Special Issue

Advances in Computational Chemistry for Reaction Mechanisms

Message from the Guest Editors

Recent developments in computational chemistry have significantly advanced the study of reaction mechanisms, providing a deeper understanding of experimental results and revealing the key factors influencing chemical reactions. This is particularly useful for investigating short-lived intermediates that cannot be observed experimentally, providing a molecular-level perspective which complements traditional methods. Additionally, the integration of artificial intelligence (AI) has greatly accelerated computational algorithms, expanding the insights derived from computational chemistry and enabling chemists to approach chemical processes from a novel perspective. This Special Issue on “Advances in Computational Chemistry for Reaction Mechanisms” seeks high-quality works focusing on reaction mechanistic studies with the help of computational chemistry. The topics include, but are not limited to, computational modeling on reaction mechanisms, catalyst design, prediction of enantioselectivity, machine learning applications for chemical reactions, and automated transition-state search algorithms, among others.

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Editor-in-Chief

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