Special Issue

Computational Chemistry for Material Research

Message from the Guest Editors

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.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.

Guest Editors

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Deadline for manuscript submissions

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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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