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Theoretical and Computational Studies of Catalytic Reactions

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Message from the Guest Editors

Catalytic reactions are of fundamental importance in energy storage and conversion. The development of more active catalysts is essential for these applications. The knowledge of catalytic reaction mechanisms is crucial in understanding the functioning of catalysts. In many technological processes, catalytic activity is limited and the specific reaction mechanisms are not fully understood; thus, the knowledge of reaction mechanisms can help to better design catalysts considering more effective catalyst development and deep discussions regarding catalytic reaction mechanisms are urgently needed. The theoretical and computational approach is more economical, time-saving, and effective than conventional experiments. Experimental kinetic research as well as theoretical and computational studies of catalytic reaction dynamics are crucial for understanding their mechanisms and the observed reaction efficiencies, which would contribute to a better design of catalysts. The use of advanced experimental techniques and modern theoretical methods are applied to elucidate catalytic reaction mechanisms and exploit better catalysts.