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Mechanism/Kinetic Modeling Study of Catalytic Reactions

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Message from the Guest Editors

Catalytical reactions are of fundamental importance in industry and biochemical systems. The knowledge of catalytic reaction mechanisms is crucial in understanding the functioning of catalysts equally in homogeneous, heterogeneous, and enzymatic catalysis. In many technological or biological processes, the specific reaction mechanisms are not fully understood and are still widely discussed. The knowledge of reaction mechanisms can help to design better catalysts or effective drugs. Experimental kinetic research and simulations of catalytic reaction dynamics are crucial for understanding their mechanisms and comprehension of the observed reaction efficiencies. The use of advanced experimental techniques and modern theoretical methods is applied to elucidate catalytic mechanisms.

This Special Issue is devoted to the mechanisms and kinetics of homogeneous, heterogeneous, and enzymatic catalytic reactions. Articles focused on research with both experimental and computational methods are welcome. Short communications are also encouraged.