# Special Issue

# Computational Photochemistry: Challenges and Possibilities

## Message from the Guest Editor

Photochemistry is the study of chemical processes initiated by the interaction between light and matter. Computational photochemistry has emerged as an indispensable theoretical paradigm. By constructing high-accuracy potential energy surfaces and executing nonadiabatic molecular dynamics simulations, it enables researchers to “witness” the complete picture of photochemical reactions at atomic and electronic scales. This, in turn, provides profound microscopic interpretations and precise predictions for experimental observations. This Special Issue aims to bring together leading global researchers to systematically showcase the latest breakthroughs and perspectives at the frontier of this field (e.g., photocatalytic water splitting, $CO_2$ photoreduction, degradation of pollutants, photodynamic therapy, photochemical transformation of small molecules, and mechanisms of luminescent materials). We aspire to create a platform for high-level academic exchange that promotes the deep integration of theoretical innovation and practical application, thereby injecting new vitality into the flourishing development of the broader field of photochemistry.

## Guest Editor

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## Deadline for manuscript submissions

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## Message from the Editor-in-Chief

As the premier open access journal dedicated to molecular chemistry, now in its 29th 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.

## Editor-in-Chief

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