Special Issue

Computational Studies of Novel Function Materials

Message from the Guest Editor

In recent years, there has been an explosion of new material discoveries. Such as low-dimensional materials, single-layer materials, multiple-layered materials, transition-metal dichalcogenides (TMD), and MXene. Those new rising materials have been investigated as catalysts, adsorbents, electrodes, and electrolytes. All these great developments of functional material discovery have led to a new era in material discovery. Computations have provided a strong ability to accelerate material discovery. For instance, computations for spectrum, stability exploration of new materials, electronic and optical properties, molecular dynamics, and adsorption ability have been employed for defining and analyzing a new material from a theoretical aspect. In light of the growing demand for new functional materials in various applications and the strong power of computations implemented in material discovery, we have decided to edit a Special Issue, "Computational Studies of Novel Function Materials".

Guest Editor

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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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