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Self-assembled monolayer by dissociative chemisorption: Methanol on Ge(100)

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The adsorption and reaction of methanol (CH_3OH) on Ge(100) has been studied using ultrahigh vacuum scanning tunneling microscopy (UHV-STM) and density functional theory (DFT) calculation. At low coverage, the high resolution STM image reveals that methanol undergoes O-H bond dissociative adsorption on a single Ge-Ge dimer. The real-time STM measurement shows that the methanol gradually grows to be molecular chain by successively dissociative adsorption along the dimer row direction as exposure of molecule increases. The saturation coverage is made by extension of these molecular chains. The DFT calculation results show that the O-H bond dissociative adsorption is kinetically more favorable than the C-O bond dissociative adsorption at room temperature, although the final product by the C-O bond dissociative adsorption is thermodynamically the most stable geometry. From STM and DFT calculation results, we conclude that the adsorption structure of methanol on Ge(100) is attributed to CH_3O-Ge-Ge-H geometry by the O-H bond dissociation on the single dimer at room temperature.