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DFT study on the partial oxidation mechanism of benzyl alcohol to benzaldehyde by O_2 on TiO_2 surface under visible-light irradiation

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The selective photocatalytic oxidation of benzyl alcohol by O_2 on the TiO_2 surface was theoretically studied by DFT calculations. Experimentally, it is well known that benzyl alcohol is oxidized to benzaldehyde, but cannot be further oxidized to benzoic acid, and TiO_2 surface itself is insensitive for the visible light, but becomes sensitive by benzyl alcohol adsorption. These phenomena were clarified by the plane wave based DFT calculations. Dehydroxylated and partially hydroxylated TiO_2 with an anatase TiO_2 (101) crystal face were modeled with a slab of $Ti_{16}O_{32}$ and $Ti_{16}O_{32}(OH)H$, respectively. It was found that the interaction of benzyl alcohol with the hydroxylated TiO_2 surface significantly induces the formation of the alkoxide species, of which the donative orbitals hybridized with the O_2 p orbital in the valence band (VB) of the TiO_2. The visible light response is attributed to the electronic transition from the donor levels created by the alkoxide species to the conduction band (CB). The dissociation of methylene C-H in the alkoxide was assisted by O_2, and this process was confirmed to be the rate-determining step. Furthermore, the hydro-peroxide (OOH) species formed by O_2 reduction can also oxidize another benzyl alcohol into benzaldehyde together with Ti-OH regeneration. It was thus clearly demonstrated that two benzaldehyde molecules were formed from two benzyl alcohols and one O_2 molecule on the TiO_2 photocatalysis.

Biography

Hisayoshi Kobayashi is a Professor of Kyoto Institute of Technology. He got his Doctorate degree from Kyoto University in 1982 under Professor Kenichi Fukui. His field of research is theoretical analysis of catalysis of metal and metal oxide surfaces. He received the Award from the Catalysis Society of Japan in 1989, and the BCSJ Award Article from the Chemical Society of Japan in 2007. He has worked at the Nippon Sheet Glass Co., and at the Kinki University as a Professor.

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