

Special Issue

Symmetry and Asymmetry in Theoretical Chemistry

Message from the Guest Editors

- Symmetry plays a fundamental role not only in art but also in nature, influencing countless phenomena at both macroscopic and microscopic levels. In quantum chemistry, symmetry leads to unique behaviors in molecules. A particularly important aspect arises when the symmetry operator commutes with the Hamiltonian, ensuring that the symmetry operation does not alter the system's energy and that the system remains invariant under the transformation.
- The symmetry of molecules has a significant impact on both reaction mechanisms and material properties, affecting processes in the bulk phase as well as at surfaces. Symmetry considerations are crucial in understanding how molecular structure influences the course of chemical reactions, catalytic activity, and adsorption behavior. Moreover, molecular symmetry has a significant impact on spectroscopic properties, including selection rules and spectral patterns, which are crucial for interpreting infrared, Raman, and electronic spectra.
- We invite submissions of original theoretical research and review articles that explore various aspects of symmetry and asymmetry in chemical compounds and processes.

Guest Editors

Prof. Dr. Amin Bakhshandeh

Prof. Dr. Karina dos Santos Machado

Prof. Dr. Emerson Gustavo de Souza Luna

Deadline for manuscript submissions

31 March 2026



Symmetry

an Open Access Journal
by MDPI

Impact Factor 2.2
CiteScore 5.3



mdpi.com/si/245886

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

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





Symmetry

an Open Access Journal
by MDPI

Impact Factor 2.2
CiteScore 5.3



[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

1. ICREA, 08010 Barcelona, Spain

2. 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, CAPus / SciFinder, Inspec, Astrophysics Data System, and other databases.

Journal Rank:

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