

Mechanism of NO_x Chemisorption on Solid Phosphotungstic Acid

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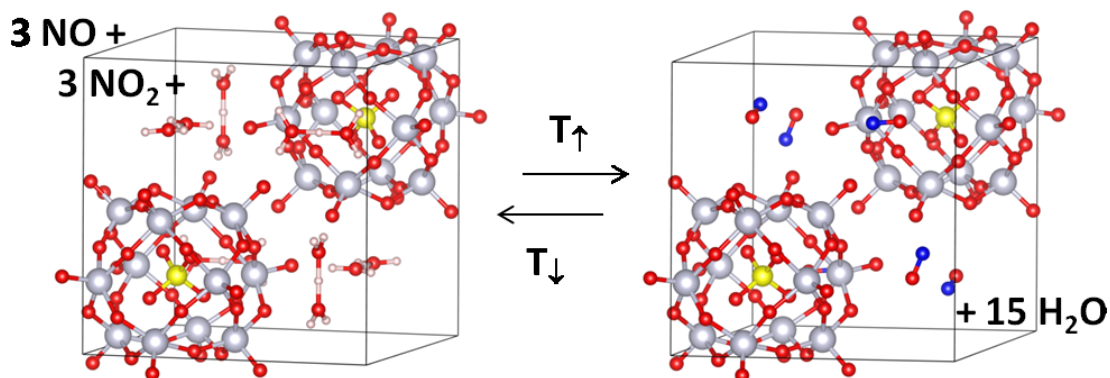
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Nitrogen oxides (NO_x) -mostly caused by the combustion of fuels- contribute to the formation of ozon, smog and acid rain. Therefore, it is desired to remove them from the exhaust gases. Phosphotungstic acid is a selective NO_x adsorbent with high adsorption capacity that could be used for this purpose.

A variety of experimental and computational approaches - including ex-situ and in-situ X-ray diffraction, neutron diffraction, NMR and DFT calculations - determined the nature of the chemisorbed NO_x species and elucidated the reaction behavior. This knowledge will allow optimization of the adsorbent material for application in after-treatment systems for NO_x elimination.



NO_x adsorption is favorable at high temperatures, whereas desorption occurs at lower temperature. A combination of experiments and DFT calculations elucidated this behavior.