

## Special Issue

# Molecular Scale Research of Energy Materials

### Message from the Guest Editor

The envisaged green transition will require, for being sustainable, the design of new materials. It involves the collection, storage, and conversion of energy, which has led to the research of a series of energy materials, such as photocatalytic materials, perovskite materials, lithium battery materials, biomass energy materials, etc.

Although the actual functioning of energy devices occurs at the macroscopic scale, this is due to chemical and physical processes originating at the molecular scale. The periodic crystalline unit comprising up to a few tens of atoms determines light absorption and charge transport. Free energy surfaces of a molecular complex in proximity to a surface determine its catalytic activity. This Special Issue is focused on experimental and theoretical/computational contributions tackling the properties at the molecular scale of the extended family of energy materials. It focuses on the latest research on energy materials from the molecular scale to the design and synthesis of energy materials, electron and ion transport mechanisms, catalytic activity, and energy conversion mechanisms.

### Guest Editor

Dr. Paolo Umari

Department of Physics and Astronomy, University of Padova, Via F. Marzolo 8, 35131 Padua, Italy

### Deadline for manuscript submissions

closed (30 October 2025)



## International Journal of Molecular Sciences

---

an Open Access Journal  
by MDPI

---

Impact Factor 4.9  
CiteScore 9.0  
Indexed in PubMed



[mdpi.com/si/203773](https://mdpi.com/si/203773)

*International Journal of  
Molecular Sciences*  
Editorial Office  
MDPI, Grosspeteranlage 5  
4052 Basel, Switzerland  
Tel: +41 61 683 77 34  
[ijms@mdpi.com](mailto:ijms@mdpi.com)

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





# International Journal of Molecular Sciences

---

an Open Access Journal  
by MDPI

---

Impact Factor 4.9  
CiteScore 9.0  
Indexed in PubMed



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



## About the Journal

### Message from the Editor-in-Chief

The International Journal of Molecular Sciences (*IJMS*, ISSN 1422-0067) is an open access journal, which was established in 2000. The journal aims to provide a forum for scholarly research on a range of topics, including biochemistry, molecular and cell biology, molecular biophysics, molecular medicine, and all aspects of molecular research in chemistry. *IJMS* publishes both original research and review articles, and regularly publishes special issues to highlight advances at the cutting edge of research. We invite you to read recent articles published in *IJMS* and consider publishing your next paper with us.

---

### Editor-in-Chief

Prof. Dr. Maurizio Battino

Department of Odontostomatologic and Specialized Clinical Sciences,  
Sez-Biochimica, Faculty of Medicine, Università Politecnica delle  
Marche, Via Ranieri 65, 60100 Ancona, Italy

---

### Author Benefits

#### Open Access:

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

#### High Visibility:

indexed within Scopus, SCIE (Web of Science), PubMed, PMC, MEDLINE, Embase, CAPlus / SciFinder, and other databases.

#### Journal Rank:

JCR - Q1 (Biochemistry and Molecular Biology) / CiteScore  
- Q1 (Organic Chemistry)