Special Issue

Computational Chemistry Approach for Materials Design

Message from the Guest Editors

Due to the intricate structures of different materials and limited in situ characterization techniques, the traditional approaches for materials design often rely on trial-and-error testing, which is laborious and inefficient. Currently, computational modelling offers a more rational way to accelerate this process. Understanding the design rules that govern materials chemistry and architecture holds the key towards rationally optimizing technologies such as batteries, fuel cells, electrolysers, and so on. This Special Issue, "Computational Chemistry Approach for Materials Design", aims to become a useful platform to report and summarize the progress achieved in this field.

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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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