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

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Deadline for manuscript submissions:
closed (31 December 2020)

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.