and length scales
- Computational approaches that incorporate non-ideal effects (solvation, defects, correlation, etc.)
- Development of new data-driven approaches within the field of computational catalysis
- Computational approaches for analyzing enzymatic and biochemical catalytic processes
- Industrial applications and direct experimental benchmarking of computational catalysis techniques

All of the accepted papers in this Special Issue will be published free of charge in open access.

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### Guest Editor

Prof. Dr. C. Heath Turner

Department of Chemical and Biological Engineering, The University of Alabama, Box 870203, Tuscaloosa, AL 35487, USA

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### Deadline for manuscript submissions

closed (31 December 2020)



## Catalysts

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*Catalysts*  
Editorial Office  
MDPI, Grosspeteranlage 5  
4052 Basel, Switzerland  
Tel: +41 61 683 77 34  
[catalysts@mdpi.com](mailto:catalysts@mdpi.com)

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## About the Journal

### Message from the Editor-in-Chief

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#### Editor-in-Chief

Prof. Dr. Keith Hohn  
Carl R. Ice College of Engineering, Kansas State University, Manhattan,  
KS, USA

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##### Rapid Publication:

manuscripts are peer-reviewed and a first decision is provided to authors approximately 15.9 days after submission; acceptance to publication is undertaken in 3.5 days (median values for papers published in this journal in the second half of 2025).