Special Issue

Computational Studies on Bioinspired Transition-Metal-Based Catalysts

Message from the Guest Editor

The relevance of oxidation and reduction reactions in biology cannot be overstated. A variety of bioinspired metal complexes based on iron, copper, manganese, molybdenum, tungsten, and nickel are capable of catalyzing a variety of oxidation and reduction reactions such as oxygen reduction, water oxidation, proton and CO2 reduction, organic molecule transformation, and energy conversion processes, often using ligands like porphyrins, phthalocyanines, and nonporphyrinic tetradentate N4 ligands.

Computational studies play a crucial role in understanding the reactivity of metal complexes and in designing new and more efficient catalysts.

This Special Issue aims to attract research work about new advances in the computational modelling of bioinspired reactions catalyzed by transition metal complexes, as well as their electronic structure characterization and design. The scope includes, but is not limited to, the following:

Computational chemistry;
Quantum mechanics;
QM/MM;
Density Functional Theory (DFT);
Catalysis;
Reaction mechanism;
Electronic structure analysis

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Editor-in-Chief

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