

Special Issue

Computational Catalysis: Methods and Applications

Message from the Guest Editors

This Special Issue titled “Computational Catalysis: Methods and Applications” aims to capture high-quality research papers and review articles that report the advances, developments and challenges in computational catalysis and catalyst design. Studies on both homogeneous and heterogeneous catalysis with inorganic and organometallic complexes are welcome, and computational predictions of the selectivity and efficiencies of catalysts are also encouraged.

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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.

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Prof. Dr. Duncan H. Gregory

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