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## Dispersion studies of VO<sub>x</sub>/WO<sub>x</sub>/TiO<sub>2</sub> catalysts: the importance of combining Raman and IR spectroscopies

The emission of nitrogen oxides (NO<sub>x</sub>) produced by fuel combustion poses a significant threat to both air quality and public health [1,2]. To address this problem, the current technology used to comply with the imposed restrictions is based on the selective catalytic reduction of NO<sub>x</sub>, with NH<sub>3</sub> (NH<sub>3</sub>-SCR) [3], where the NO<sub>x</sub> and NH<sub>3</sub> react in the presence of O<sub>2</sub>, to produce N<sub>2</sub> and H<sub>2</sub>O [3–5]. The commonly used catalysts for NH<sub>3</sub>-SCR in stationary plants and heavy-duty diesel vehicles are based on vanadium oxide supported on anatase TiO<sub>2</sub> with tungsten (W) used as promoter (VO<sub>x</sub>/WO<sub>x</sub>/TiO<sub>2</sub>) [5].

This work utilizes Raman and infrared (IR) spectroscopy to study the dispersion of  $VO_x$  and  $WO_x$  species on the TiO<sub>2</sub> surface, a critical factor for catalyst performance.

Raman spectroscopy is commonly employed to evaluate the dispersion of VO<sub>x</sub> and WO<sub>x</sub> species on the TiO<sub>2</sub> surface and the corresponding monolayers through the identification of V<sub>2</sub>O<sub>5</sub> and WO<sub>3</sub> crystalline phases, but distinguishing between V-O-V and V-O-W signals in mixed VO<sub>x</sub>/WO<sub>x</sub>/TiO<sub>2</sub> systems is challenging.

The use of resonance-enhanced Raman signals, alongside complementary IR data, provides valuable insights into surface species distribution.

Our results indicate crystalline phases of  $V_2O_5$  and  $WO_3$  at surface densities of 6.4 V and 5.3 W atoms/nm<sup>2</sup>, respectively, as measured by Raman, while IR-based titration of Ti<sup>4+</sup> surface sites on TiO<sub>2</sub> with CO molecules, yielded slightly different values of 5.7 V and 5.2 W atoms/nm<sup>2</sup>. Interestingly, WO<sub>3</sub> appears before full surface coverage of TiO<sub>2</sub>, suggesting early agglomeration, while  $V_2O_5$  emerges after complete surface saturation. These findings highlight the necessity of combining both Raman and IR techniques to fully characterize the dispersion of oxides on catalyst surfaces, providing a more accurate understanding of monolayer formation and catalytic behavior.

## References

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