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First-Principles Studies on Deoxidizing Mechanism of V_2O_5 via Hydrogen[1] YANNING ZHANG, University of Electronic Science and Technology of China, MENGTING JIN, Chengdu Green Energy and Green Manufacturing Technology RD Center — With its high melting point, good plasticity and good corrosion resistance at low temperatures, vanadium has been widely used in the industries of iron and steel, aviation, energy storage, etc. However, the traditional manufacturing technologies of pure vanadium are usually connected with complex manufacturing processes, high costs and serious environment pollution, which more or less hindered its further applications. Recently, hydrogen gas has been considered as a promising reducing agent of V_2O_5, but experimental studies of deoxidization process of V_2O_5 single crystal surfaces were found to be extremely difficult. In this work, we perform extensive *ab initio* studies on the structural and electronic properties of different V_2O_5 surfaces, as well as the adsorption sites, diffusion and desorption processes of H on these surfaces as a dependence of depth. We found that H atoms adsorb at oxygen site to form surface hydroxyl (OH^-) and further to form H_2O on V_2O_5(010) surfaces, and the latter is easier to be desorbed compared with the former. But the desorption of H_2O causes significant surface reconstructions, which makes the further deoxidization of V_2O_5 difficult, particularly on the V_2O_5 single-layer. Our theoretical results are instructive for understandings of the reduction mechanism of V_2O_5 by using a green agent of H_2, and furthermore for the design of new experiments.

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