molecules

an Open Access Journal by MDPI

IMPACT FACTOR 4.2

Indexed in: PubMed

CITESCORE 7.4

Computational Design and Modelling of Organic Materials for Energy Applications

Guest Editor:

Dr. Daniele Padula
Department of Biotechnology, Chemistry and Pharmacy, University of Siena, 53100 Siena, Italy

Deadline for manuscript submissions:
closed (15 May 2021)

Message from the Guest Editor

Dear Colleagues,

Thanks to their versatility, organic semiconductors play a central role in the search for solutions to some of the most fascinating problems in energy research. The quest for efficient and stable singlet fission materials or photocatalysts, the rationalization of the impact of three-dimensional order and disorder on charge mobility, and the elucidation of general design principles for emissive (TADF, AIE) candidates are only some of the challenges that our community is facing.

The objective of this Special Issue is to gather contributions that advance the design of organic materials or shed light on theoretical aspects of the physical processes involved, from a computational perspective.

We welcome communications, full papers, and reviews on the aforementioned topics.

Dr. Daniele Padula
Guest Editor

molecules

IMPACT FACTOR 4.2 | Indexed in: PubMed | CITESCORE 7.4

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

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