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Computational Chemistry for Material Research

Guest Editors:

Dr. Tian Wang

Dr. Cheng Zhong

Dr. Tianyuan Zhang

Dr. Xiaohua Wang

Deadline for manuscript submissions:
closed (30 November 2023)

Message from the Guest Editors

Dear Colleagues,

Recent advances in computational chemistry have stimulated their application in material research, such as in the prediction of thermodynamic properties for catalysts, X-ray absorption spectroscopy (XAS), mechanical and elastic properties, and ion mobilities for batteries. Computational chemistry bridges theory and experimental insight for material research.<false,>This Special Issue aims to cover the large scale of materials and answer the questions that experiments are unable to. Fields to be covered that involve computational study include the following:

- Prediction of novel heterogeneous catalysts for HER, ORR, OER, NRR, etc.
- Prediction of novel anode and cathode materials for Li- and Na-ion batteries.
- Prediction and verification of lanthanide and transition-metal X-ray absorption spectroscopy, especially their L and M edges.
- Development of novel methodologies for the accurate prediction of semiconductor band gap energies.
- Fast algorithms for fast potential energy surface (PES) scanning.

Dr. Tian Wang
Dr. Xiaohua Wang
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Dr. Tianyuan Zhang
Guest Editors

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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.

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Contact Us

Molecules Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland

Tel: +41 61 683 77 34
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