inorganics

an Open Access Journal by MDPI

IMPACT FACTOR 2.9

CITESCORE 4.0

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

Guest Editor:

Dr. Markus Bursch
Max-Planck-Institut für Kohlenforschung, Kaiser-Wilhelm-Platz 1, D-45470 Mülheim an der Ruhr, Germany

Deadline for manuscript submissions:
closed (15 February 2023)

Message from the Guest Editor

Dear Colleagues,

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.

inorganics

IMPACT FACTOR 2.9

CITESCORE 4.0

an Open Access Journal by MDPI

Editor-in-Chief

Prof. Dr. Duncan H. Gregory
School of Chemistry, University of Glasgow, University Avenue, Glasgow G12 8QQ, UK

Message from the Editor-in-Chief

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.

Author Benefits

Open Access: free for readers, with article processing charges (APC) paid by authors or their institutions.
High Visibility: indexed within Scopus, SCIE (Web of Science), CAPlus / SciFinder, and other databases.
Journal Rank: JCR - Q2 (*Chemistry, Inorganic & Nuclear*) / CiteScore - Q2 (*Inorganic Chemistry*)

Contact Us

Inorganics Editorial Office
MDPI, St. Alban-Anlage 66
4052 Basel, Switzerland

Tel: +41 61 683 77 34
www.mdpi.com

mdpi.com/journal/inorganics
inorganics@mdpi.com
𝕏@inorganics_MDPI