Special Issue

Machine Learning in Catalyst Design and Synthesis

Message from the Guest Editor

The Special Issue "Machine Learning in Catalyst Design and Synthesis" aims at highlighting the transformative impact of machine learning (ML) on the field of catalysis. ML techniques have revolutionized the way researchers approach catalyst design and synthesis, enabling the rapid discovery of new materials and the optimization of reaction conditions. By integrating computational modeling, experimental data, and advanced ML algorithms, this interdisciplinary field is accelerating breakthroughs in areas such as CO2 reduction, hydrogen production, and sustainable chemical processes. This Special Issue welcomes original research articles, reviews, and perspectives that explore the application of ML in catalyst design, including the development of predictive models, the optimization of synthesis protocols, and the discovery of novel catalytic materials. Through this collection, we aim at showcasing cutting-edge advancements and fostering collaboration across computational and experimental domains, advancing the frontiers of catalysis research.

Guest Editor

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