# Special Issue

# Theoretical Research on Bonding Analysis and Weak Interactions

### Message from the Guest Editors

The physical origin of the chemical bond remains an active field of research. Methods to compute and analyze covalent and non-covalent interactions from the molecular wavefunction have met a surge in development in recent years. Applications of these methods have been pivotal in describing bonding in many chemical systems such as protein–ligand binding, molecular diffusion, and molecular assemblies. This Special Issue aims to gather the recent developments and applications of ab initio derived methods to compute and interpret the electronic interactions in molecular systems.

### Guest Editors

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### Deadline for manuscript submissions

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## 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.

## Editor-in-Chief

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