



an Open Access Journal by MDPI

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

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)**

### Message from the Guest Editors

Dear Colleagues,

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.



[mdpi.com/si/8695](https://mdpi.com/si/8695)

# Special Issue



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, Grosspeteranlage 5  
4052 Basel, Switzerland

Tel: +41 61 683 77 34  
[www.mdpi.com](http://www.mdpi.com)

[mdpi.com/journal/molecules](http://mdpi.com/journal/molecules)  
[molecules@mdpi.com](mailto:molecules@mdpi.com)  
[X@Molecules\\_MDPI](#)