Special Issue

The State of the Art and Future Perspectives on Computational Catalysis

Message from the Guest Editors

Computational chemistry has emerged as an essential tool in deciphering various chemical transformations, ranging from pure organic rearrangements to catalytic processes. It continues to play a pivotal role in enhancing scientists' understanding of the many reactions they investigate. Despite its vast contributions, there are still inherent limitations regarding the tools available and the size of the systems that can be effectively studied. This Special Issue focuses on (but is not limited to) two main approaches to computational catalysis: the classical interpretation at the molecular level of chemical reactions, and a recently emerging approach for discovering new catalysts by computational methodologies (for example, machine learning), making use of large amounts of data. In this Special Issue, we aim to offer a collection of narratives that not only highlight the significance of computational chemistry, but also address the unmet needs within the chemistry community. Our goal is to foster further development and expansion in the field of homogeneous and heterogeneous catalysis.

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Deadline for manuscript submissions

closed (15 April 2025)

Catalysts

an Open Access Journal by MDPI

Impact Factor 4.0
CiteScore 7.6

mdpi.com/si/218610

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