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Comparative study of cycloaddition reactions of ethylene and acetylene on Ge(100)

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The interaction of unsaturated hydrocarbon molecules, such as acetylene (C_2H_2) and ethylene (C_2H_4) with group Ⅳ semiconductor surfaces have been the subject of numerous investigations. In reviewing earlier works, these molecules show various adsorption structures on top structure (adsorbed on top of the Ge dimer), end-bridge structure(bound to the one side of two adjacent Ge dimers), bridge structure(tetracoordinated to two adjacent dimers), and paired end bridge structure(consisted of two end bridge structure across two adjacent dimers).

In this presentation, I will focus on three new points of these adsorption structures and interactions of ethylene/Ge(100) and acetylene/Ge(100) investigated using real-time scanning tunneling microscopy (STM) and density-functional theory (DFT) calculations. First, the diffusion of ethylene and acetylene on Ge(100) surface was investigated in the temperature range between 300 K and 550 K. The activation energy for thermal motion was determined by imaging individual molecular displacements with a scanning tunneling microscopy. And the attractive interactions between adsorbed molecules gave rise to the formation of dimers and longer chains. Second, I will compare the strength of attractive interaction between ethylene-ethylene and acetylene-acetylene. I also elucidate the reason inducing the different attractive interaction using DFT calculation. Finally, I will introduce the new method inducing 1D long range molecular line by inducing selective molecular adsorption and desorption.

This work is focused on the fundamental reaction chemistry and the development of strategies to obtain selectively attached monolayer for applications in molecular electronics, chemical sensing, and ultra thin film deposition.