

Special Issue

10th Anniversary of Catalysts: Achievements in Computational Catalysis Techniques and Applications

Message from the Guest Editors

In 2021, Catalysts will reach a significant milestone in its history by welcoming its tenth anniversary. In order to celebrate this special occasion, we will be launching a Special Issue entitled “10th Anniversary of Catalysts: Achievements in Computational Catalysis Techniques and Applications.”

Computational catalysis has emerged as one of the fastest growing research fields in the last decade, and it now represents a critical tool for the analysis of chemical mechanisms and active sites. As the field of computational catalysis continues to expand, the gap between models and reality is beginning to narrow. We are particularly interested in articles that investigate the secondary effects influencing catalysis and reaction mechanisms. This includes the role of structural defects, the solvation environment or neighbor-neighbor effects, deactivation events, and work that incorporates system features encountered at finite temperatures. Furthermore, we are interested in new techniques and applications that enable extended time scale analyses, as well as high throughput screening techniques that involve machine learning or descriptor-based protocols.

Guest Editors

Prof. Dr. C. Heath Turner

Prof. Dr. Tibor Szilvási

Prof. Dr. Wei An

Prof. Dr. Yaqiong Su

Deadline for manuscript submissions

closed (31 December 2021)



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Catalysts
Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
catalysts@mdpi.com

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

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