Stability of V2O5 Supported on Titania in the Presence of Water, Bulk Oxygen Vacancies, and Adsorbed Oxygen Atoms

A catalyst consisting of vanadium oxide submonolayers supported on rutile titanium dioxide is used for a variety of reactions. One important question is the difference between the activity of monomeric clusters (having one vanadium atom) and polymeric clusters (having more than one vanadium atom). In the case of oxidative dehydrogenation of alkanes and methanol, the reaction produces water, oxygen vacancies, and hydrogen atoms bound to the surface. For this article we use density functional theory to examine how the presence of these species on the surface affects a V2O5 cluster, which we assume to be a representative of a polymeric species. We find that often the presence of other species on the surface can change the composition of the cluster or break it up into two monomeric clusters.