Special Issue

Density Functional Theory Modeling for Metallic Corrosion Science

Message from the Guest Editor

Corrosion science has traditionally relied on experimental approaches to understand degradation mechanisms and develop protective strategies for materials. However, Density Functional Theory (DFT) has emerged as a powerful tool to complement experiments, offering atomic-scale insights into corrosion phenomena in recent years. This Special Issue focuses on recent advances in **DFT modeling** applied to **metallic corrosion**, bridging atomic-scale understanding with practical corrosion mitigation. The Special Issue aims to gather contributions that elucidate **electron-level mechanisms** governing corrosion phenomena and the effects of alloy composition, environment, and inhibitors. Its scope can be organized into key sections:

- **Corrosion Inhibitors and Organic Adsorption**
- **Passivation and Oxide Films**
- **Electrochemical Interfaces**
- **Alloy Design and Microstructural Effects**
- **Methodological Advances**

The Special Issue will demonstrate how **first-principles modeling** can unravel corrosion mechanisms, accelerate inhibitor discovery, and predict material performance. It will serve as a reference for both theoreticians and experimentalists seeking to bridge atomic-level understanding with real-world corrosion behavior.

Guest Editor

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About the Journal

Message from the Editor-in-Chief

Metallic materials play a vital role in the economic life of modern societies; contributions are sought on fresh developments that enhance our understanding of the fundamental aspects related to the relationships between processing, properties and microstructure – disciplines in the metallurgical field ranging from processing, mechanical behavior, phase transitions and microstructural evolution, nanostructures, as well as unique metallic properties – inspire general and scholarly interest among the scientific community.

Editor-in-Chief

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