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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Message from the Editor-in-Chief

As the premier open access journal dedicated to molecular chemistry, now in its 29th year of publication, the papers published in *Molecules* span from classical synthetic methodology to natural product isolation and characterization, as well as physicochemical studies and the applications of these molecules as pharmaceuticals, catalysts, and novel materials. Pushing the boundaries of the discipline, we invite papers on all major fields of molecular chemistry and multidisciplinary topics bridging chemistry with biology, physics, and materials science, as well as timely reviews and topical issues on cutting-edge fields in all of these areas.

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