Special Issue

Theoretical Excited-State Chemistry: New Developments and Cutting-Edge Applications

Message from the Guest Editors

Chemical excited states are at the basis of new developments such as luminescent devices, fluorescence markers, energy generating and converting materials or photochemical synthetic methods, and they play a key role in biological contexts such as photosynthesis, photoactive proteins, or the reaction of DNA with light. They are also very challenging from the point of view of theory. In this Special Issue, we aim to provide a broad overview of the state of the art covering both applications and method development. This includes applications such as excited states of biomolecules, fluorescent markers, luminescent molecules and materials, photocatalysis, aggregation-induced emission, solar cell components and others, and methodological issues related with the description of excited states, their potential energy surfaces and dynamics. We hope that the forthcoming Issue will set the stage for new developments and open new perspectives in the field.

Guest Editors

Prof. Dr. Lluís Blancafort

Institut de Química Computacional i Catàlisi and Departament de Química, Universitat de Girona, Facultat de Ciències, C/M. Aurèlia Campmany 69, 17003 Girona, Spain

Dr. Annapaola Migani

Institut de Química Computacional i Catàlisi and Departament de Química, Universitat de Girona, Facultat de Ciències, C/M. Aurèlia Campmany 69, 17003 Girona, Spain

Deadline for manuscript submissions

closed (31 March 2019)

Molecules

an Open Access Journal by MDPI

Impact Factor 4.6
CiteScore 8.6
Indexed in PubMed

mdpi.com/si/8695

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

About the Journal

Message from the Editor-in-Chief

As the premier open access journal dedicated to molecular chemistry, now in its 29th 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 all major fields of molecular chemistry and multidisciplinary topics bridging chemistry with biology, physics, and materials science, as well as timely reviews and topical issues on cutting-edge fields in all of 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).

MDPI