Special Issue

Theoretical and Experimental Studies on Metal–Organic Frameworks: Structures, Optical Properties and Applications

Message from the Guest Editors

Metal–organic frameworks (MOFs) are a class of compounds consisting of metal ions or clusters coordinated to organic ligands to form one-, two-, or three-dimensional structures. The synthesis and properties of MOFs constitute the primary focus of computational and material chemistry. A wide range of potential applications of these MOFs has been identified in the fields of gas separation, water remediation, catalysis, conducting solids, as supercapacitors., etc. This Special Issue welcomes contributions, original research or review articles on all aspects related to the structure and optical properties of MOFs. This Special Issue will include research articles on MOFs using various simulation calculations and chemical analyses, with the opportunity to present purely computational studies, as well as computational studies with experimental validations.

Guest Editors

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Message from the Editor-in-Chief

As the premier open access journal dedicated to molecular chemistry, now in its 29th 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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