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Simulation-Aided Materials Design for Electrocatalysis

Guest Editor:

Dr. Junxian Liu
School of Mechanical, Medical & Process Engineering, Faculty of Engineering, Queensland University of Technology, Brisbane, QLD, Australia

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Message from the Guest Editor

To accelerate the advancement of affordable and environmentally friendly electrocatalysts, it is crucial to embrace numerical simulations for directly accessing information about electrochemical reactions.

This Special Issue aims to present research findings obtained through theoretical simulations, including the following:

1. Theoretical Simulations: Utilizing computational methods such as density functional theory, molecular dynamics, or quantum mechanics/molecular mechanics to investigate diverse electrocatalysis processes.
2. Electrocatalyst Design: The rational design and optimization of electrocatalysts for energy conversion and storage applications, including fuel cells, batteries, and electrolyzers, with insights derived from theoretical simulations and collaborative experimental–theoretical research.
3. Reaction Mechanisms: Investigations into reaction mechanisms at the atomic and molecular levels, elucidating the underlying processes of electrocatalytic reactions.
4. Materials Discovery: Explorations of new materials and nanostructures with enhanced electrocatalytic properties, including the development of novel catalysts for sustainable energy solutions.

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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.

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

Tel: +41 61 683 77 34
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inorganics@mdpi.com
𝕏@inorganics_MDPI