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Determination of Molybdenum Species Evolution during Non-Oxidative Dehydroaromatization of Methane and its Implications for Catalytic Performance

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Methane dehydroaromatisation reaction (MDA) is of increasing industrial interest to convert methane directly into benzene, valuable precursor for the chemical industry. Mo-containing zeolites are promising catalysts for MDA, Mo species activate methane while the zeolite pores provide shape selectivity to benzene; however, the rapid material deactivation due to carbon deposit accumulation compromises the commercialisation of the reaction.
In order to shed light into the catalyst working mechanism/deactivation, the evolution of Mo species in Mo/zeolites has been investigated by means of operando X-ray absorption/diffraction techniques (XAS/XRD). XAS results revealed that in contact with methane, initial tetrahedral Mo-oxo species attached to the zeolite are carburised to MoxCy, which showed to be selective to aromatics. XAS/XRD studies evidenced the detachment of MoxCy from the zeolite and their migration outside the pores; this would result in the loss of shape selectivity to aromatics explaining the increased carbon deposit formation overtime and catalyst deactivation. At short reaction times, MoOx and MoOxCy species are believed to coexist and to show selectivity to ethylene, also of interest for the chemical industry. Collaboration with SuperXAS to perform modulated quick-XAS measurements combined with multivariate curve resolution (MCR) analysis will help to discriminate among the different Mo species evolving under reaction conditions and to evaluate their selectivity/stability.

Position

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