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.

Guest Editor

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Message from the Editor-in-Chief

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Rapid Publication:

manuscripts are peer-reviewed and a first decision is provided to authors approximately 16.6 days after submission; acceptance to publication is undertaken in 2.7 days (median values for papers published in this journal in the first half of 2025).