Cost-Effective Catalysis on Early Transition Metal Carbides

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Most of the reactions carried out in the industry are catalyzed on the surface of materials, which oftentimes are late transition metals, given its ideal properties as catalytic active phases. However, coinage and Pt-group metals can be quite expensive mainly due to their scarcity, which leaded to the utilization of metal nanoparticles supported on oxide supports, thus partially alleviating the economic burden.

Early transition metal carbides have been introduced in the last decade as a low-cost alternative to late transition metals. Beyond the comparable electric and thermic conductivities, they present physical robustness, and, eventually, a catalytic activity comparable, or even superior, to late transition metals.[1] Here we show, by *ab initio* density functional calculations combining experimental results, how different surfaces of such carbides are adequate catalytic active phases for a variety of reactions, including the water-gas-shift reaction[2] and the dissociation of small molecules, such as O_2 and even CO_2.[3] Moreover, theses carbides result to be excellent supports for late transition metal clusters, playing also the role of promoters; the carbide surface is able to polarize the late transition metal electron density,[4] leading to an enhanced catalytic activity, as shown to be critical in the decomposition of sulfur-containing species such as SO_2 and tiophene.[5,6] Future fields of applications are envisaged.

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