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Transient *operando* study on the NH_3/NH_4^+ interplay in V-SCR monolithic catalysts

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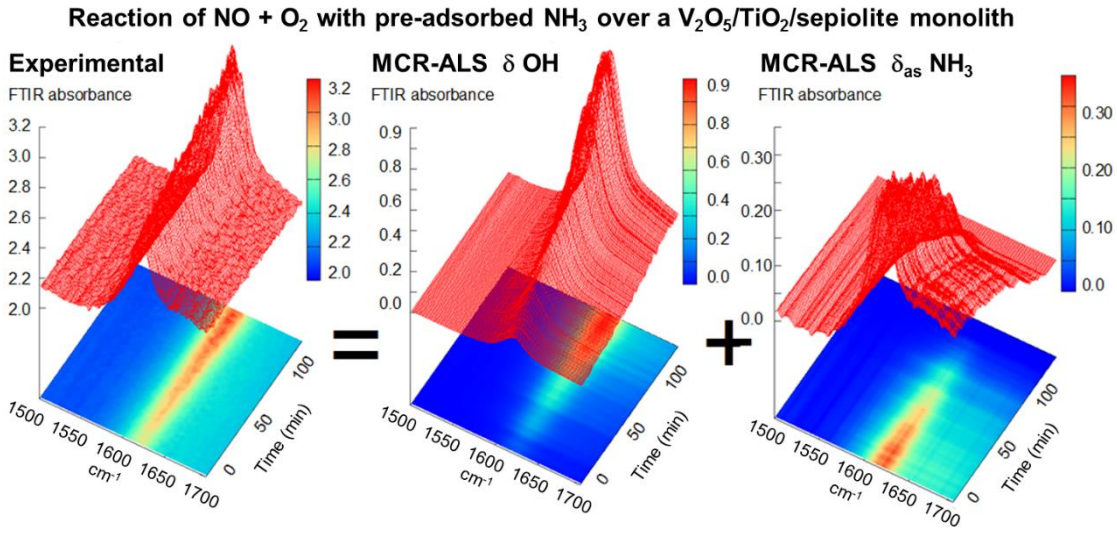
Graphical abstract



Highlights

- Transmission IR *operando* rig to follow NH_3-to-$NO+O_2$ transient on V-SCR honeycomb
- Chemometrics resolves adsorbed H_2O and NH_3 contributions to ~ 1620 cm^{-1} IR band
- Water formed upstream hydrolyzes dispersed vanadia creating Brønsted acid sites
- Spatial effects in integral reactor complement fundamental observations on powder

1 Abstract

The assessment of an integral catalytic reactor facilitating *operando* spectroscopic measurements on a monolith has been carried out using NH_3-SCR on a vanadia-based catalyst as a probe reaction. The NH_3-SCR mechanism is revisited by studying the adsorbed ammonia and ionically bound ammonium ions and their relations to Lewis and Brønsted acid sites during reaction. The simultaneous presence of molecular water and ammonia adsorbed on the surface is intrinsic to low temperature NH_3-SCR, and their IR absorption bands overlap in the bending region around 1600 cm^{-1}. This has to be tackled in order to genuinely reproduce real reaction conditions and simultaneously extract relevant spectroscopic data of a working