Special Issue

Theoretical Inorganic Chemistry

Message from the Guest Editor

The advent of a multitude of molecular modeling software packages along with powerful computers boosted the field of theoretical inorganic chemistry to another level, realizing its departure from the long-standing era of the simple ad hoc models, developed by chemists to explain various properties of inorganic compounds. Today, molecular modeling methods such as ab initio, semiempirical, DFT, molecular dynamics/mechanics, and QM/MM are applied to simulate and provide in-depth studies on a broad range of chemical, physical, and biological phenomena of importance in chemical reactivity, catalytic activity, bioactivity, photophysics, electronic and nuclear magnetic resonance spectroscopy, and linear and nonlinear optics etc. of inorganic compounds. This Special Issue aims to collect original, high-quality theoretical studies of inorganic compounds based on molecular modeling methods.

Guest Editor

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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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