molecules

an Open Access Journal by MDPI

IMPACT FACTOR 4.6

Indexed in: PubMed

CITESCORE 6.7

Molecular Reactivity: Theoretical Study and Interpretation of Experimental Results (II)

Guest Editors:

Prof. Dr. Marzio Rosi
Department of Civil and Environmental Engineering, Università degli Studi di Perugia, Perugia, Italy

Prof. Dr. Stefano Falcinelli
Department of Civil & Environmental Engineering, Universita degli Studi di Perugia, Perugia, Italy

Deadline for manuscript submissions:
30 November 2024

Message from the Guest Editors

Dear Colleagues,

This Special Issue aims to collect papers investigating recent theoretical and experimental efforts exploiting new insights, methods, and techniques applied to the study of the microscopic dynamics of elementary chemical reactions. In particular, an overview of the most powerful calculation methods currently available will be published for the identification and characterization of the nature and strength of intermolecular interactions able to describe chemical reactivity. Topics include reactions between neutral species of interest in combustion, including ion–molecule reactions and those involving excited and radical species, from processes relevant for surface physics to the fundamentals of gas-phase stereodynamics, up to the physical chemistry of plasmas, planetary ionospheres, and astrochemistry, as well as complex systems of biochemical interest.

Keywords: potential energy surface; molecular reaction dynamics; theoretical chemistry ab initio calculations; combustion; astrochemistry; astrobiology; atmospheric chemistry; catalysis; calculation of kinetic parameters; modeling dust and icy grain structures and properties

molecules

IMPACT FACTOR 4.6 | Indexed in: PubMed | CITESCORE 6.7

an Open Access Journal by MDPI

Editor-in-Chief

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

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.

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, MEDLINE, PMC, Reaxys, CaPlus / SciFinder, MarinLit, AGRIS, and other databases.
Journal Rank: JCR - Q2 (*Chemistry, Multidisciplinary*) / CiteScore - Q1 (*Chemistry (miscellaneous)*)

Contact Us

Molecules Editorial Office
MDPI, St. Alban-Anlage 66
4052 Basel, Switzerland

Tel: +41 61 683 77 34
www.mdpi.com

mdpi.com/journal/molecules
molecules@mdpi.com
𝕏@Molecules_MDPI