



Theoretical Study of Inorganic Complexes

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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.





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Message from the Editor-in-Chief

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