

## Special Issue

# Quantum Chemical Calculations of Molecular Reaction Processes, 2nd Edition

### Message from the Guest Editors

Theoretical chemical calculations are becoming increasingly important in molecular science and are indispensable for elucidating complex chemical reaction processes and quantitatively predicting observations. The accuracy of quantum chemical calculations has been supported by developments in electronic state theory and the increasing speed of computers. In quantum chemical calculations for reactions, novel algorithms have been developed to reveal reaction pathways, and eventually artificial intelligence will be used to a great extent for molecular design. In this Special Issue, we will feature papers that use quantum chemical calculations to reveal the reaction processes of molecules. As an open access journal, we will make the potential of quantum chemical calculations widely known to the world by publishing the latest results on using computers to understand the complex world of chemistry.

### Guest Editors

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### Deadline for manuscript submissions

closed (31 March 2026)



## Molecules

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## About the Journal

### 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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### Editor-in-Chief

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