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Computational Design and Modelling of Organic Materials for Energy Applications

Guest Editor:

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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

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Editor-in-Chief

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Message from the Editor-in-Chief

As the premier open access journal dedicated to molecular chemistry, now in its 30th 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.

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