

Footprints of water molecules on Si(001) and co-adsorption configurations obtained via low temperature scanning tunneling microscopy

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Water adsorption on Si(001)-c(4x2) surface is investigated at low temperature by using scanning tunneling microscope (STM) and ab initio pseudopotential calculations. H₂O configurations of single and cluster of two molecules reveal “Y”, “X” and “W” depressions as footprints on the surface. Atomic structures of H₂O molecules, which are dissociatively adsorbed on the Si(001)-c(4x2) surface, are studied with simulated and STM images of the filled states. The generation processes of the growth configurations are systematically considered with elapsed time.