

CLUSTER APPROACH TO CHEMISORPTION AND CATALYSIS

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We present here the results of DFT calculations on the chosen three examples to show the ultimate importance of proper modeling of structure and chemical activity of transition metal and metal oxide catalysts.

First we consider the formation of oxygen vacancy site on rutile $\text{TiO}_2(110)$ and its interaction with molecular oxygen. The experimental TPD observation on triply exceeding concentration of O_2 per vacancy site at low temperature saturation coverage can be well explained without making an assumption on the formation of O_4 particle at the vacancy site if one properly address the mechanism of formation of precursor defect sites on rutile $\text{TiO}_2(110)$. Next the mechanism of the selective oxidation of methanol into formaldehyde over vanadia supported on silica and titania catalysts will be discussed. An improper use of cluster models mimicking an intrinsic support structure may result in the failure to explain the experimental findings on selective oxidation of methanol into formaldehyde over these modified oxide catalysts. Finally, an attractive bonding interaction not only for bromine and $\text{Pt}(111)$ but also for all the three adsorption modes of NO on the $\text{Pt}(111)$ surface will be explained within the conventional cluster approach.

Based on these results obtained, some discrepancies with the results of other theoretical studies in literature will be critically pointed out.