Special Issue

Computational Study and Molecular Modeling in Materials Chemistry

Message from the Guest Editors

Rapid advances in computational technology and the decreasing cost of computing have revolutionized the field of chemistry, enabling researchers to explore complex molecular interactions and phenomena with unprecedented precision. Computational methods allow the detailed analysis of molecular structures, dynamics and properties, providing insights that are often difficult to obtain through experimental approaches alone. This Issue aims to showcase cutting-edge research using computational tools to address pressing questions in materials science, bridging the different descriptions of similar chemical phenomena across disciplines including physical chemistry, DFT calculation; machine learning and catalysis. We welcome original research articles, short communications and selected review articles that present novel methods or findings in computational materials and molecular modeling.

Guest Editors

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Dr. Osvaldo Yáñez

Dr. Kerry Wrighton-Araneda

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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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manuscripts are peer-reviewed and a first decision is provided to authors approximately 16.1 days after submission; acceptance to publication is undertaken in 2.6 days (median values for papers published in this journal in the first half of 2025).