

## Special Issue

# Development and Application of Computational Chemistry Methods

### Message from the Guest Editors

Computational chemistry has emerged as a pivotal field in modern science, revolutionizing our ability to model and understand complex chemical phenomena. As computing facilities, algorithms complexity, and analysis tools continue to improve, computational techniques offer unprecedented opportunities for fundamental and applied research. This Special Issue aims to collect the latest advancements in these approaches, highlighting recent innovations in theoretical and computational methodologies and presenting how they enhance our understanding of chemical systems and drive new experimental investigations. By featuring contributions that showcase advances in algorithms, software, and simulations, this issue wants to provide a comprehensive overview of how computational chemistry is shaping the future of scientific inquiry and technological progress. For more information on the Special Issue, please visit LINK

[https://www.mdpi.com/journal/applsci/special\\_issues/O84A1U5094](https://www.mdpi.com/journal/applsci/special_issues/O84A1U5094)

### Guest Editors

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Dr. Marco Romanelli

### Deadline for manuscript submissions

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## Applied Sciences

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## About the Journal

### Message from the Editor-in-Chief

As the world of science becomes ever more specialized, researchers may lose themselves in the deep forest of the ever increasing number of subfields being created. This open access journal Applied Sciences has been started to link these subfields, so researchers can cut through the forest and see the surrounding, or quite distant fields and subfields to help develop his/her own research even further with the aid of this multi-dimensional network.

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### Editor-in-Chief

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