Special Issue

Density Functional Theory (DFT) and Semi-empirical Quantum Mechanical (SQM) Methods in Organometallic Chemistry

Message from the Guest Editor

In recent decades, Kohn–Sham density functional theory (DFT) has become the workhorse of computational chemistry, and numerous methods with different focus have been developed. Moreover, modern semi-empirical quantum mechanical (SQM) methods are also seeing more and more applications in various fields of organometallic chemistry due to their outstanding efficiency and their improved reliability in describing organometallic systems. Both represent valuable tools for detailed studies of a wide variety of chemical problems, and their predictive power enables rapid and targeted scientific progress. Accordingly, these methods allow a deep understanding of the very nature of organometallic molecules and reactions far beyond the limits of the experiment. This Special Issue aims to highlight cutting-edge applications and methodological developments of DFT and SQM methods regarding chemical challenges in the field of molecular organometallic chemistry.

Guest Editor

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Inorganic chemistry remains a lynchpin of modern chemistry, not only embracing the function and reactivity of combinations of most elements of the periodic table, but also providing a footing for studies of materials, catalysts, drugs, fuels and industrial chemicals. Arguably, the role and reach of inorganics in society have never been as great as today. Adventurous research at the heart and at the extremes of inorganic chemistry is vital to further advances and Inorganics offers authors the opportunity to publish exciting new research in an open access format.

Editor-in-Chief

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