

Special Issue

Experimental and Theoretical Studies of Active Sites in Catalysts

Message from the Guest Editors

Tremendous progress has been achieved for developing and improving catalysis technology in the past century. However, in the past, the development of new catalysts largely relied on trial-and-error experiments, which is a tedious and costly approach. One of the major challenges that limit intelligent catalyst design was the difficulty in identifying the active sites and unraveling their roles in reaction mechanisms. However, recent advances in experimental and computational techniques have made it possible to better characterize active sites and determine their functionality in reaction pathways. This progress has opened the door toward a more detailed understanding of catalytic chemistry, and hence allows for the intelligent design of novel catalysts. This Special Issue will focus on the latest research on the synthesis and characterization of active sites, as well as the investigation of the effects of active sites in catalytic reactions. All experimental and computational studies falling within the scope are welcome for submission.

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