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Hydrogen elimination and migration reactions in the desorption of alcohols on Si(100) surfaces

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The thermal decomposition of alcohols on clean Si(100)-2×1 in ultra-high vacuum has been examined using temperature programmed desorption (TPD), integrated desorption mass spectrometry (IDMS), and low energy electron diffraction (LEED). The adsorption of an alcohol on clean Si(100) has been expected to make an alkoxy species with adsorbed hydrogen. The alkoxy species formed on Si(100) are stable up to temperatures of about 500 K. Above 500 K the alkoxy species with γ -hydrogens decompose on Si(100) via the γ -hydrogen elimination mechanism to yield alkene in the gas phase, together with adsorbed hydrogen. In contrast, the alkoxy species with no γ -hydrogen decompose on Si(100) via the hydrogen migration mechanism to yield an alkane in the gas phase. The hydrogen migration mechanism was confirmed by the thermal study of the deuterium-labeled molecules. The H₂ gas is evolved by the recombinative desorption of hydrogen atoms that are generated by the adsorption of alcohols and/or the decomposition of alkoxy species.