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Born-Oppenheimer Molecular Dynamics Simulation of Pentanoic Acid Adsorption on α-Al_2O_3

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Abstract

Adsorption of a single pentanoic acid ($C_5H_{10}O_2$) molecule on (0001) α-Al_2O_3 in a vacuum was explored with the aid of Born-Oppenheimer molecular dynamics simulations. Computer simulations were carried out considering two different situations, namely a clean Al/O-terminated surface and, also, a (0001) α-Al_2O_3 surface saturated with doubly-coordinated, isolated hydroxyls. In the first case, pentanoic acid adsorbs dissociatively, with the creation of an isolated surface hydroxyl, while the oxygen from the molecule's former carbonyl makes a bond to a nearby surface Al. On the other hand, pentanoic acid adsorbs on hydroxylated alumina by making a strong hydrogen bond to a surface oxygen, with the molecule aligning itself nearly parallel to the surface after full relaxation. For each case (i.e., pentanoic acid adsorption on Al/O-terminated or hydroxylated corundum surface), the different adsorption mechanism has a marked impact on the respective calculated infrared absorption spectrum, which can be of further use as an analytical tool to determine the underlying adsorption mechanism in actual experiments.

Keywords: α-Al_2O_3, pentanoic acid, adsorption, molecular dynamics

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