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Dynamic surfaces of MAX phase and MXene in catalytic processes

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The MAX phases are novel structural and functional ceramics with a layered ternary carbides structure discovered in the ‘60s.(1) They are so-called MAX because of their composition: namely, Mn+1AXn, where M is an early transition metal, A is mainly a group IIIA or IVA (i.e., groups 13 or 14) element, X is C and/or N, and n= 1 - 4. The applications of solid MAX phases are narrow due to their metallic, high-temperature stabilities, and superior mechanical properties, but when they are exfoliated into 2D MXenes they exhibit quite different electronic, magnetic, optical, and electrochemical properties that are rarely seen in their original MAX phases.(2)
These newly discovered 2D metal carbides (MXenes), and their 3D parents (MAX phase), hold promises to possess interesting catalytic properties (3) due to a bouquet of particular properties such as good electronic conductivity, hydrophilicity, resistance to chemical attack and oxidation under high-temperature conditions. These properties are strongly related to their very rich surface functionality formed during wet-etching synthesis of MXenes from MAX phases, when functional groups such as –O,–OH, and –F are formed on the surface.
Yet, little is known about the dynamics of the surface and structural changes that these systems undergo during catalysis and lead to efficient catalyst function. Recently, we investigated at the X07DB-In Situ Spectroscopy beamline at the Swiss light source synchrotron the dynamics of the surface and subsurface rearrangements of the MAX phase (Ti3SiC2) and MXene (Ti3C2Tz) under steady state O2 and/or CH4 environment at different temperatures (between room temperature and 350 ˚C). In this way, the impact of reduction and oxidation conditions was assessed. Sensitive surface and subsurface in situ XPS spectra were obtained at different kinetic photoelectron energies (300 and 600 eV). The influence of water on surface dynamics was also studied. As expected, the surface is “alive”and reversible surface modifications were observed, indicating the presence of a possible “memory”phenomenon.
The most important outcome of this study was the appearance of OH surface species in the presence of CH4 onto the MXene surface. One possible explanation for this finding is that CH4 might be activated on the metal species, then one C–H bond is broken and the resulting H is immediately attached to the O species on the surface. Furthermore, a good stability of the of MAX phase and MXene throughout the AP-XPS experiments was confirmed. These are valuable findings for further understanding of the MAX phase and MXene behaviour in catalytic processes.

if ”Other”, please specify:

I apply for a travel grant

No

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