

Special Issue

10th Anniversary of *Computation*–Computational Chemistry

Message from the Guest Editors

Computational chemistry is crucial for understanding the relationship between atomic structure and material properties. Many papers, including in this journal, have been published on this topic. Simulations often simplify computations through idealizations. Methodology analysis is critical for enhancing computation quality, particularly for electronic structure using density functional theory (DFT) based on functionals.

Determining which functionals align with experimental data is crucial. Additional important factors include temperature, pressure, magnetism, substitutions, and relativistic effects (for heavy elements). Accuracy is essential for evaluating similar cases like magnetic anisotropy. Improving efficiency enables exploration of complex structures representing real systems.

Systematic studies unveil trends, enhancing structure-property relations with new insights. We plan to publish a Special Issue addressing current challenges and future innovations. Solid-state research, numerical analysis, machine learning, AI, computational biology, and bioinformatics are also significant in computational chemistry.

Guest Editors

Prof. Dr. Karlheinz Schwarz

Theoretical Chemistry Group, Materials Chemistry, TU Wien, A-1060 Vienna, Austria

Prof. Dr. Henry Chermette

Institut des Sciences Analytiques, Université de Lyon, UMR 5280, CNRS, Université Lyon 1 - 5, rue de la Doua, F-69100 Villeurbanne, France

Deadline for manuscript submissions

closed (30 November 2023)



Computation

an Open Access Journal
by MDPI

Impact Factor 1.9
CiteScore 4.1



mdpi.com/si/161051

Computation
Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
computation@mdpi.com

[mdpi.com/journal/
computation](https://mdpi.com/journal/computation)





Computation

an Open Access Journal
by MDPI

Impact Factor 1.9
CiteScore 4.1



[mdpi.com/journal/
computation](https://mdpi.com/journal/computation)



About the Journal

Message from the Editor-in-Chief

You are invited to submit the results of your research for consideration and publication in *Computation*, an international open access journal, which is published monthly online by MDPI.

The editorial board and staff of *Computation* are dedicated to establishing a benchmark journal for the world scientific and engineering communities for original research articles, reviews, conference proceedings (i.e., peer reviewed full articles), and communications, in the cutting-edge areas of computational biology, computational chemistry, computational social science and computational engineering.

Editor-in-Chief

Prof. Dr. Ali Cemal Benim

Center of Flow Simulation (CFS), Department of Mechanical and Process Engineering, Duesseldorf University of Applied Sciences, D-40476 Duesseldorf, Germany

Author Benefits

High Visibility:

indexed within Scopus, ESCI (Web of Science), CAPIus / SciFinder, Inspec, dblp, and other databases.

Journal Rank:

JCR - Q2 (Mathematics, Interdisciplinary Applications) /
CiteScore - Q1 (Applied Mathematics)

Rapid Publication:

manuscripts are peer-reviewed and a first decision is provided to authors approximately 14.8 days after submission; acceptance to publication is undertaken in 5.6 days (median values for papers published in this journal in the second half of 2025).