**Deciphering the mechanism of oxo-V(V) species prevalence on TiO2 support under different environments.**

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**ABSTRACT**

Nowadays, following the strategy of emission control, the utilization of catalysts to mitigate multi-pollutants, including NOx, has been adopted. Within this frame, the knowledge-based design and operation of commercially used catalysts is paving the way for studing structure-reactivity relationships for several materials. Specifically, large research effort has been directed towards understanding the selectivity of V2O5/TiO2 SCR catalysts by studying the metal oxide configurations on the support [1], [2]. Although a variety of Raman studies describes the heterogeneity of surface vanadia structures at sub-monolayer coverage[3], fundamental issues regarding how the surface loading, the oxide support and the different environments do affect the surface vanadia species still remain [4] .

A rigorous study of the dispersed oxo-V(V) species on TiO2 support (Degussa P25, anatase), under dehydrated conditions, for catalysts with sub-monolayer coverage, aims to interpret the temperature and the loading effect on the deposited VOx configurations prevalence. The equilibrium deposition filtration method (EDF) was selected as a molecular-level approach to synthesize VOx/TiO2 supported catalysts. Then, the combination of *in situ* Raman and IR studies, under oxidative conditions, for a temperature range below the calcination point, constitutes the spectroscopic tool to discriminate the local structures of the deposited VVOx species. Special attention has been drawn to the impact of support surface hydroxyls retained after calcination on the prevalence of each species, by means of a neoteric Raman study under static equilibrium conditions. Additionaly, the combined exploitation of *in situ* Raman with 18O/16O isotope exchange sheds further light on the termination configuration of the dispersed (VOx)n sites under oxidative dehydrated environment. Lastly, the temperature and loading evolution study under flowing NH3 stands as a starting point towards deciphering the mechanism governing the SCR process.

Therefore, this study validates the scenario of tuning in a reversible and reproducible manner the prevalent (VOx)n sites dispersed on titania, and hence their catalytic behaviour, by controlling the temperature and the surface coverage.

**KEYWORDS:** vanadia/titania catalysts ; local structures; temperature evolution; in situ spectroscopy; surface hydroxyls

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