

Understanding the catalytic activity of molybdenum carbide surfaces: *what we can learn from surface-mobility of reaction intermediates*

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Abstract

Transition metal carbides (TMCs) are recognised as the cheap alternative to the rare-expensive noble metals such as platinum, palladium, and Ruthenium [1]. This is obvious from similar electronic properties these materials share with noble metals. As a result, there has been great interest in the application TMCs in catalysis, in particular molybdenum carbides as catalysts and catalyst support materials. Many studies show molybdenum carbides as highly active CO₂ activation, dehydrogenation, and water gas shift (WGS) catalysts (and supports) [1-3].

In recent works of Ma and co-authors, α -MoC supported Pt and Au clusters showed extraordinary activities towards hydrogen production via the WGS reaction at ambient temperatures [2,3]. However, with limited surface coverage of α -MoC surfaces with Pt/Au, the observed activity quickly diminishes. Experimental work suggests that this deactivation (rapid decrease in activity) is associated with partial surface oxidation – occurring due to stable and immobile hydroxyl intermediates. Limited density functional theory (DFT) calculations are performed to understand the activity of these systems. However, the mobility of various reaction intermediates on these surfaces remains relatively unexplored. Furthermore, the assumed surface is based on experimental observation – this however does not exclude the presence of other surfaces. We have used the CHPC (CPU nodes) resources to explore the mobility and reactivity of various reaction intermediates on α -MoC(111) surface. Additional data over the more stable α -MoC(100) has also been generated. To our surprise, over the observed surface all reaction intermediates are extremely mobile while over the α -MoC(100) surface the converse is true. In this talk we will discuss these findings and their implication on catalyst design where α -MoC is considered as either an active phase or catalyst support.

References

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