Special Issue

Theory and Simulations of Single-Molecule Magnets

Message from the Guest Editor

Molecular magnets are systems with a series of transition metal atoms surrounded by ligands. The magnetic properties of these molecules, which can be used to design magnetic storage and spintronic devices, depend on the interplay between properties such as super-exchange, spin–orbit coupling, and the crystal field. The correct prediction of these properties using ab initio methods is, however, not easy, and theoretical results often differ from experimental ones. In this issue, we cover the latest developments of simulations of single-molecular magnets using ab initio methods.

Guest Editor

Prof. Dr. Victor M. García-Suárez
Centro de investigacion en Nanomateriales y Nanotecnologia (CINN), University of Oviedo, El Entrego, Spain

Deadline for manuscript submissions

closed (15 June 2021)

Molecules

an Open Access Journal by MDPI

Impact Factor 4.6
CiteScore 8.6
Indexed in PubMed

mdpi.com/si/58438

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

mdpi.com/journal/molecules

Molecules

an Open Access Journal by MDPI

Impact Factor 4.6
CiteScore 8.6
Indexed in PubMed

mdpi.com/journal/molecules

MDPI

About the Journal

Message from the Editor-in-Chief

As the premier open access journal dedicated to experimental organic chemistry, and now in its 25th year of publication, the papers published in *Molecules* span from classical synthetic methodology to natural product isolation and characterization, as well as physicochemical studies and the applications of these molecules as pharmaceuticals, catalysts and novel materials. Pushing the boundaries of the discipline, we invite papers on multidisciplinary topics bridging biochemistry, biophysics and materials science, as well as timely reviews and topical issues on cutting edge fields in all these areas.

Editor-in-Chief

Prof. Dr. Thomas J. Schmidt
Institute of Pharmaceutical Biology and Phytochemistry, University of Münster, Corrensstrasse 48, D-48149 Münster, Germany

Author Benefits

High Visibility:

indexed within Scopus, SCIE (Web of Science), PubMed, MEDLINE, PMC, Reaxys, CaPlus / SciFinder, MarinLit, AGRIS, and other databases.

Journal Rank:

JCR - Q2 (Biochemistry and Molecular Biology) / CiteScore - Q1 (Organic Chemistry)

Rapid Publication:

manuscripts are peer-reviewed and a first decision is provided to authors approximately 16.1 days after submission; acceptance to publication is undertaken in 2.6 days (median values for papers published in this journal in the first half of 2025).