Special Issue

DFT Study on Electrocatalysis

Message from the Guest Editor

A suitable catalyst that is characterized by high activity and selectivity plays a key role in important electrochemical catalytic reactions, including carbon dioxide reduction, H2O2 generation, N2 reduction, water splitting, fuel cell electrocatalysis, ammonia synthesis, and so on. These reactions are critical for the development of clean technologies. An important issue in the design of high-performance electrocatalysts is understanding the reaction mechanisms and identifying factors limiting activity and selectivity. The use of computational techniques, e.g., density functional theory, high throughput calculations, and machine learning, represents a powerful tool that plays a crucial role in the development of electrocatalysts for different reactions. These approaches provide insights for understanding the properties of fundamental materials and design of new catalyst materials. This Special Issue will present the most recent and significant developments in computational catalysts. Original papers on the above topics and short reviews are welcome for submission.

Guest Editor

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