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The Adsorption and Desorption of NH_3 on Rutile TiO_2(110)–1×1 Surfaces

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The adsorption of molecular NH_3 on rutile TiO_2(110)-1×1 surfaces was investigated using a temperature-programmed desorption (TPD) technique combined with a molecular beam apparatus. A quantitative investigation into the TPD spectra of NH_3 was made for NH_3 adsorbed on two kinds of rutile TiO_2(110)-1×1 surfaces with the oxygen vacancy (V_O) concentration of ~0% (p-TiO_2(110)) and ~5% (r-TiO_2(110)), respectively. On both surfaces, non-dissociative adsorption of NH_3 was inferred from a quantitative analysis on the amount of adsorbed NH_3 and those desorbed. With increasing coverage, the monolayer desorption feature shifted from 400 K toward lower temperatures until it saturates at 160 K, suggesting a repulsive nature in the interaction between NH_3 molecules. At the very low coverage regime, the desorption features were found to extend up to 430 K and 400 K on p-TiO_2(110) and p-TiO(110), respectively. As a result, the saturation coverage of monolayer of NH_3 was higher on the p-TiO_2(110) surface than on the p-TiO(110) by about 10%. The desorption energy (E_d) of NH_3 obtained by inversion of the Polanyi-Wigner equation indicated that the difference between the E_d's of NH_3 (that is, E_d(on p-TiO_2(110)) - E_d(on p-TiO(110)) was 14 kJ/mol at $\theta(NH_3)$ = 0 and decreased to 0 as the coverage approached to a monolayer. The observed adsorption behavior of NH_3 was interpreted using an interaction model between NH_3 and surface defects on TiO_2 such as V_O's and Ti^{3+} interstitials.

Keywords: TiO_2(110), NH_3, Temperature-programmed desorption, TPD, Desorption energy