



## Simulation-Aided Materials Design for Electrocatalysis

Guest Editor:

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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

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## Message from the Editor-in-Chief

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