

Special Issue

Applications of Density Functional Theory in Inorganic Chemistry

Message from the Guest Editor

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

Guest Editor

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About the Journal

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.

Editor-in-Chief

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manuscripts are peer-reviewed and a first decision is provided to authors approximately 16.6 days after submission; acceptance to publication is undertaken in 2.5 days (median values for papers published in this journal in the first half of 2025).