inorganics

an Open Access Journal by MDPI

IMPACT FACTOR 3.1

CITESCORE 2.8

Applications of Density Functional Theory in Inorganic Chemistry

Guest Editor:

Prof. Dr. Athanassios C. Tsipis
Laboratory of Inorganic and General Chemistry, Department of Chemistry, University of Ioannina, 45110 Ioannina, Greece

Deadline for manuscript submissions:
closed (15 April 2019)

Message from the Guest Editor

Dear Colleagues,

Recent improvements in the design of faster and more efficient algorithms have placed powerful computational quantum chemistry tools in the hands of all chemists. Nowadays, Density Functional Theory (DFT) calculations has become as useful to the bench chemist as spectrometers and vacuum lines. Being practically a "virtual inorganic chemistry lab", DFT has been applied to predict the behavior of a broad range of chemical, physical, and biological phenomena of importance in chemical reactivity, catalytic activity, bioactivity, photophysics, electronic and nuclear-magnetic resonance spectroscopy, linear and nonlinear optics, etc. This Special Issue aims to collect original, high quality DFT studies focused on diverse research areas in inorganic, organometallic and coordination chemistry. Topics include but are not limited to:

- Structural, bonding and spectroscopic properties of inorganic compounds
- Catalysis (mechanistic studies)
- Electronic spectroscopy
- Heavy-nucleus NMR spectroscopy
- Small molecule activation
- Organometallic reactivity
- Bioinorganic chemistry

Prof. Dr. Athanassios C. Tsipis
Guest Editor

mdpi.com/si/17081

inorganics

an Open Access Journal by MDPI

IMPACT FACTOR 3.1

CITESCORE 2.8

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 and 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