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Comparative study of the adsorption of aromatic pollutants onto TiO₂ (100) surface via molecular simulation

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Simulation of the saturated anatase TiO₂ bulk cluster

The extended saturated three layer cluster, Ti₃₆O₉₀H₃₆, has been simulated through the MSINDO method. Subsequently, it is used for modeling the (100) anatase surface, which is normally observed in powder materials [U. Diebold, Surf. Sci. Rep. 48 (2003) 53]. The cluster models are often selected for local processes such as adsorption of single atoms and molecules. The free cluster approach, however, has some disadvantages. For example, cluster atoms with lower coordination than in the bulk or at the surface, so-called border atoms, show artifacts like dangling bonds [M. Witko, K. Hermann, R. Tokarz, Catal. Today 50 (1998) 553]. Such type of artifacts cause spin localization at low-coordinated corner and edge atoms, which, consequently, exhibits an artificial lowering of the energy [T. Homann, T. Bredow, K. Jug, Surf. Sci. 515 (2002) 205] . In order to avoid such boundary effects we have saturated all peripheral oxygen atoms of free Ti₃₆O₇₂ cluster with hydrogen atoms and all less than five fold coordinated titanium atoms with OH groups so that the cluster, Ti₃₆O₉₀H₃₆, is formally saturated with water (Fig.1). This technique is often applied to metal oxides of partially covalent nature [K. Jug, Int. J. Quantum Chem. 58 (1996) 283] , and is appropriate particularly for semiconductors.

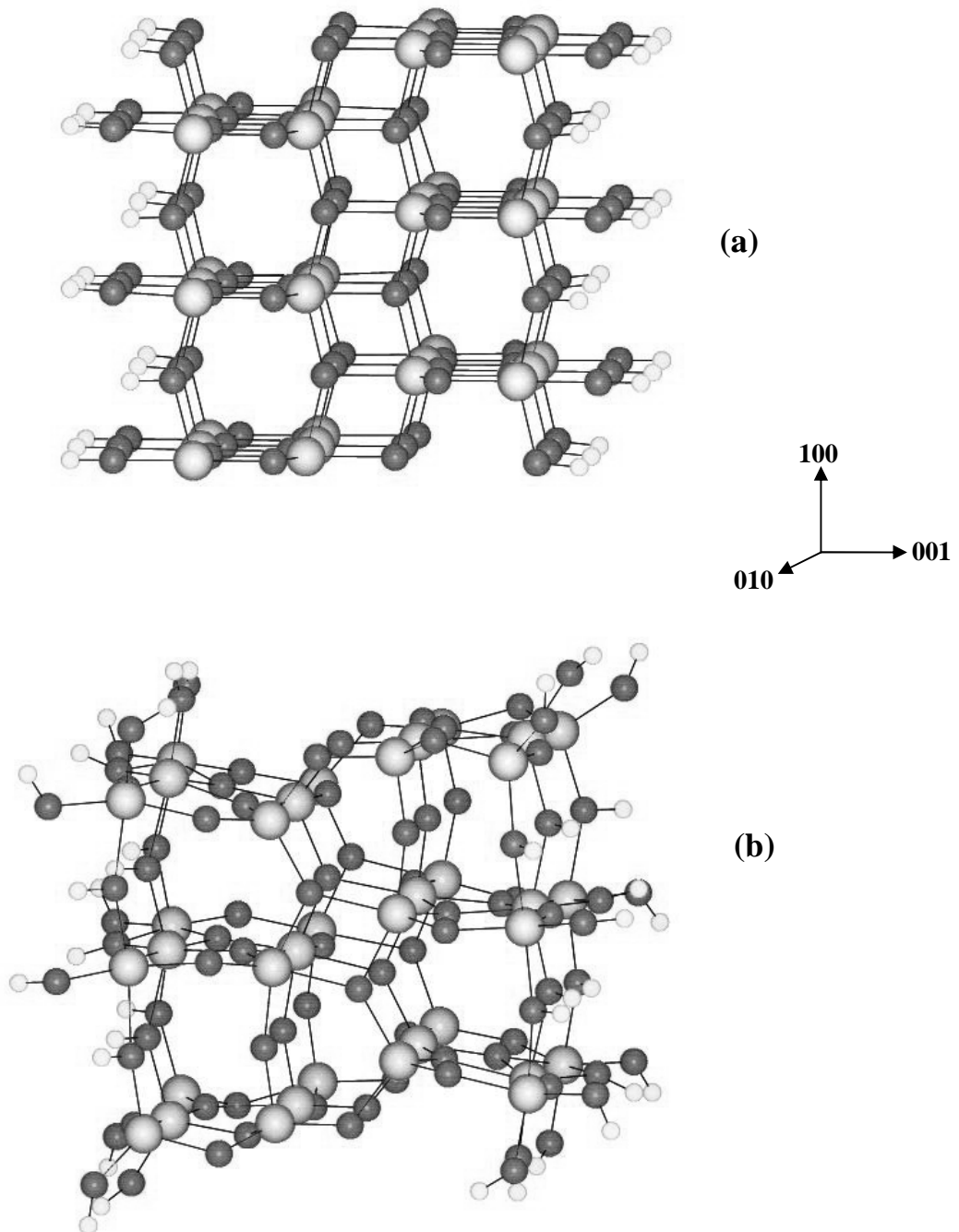


Figure 1. (a) Non-relaxed saturated $\text{Ti}_{36}\text{O}_{90}\text{H}_{36}$ cluster; (b) Minimum energy structure of $\text{Ti}_{36}\text{O}_{90}\text{H}_{36}$. Large light spheres represent titanium atoms, the dark spheres represent oxygen atoms and small light spheres represent hydrogen atoms .