

## Special Issue

# Theoretical Inorganic Chemistry

### Message from the Guest Editor

The advent of a multitude of molecular modeling software packages along with powerful computers boosted the field of theoretical inorganic chemistry to another level, realizing its departure from the long-standing era of the simple ad hoc models, developed by chemists to explain various properties of inorganic compounds. Today, molecular modeling methods such as ab initio, semiempirical, DFT, molecular dynamics/mechanics, and QM/MM are applied to simulate and provide in-depth studies on a broad range of chemical, physical, and biological phenomena of importance in chemical reactivity, catalytic activity, bioactivity, photophysics, electronic and nuclear magnetic resonance spectroscopy, and linear and nonlinear optics etc. of inorganic compounds. This Special Issue aims to collect original, high-quality theoretical studies of inorganic compounds based on molecular modeling methods.

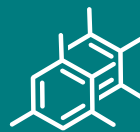
### Guest Editor

Prof. Dr. Athanassios C. Tsipis

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### Deadline for manuscript submissions

closed (31 May 2021)



## 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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#### Journal Rank:

JCR - Q2 (Biochemistry and Molecular Biology) / CiteScore - Q1 (Organic Chemistry)

#### Rapid Publication:

manuscripts are peer-reviewed and a first decision is provided to authors approximately 15.1 days after submission; acceptance to publication is undertaken in 2.6 days (median values for papers published in this journal in the second half of 2025).