catalysts

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From Low-Dimensional Molecular Dynamics to High-Order Machine Learning: Advances in Computational Simulations in Catalysts

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Message from the Guest Editors

Dear Colleagues,

Given the importance of catalysts in the energy industry, they have been extensively investigated by experimental and numerical methods. With the development of computational algorithms and computer hardware, large-scale simulations have enabled influential studies with more atomic details reflecting microscopic mechanisms. We welcome recent research on computational studies including energy conversion, energy transfer, material growth, dehydrogenation, hydrogenation, oxidation reactions, and recombination of carbon materials that can guide catalyst calculations.

Machine learning has attracted increasing interest in recent years, and its combination with the field of catalysts has inspired promising development approaches. Its applications in machine learning potential, catalyst design, performance prediction, structure optimization, and classification are also welcome in this Special Issue. This Special Issue aims to collect a list of articles and reviews that provide state-of-the-art insights into recent developments in computer-aided studies in catalysts and energy.