Effects of Crystal Phase and Reduction Treatment on the Mercury Oxidation Activity of VO_x/TiO_2 Catalyst: A DFT Study

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Mercury (Hg) has been considered hazardous because of its toxicity and bioaccumulation property. Stationary combustion source still emits significant amounts of flue gas containing the elemental form of Hg (Hg^0). Although the Hg^0 is very difficult to remove as it is insoluble and hard to capture without additional treatments, VO_x/TiO_2 catalyst, known as SCR catalyst, can oxidize the Hg^0 into Hg^{2+} which is soluble and easily removed. Here, Hg oxidation activity was investigated using density functional theory (DFT) calculations based on the Eley-Rideal (E-R) mechanism. By using reduced and bare TiO_2 with anatase phase and those with rutile phase, the effects of TiO_2 phase and reduction treatment on the activity were studied; notably, the oxygen vacancy on the reduced TiO_2 led to structural transformation of V_2O_5, thus changing the oxidation state of V from 5+ to 4+. This work demonstrates the necessity of cautious pre-treatment of TiO_2 support and gives a guidance about which TiO_2 phase should be chosen to achieve improved Hg oxidation activity.