Understanding the acid behavior of monomeric V on TiO_2 from DFT calculation and DRIFT experiments

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V_2O_5/TiO_2 system is widely used in various reactions including ethanol partial oxidation, oxidative dehydrogenation of light alkanes, and selective catalytic reduction of NO_x. Since the adsorption of reactants on the catalyst surface is known to be an inevitable step in many reactions, there are many reports correlating the acidity of the catalyst and the catalytic performance. Therefore, understanding the acidic nature of the V/TiO_2 surface is quite important in anticipating catalytic behavior. In this study, we optimized the configuration of monomeric vanadium oxides on anatase TiO_2(101) surface using DFT calculations to find out the adsorption sites of NH_3 molecules. These results explained the formation of Bronsted acid sites on V/TiO_2 surface, which are not observed in pure TiO_2. Combined DRIFT study also demonstrates that monomeric V can act as a Lewis acidic site as well as Bronsted acidic site.