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Initial adsorption structure of ethylene on Si(001) surface at room temperature

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Ethylene (C_2H_4) on the Si(001) surface has been a subject of numerous investigations over a decade. Despite a wealth of experimental and theoretical studies, the adsorption structures are not clearly understood yet. In order to elucidate this controversial issues clearly, C_2H_4 molecules have been non-dissociatively chemisorbed on Si(001)-(2×1) surface at room temperature with an exposure of 100L, and C2H4 on Si(001) surface structure has been investigated by coaxial impact collision ion scattering spectroscopy (CAICISS). To determine the adsorption structure of the C_2H_4 molecules definitely, the computer simulation with the two-dimension trajectory count method has been performed for the recently proposed most possible four single molecular adsorption configurations (di-σ on-top, di-σ end-bridge, tetra-σ p-bridge, and tetra-σ r-bridge). The CAICISS spectra and simulation results show that the di-σ on-top structure is better fit than the di-σ end-bridge and two tetra-structures. It is found that the bond length of Si dimer separation on the Si(001) surface with the adsorption of C_2H_4 is 2.35 Å, this implies that the bonding of Si dimers stays intact. It is also found that the bonding length of C-Si and C-C is 1.81 ± 0 01 Å and 1.61 ± 0.01 Å, respectively.