(SP-09)

Adsorption Geometry of Multifunctional Organic Molecule: *cis*-2-butene-1,4-diol on Si(100)-2×1

Sung-Soo Bae, Sehun Kim
Department of Chemistry and School of Molecular Science (BK 21),
Korea Advanced Institute of Science and Technology

Adsorption of *cis*-2-butene-1,4-diol (cBeDo, HO-H_2C-HC=CH-CH_2-OH) on Si(100)-2×1 has been studied using ultrahigh vacuum-scanning tunneling microscopy (UHV-STM) and *ab initio* calculations. At low coverage, the STM study shows that cBeDo adsorbs onto the Si(100) with two distinct bright features: (i) on-top (OT) geometry at a single Si-Si dimer, (ii) end-bridge (EB) geometry between two adjacent Si dimers within the same dimer row. High resolution STM images reveal that the OT and EB geometries are formed by two Si-O covalent bonds through two O-H bond dissociation of cBeDo. The *ab initio* calculation results that the OT and EB geometries of the adsorbed cBeDo are energetically more stable than other adsorbed geometries on Si(100)-2×1. These calculated results are in good agreement with the STM results.