Accepted Manuscript

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PII: S0167-5729(18)30041-4

DOI: 10.1016/j.surfrep.2018.06.002

Reference: SUSREP 462

To appear in: *Surface Science Reports*

Received Date: 5 May 2018

Revised Date: 28 June 2018

Accepted Date: 30 June 2018

Please cite this article as: J. Zhang, J.W. Medlin, Catalyst design using an inverse strategy: From mechanistic studies on inverted model catalysts to applications of oxide-coated metal nanoparticles, *Surface Science Reports* (2018), doi: 10.1016/j.surfrep.2018.06.002.

Catalyst design using an inverse strategy: From mechanistic studies on inverted model catalysts to applications of oxide-coated metal nanoparticles

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Abstract

Metal-oxide interfaces are of great importance in catalytic applications since each material can provide a distinct functionality that is necessary for efficient catalysis in complex reaction pathways. Moreover, the synergy between two materials can yield properties that exceed the superposition of single sites. While interfaces between metals and metal oxides can play a key role in the reactivity of traditional supported catalysts, significant attention has recently been focused on using “inverted” oxide/metal catalysts to prepare catalytic interfaces with unique properties. In the inverted systems, metal surfaces or nanoparticles are covered by oxide layers ranging from submonolayer patches to continuous films with thickness at the nanometer scale. Inverse catalysts provide an alternative approach for catalyst design that emphasizes control over interfacial sites, including inverted model catalysts that provide an important tool for elucidation of mechanisms of interfacial catalytic reactions and oxide-coated metal nanoparticles that can yield improved stability, activity and selectivity for practical catalysts.

This review begins by providing a summary of recent progress in the use of inverted model catalysts in surface science studies, where oxides are usually deposited onto the surface of metal single crystals under ultra-high vacuum conditions. Surface-level studies of inverse systems have yielded key insights into interfacial catalysis and facilitated active site identification for important reactions such as CO oxidation, the water-gas shift reaction, and CO_2 reduction using well-defined model systems, informing strategies for designing improved technical catalysts. We then expand the scope of inverted catalysts, using the “inverse” strategy for preparation of higher-surface area practical catalysts, chiefly through the deposition of metal oxide films or particles onto metal nanoparticles. The synthesis techniques include encapsulation of metal nanoparticles within porous oxide shells to generate core-shell type catalysts using wet chemical techniques, the application of oxide overcoat layers through atomic layer deposition or similar techniques, and spontaneous formation of metal oxide coatings from more conventional catalyst geometries under reaction or pretreatment conditions. Oxide-coated metal nanoparticles have been applied for improvement of catalyst stability, control over transport or binding to active sites, direct modification of the active site structure, and formation of bifunctional sites. Following a survey of recent studies in each of these areas, future directions of inverted catalytic systems are discussed.

Keywords: metal-oxide interfaces; core-shell structure; atomic layer deposition; strong metal-support interactions; sintering; bifunctional catalyst

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