# Special Issue

# Symmetry/Asymmetry in Computational and Theoretical Chemistry

## Message from the Guest Editors

Theoretical chemistry significantly influences the understanding of molecular structures, predicts chemical reactions, simplifies chemical problems, and aids in predicting molecular behavior. Techniques like symmetry projection and spectral shift enhance the accuracy and efficiency of quantum calculations. In contrast, asymmetry introduces unique properties such as chirality, which is essential in chemical species and plays a vital role in designing selective catalysts and reagents. This balance between symmetry and asymmetry underscores their roles in addressing the complexity of chemical systems and offering valuable insights for advancements in chemical research. To highlight symmetry/asymmetry in computational and theoretical chemistry, we invite you to participate with a review or original research article in this Special Issue of the MDPI Symmetry journal. We believe that you would make an excellent contribution in this area. All contributions, including surface science, nanoscience, scanning tunneling microscopy, and experimental/theoretical studies, are welcome if they demonstrate significant innovation in chemical physics.

## Guest Editors


Prof. Dr. Youness Benjalal

Chemical Science and Engineering Research Team (ERSIC), Department of Chemistry, Polydisciplinary Faculty of Beni Mellal (FPBM), Sultan Moulay Slimane University (USMS), Beni Mellal 23000, Morocco

Dr. Ahmed Fatimi

Chemical Science and Engineering Research Team (ERSIC), Department of Chemistry, Polydisciplinary Faculty of Beni Mellal (FPBM), Sultan Moulay Slimane University (USMS), Beni Mellal 23000, Morocco


## Deadline for manuscript submissions

31 December 2026


# Symmetry

an Open Access Journal by MDPI

Impact Factor 2.2
CiteScore 5.2

mdpi.com/si/227533

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

mdpi.com/journal/symmetry

# Symmetry

an Open Access Journal by MDPI

Impact Factor 2.2
CiteScore 5.2

mdpi.com/journal/symmetry

MDPI

# 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 )