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Photoemission study on the reactivity of organic molecules on chemically modified TiO2(001) surfaces

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Adsorption and subsequent catalytic reactions of ethanol and acetaldehyde on chemically modified rutile TiO2(001) surfaces are probed by x-ray photoemission spectroscopy (XPS) using synchrotron radiation. TiO2 is a well-known photocatalyst for various catalytic reactions including oxidation of organic molecules. In this respect, the surface atomic structure has been found to play a vital role in determining the catalytic reactivity and selectivity of TiO2. In this study, we employ an atomically well-ordered reduced TiO2(001) surface which is prepared in a UHV chamber by repeated Ar+ -sputtering and annealing (900 K) cycles. We systematically modify the surface by treating the surface with H2O or O2 at room temperature (RT). The catalytic reactivity of the surface-modified TiO2(001) is evaluated by dosing ethanol/acetaldehyde onto the surface at RT and by subsequent annealing to higher temperatures (400～600 K). XPS spectra of C 1s core level are intensively used to probe any change in the oxidation state of carbon atoms. We find that the reactivity as well as the saturation coverage are significantly affected by the RT-treatment of the TiO2 surface with H2O or O2. For both reactant molecules (ethanol/acetaldehyde), oxidation reactions are found to be enhanced on the O2-treated surface compared with the reduced or H2O-treated surfaces. Possibly reaction pathways are discussed based on the observed XPS spectra.