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Diverse Active Sites and Extensive Surface Binding Curves in

Abstract

The Sabatier principle has long guided our understanding of catalytic activity, suggesting that optimal catalysts should bind reactants neither too weakly nor too strongly. However, recent advances in catalysis reveal a more complex picture involving site heterogeneity and broad surface-binding isotherms. Modern catalytic systems often feature diverse active sites with varying electronic and geometric properties, leading to a range of catalytic behaviors that extend beyond the scope of the Sabatier principle. Additionally, surface-binding isotherms in these systems are increasingly broad and multi-modal, reflecting a spectrum of interactions with the catalyst surface. This article explores these advanced concepts, emphasizing the need for a more nuanced understanding of catalysis that incorporates dynamic site interactions and multi-scale modeling. By moving beyond the traditional Sabatier framework, researchers can design more efficient and tailored catalysts, enhancing both performance and sustainability in industrial processes.

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e interaction between the catalyst and its support material can lead to the formation of diverse active sites.

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