

## Special Issue

# Theoretical Chemistry and Quantum Chemical Computation: New Perspectives on Symmetry and Asymmetry in Molecular Systems

### Message from the Guest Editors

Theoretical chemistry, supported by advanced quantum chemical methods, is fundamental to understanding molecular structure, chemical reactivity, and the intricate behavior of molecules. These tools provide crucial insights into the principles governing symmetry and asymmetry in chemical systems. For this Special Issue of *Symmetry*, titled “Theoretical Chemistry and Quantum Chemical Computation: New Perspectives on Symmetry and Asymmetry in Molecular Systems”, we welcome original research exploring symmetry-related aspects of molecular structure, electronic properties, and reactivity. Topics include asymmetric synthesis, chiral catalysts, enantiomer separation, X-ray crystallography, molecular clusters, coordination chemistry, and related fields. We encourage you to contribute and share your findings in this innovative field.

---

### Guest Editors

Dr. Jelena Živković

Innovative Centre of the Faculty of Chemistry, Studentski trg 12-16,  
11000 Belgrade, Serbia

Dr. Dušan Dimić

Faculty of Physical Chemistry, University of Belgrade, Studentski trg 12-16,  
11000 Belgrade, Serbia

---

### Deadline for manuscript submissions

28 February 2027



## Symmetry

---

an Open Access Journal  
by MDPI

---

Impact Factor 2.2  
CiteScore 5.2



[mdpi.com/si/243227](https://mdpi.com/si/243227)

*Symmetry*  
Editorial Office  
MDPI, Grosspeteranlage 5  
4052 Basel, Switzerland  
Tel: +41 61 683 77 34  
[symmetry@mdpi.com](mailto:symmetry@mdpi.com)

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





# Symmetry

---

an Open Access Journal  
by MDPI

---

Impact Factor 2.2  
CiteScore 5.2



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



## About the Journal

### Message from the Editor-in-Chief

Symmetry is ultimately the most important concept in natural sciences. It is not surprising then that very basic and fundamental research achievements are related to symmetry. For instance, the Nobel Prize in Physics 1979 (Glashow, Salam, Weinberg) was received for a unified symmetry description of electromagnetic and weak interactions, while the Nobel Prize in Physics 2008 (Nambu, Kobayashi, Maskawa) was received for the discovery of the mechanism of spontaneous breaking of symmetry, including CP symmetry. Our journal is named *Symmetry* and it manifests its fundamental role in nature.

---

### Editor-in-Chief

Prof. Dr. Sergei Odintsov  
ICREA, 08010 Barcelona and Institute of Space Sciences (IEEC-CSIC),  
C. Can Magrans s/n, 08193 Barcelona, Spain

---

### Author Benefits

#### Open Access:

free for readers, with article processing charges (APC) paid by authors or their institutions.

#### High Visibility:

indexed within SCIE (Web of Science), Scopus, CAPlus / SciFinder, Inspec, Astrophysics Data System, and other databases.

#### Journal Rank:

JCR - Q2 (Multidisciplinary Sciences) / CiteScore - Q1  
(General Mathematics)