Special Issue

Theoretical Study of Inorganic Complexes

Message from the Guest Editor

Inorganic complexes present very large domains of applications from chemistry and biology to solid state physics. Indeed, transition metal complexes are not only commonly used as catalysts in chemical syntheses but some of them have been shown to drive biological processes. Moreover, regarding their photophysical properties, transition metal complexes are widely used in electronic devices like OLED or sensors. Some complexes can also lead to single molecule magnets (SMM). Theoretical investigations of the chemical, biochemical, catalytic, or photophysical properties of inorganic complexes using quantum chemistry methods are very common today. It is well known that these investigations could not only explain observed phenomena but could also predict new properties before experiments and help the design of improved complexes for aimed applications. In all cases, these theoretical studies permit the rationalization of experimental data. This Special Issue aims to collect original contributions or mini-reviews on the topics mentioned above relative to the theoretical study of inorganic complexes. There is no restriction on the length of the papers.

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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