Special Issue

Computational Chemistry in Homogeneous and Heterogeneous Catalysis and Surface Chemistry

Message from the Guest Editors

Computational chemistry has emerged as one of the fastest growing and developing branches in chemistry. It has developed from initially treating small molecules with a handful of electrons to accurately modelling large systems with hundreds of atoms and predicting their various chemical and physical properties. The field has received significant recognition, with multiple Nobel prizes, from Kohn and Pople in 1998 to Baker, Hassabis and Jumper in 2024. Indeed, for decades, catalysis has played a crucial role in the development of human civilization. Catalytic technologies have been shown to have huge importance in industrial production, biological systems, environmental protection and green chemistry.

The aim of this Special Issue is to provide readers with an overview of applications of computational chemistry in studying various homogeneous and heterogeneous catalytic reactions.

Reviews, full papers and short communications covering the theory and application of computational studies of both catalytic and surface reactions are equally welcome.

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Message from the Editor-in-Chief

As the premier open access journal dedicated to molecular chemistry, now in its 30th year of publication, the papers published in *Molecules* span from classical synthetic methodology to natural product isolation and characterization, as well as physicochemical studies and the applications of these molecules as pharmaceuticals, catalysts, and novel materials. Pushing the boundaries of the discipline, we invite papers on all major fields of molecular chemistry and multidisciplinary topics bridging chemistry with biology, physics, and materials science, as well as timely reviews and topical issues on cutting-edge fields in all of these areas.

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