Abstract Submitted
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Dissociation pathways and multiple adsorption configurations of ammonia on Si(001)\(^1\) HANCHUL KIM, Korea Research Institute of Standards and Science, OPTI NAGUAN CHUNG, SUKMIN CHUNG, Pohang University of Science and Technology, JA-YONG KOO, Korea Research Institute of Standards and Science — The adsorption of ammonia (NH\(_3\)) molecules on the Si(001) surface has been investigated by combining the scanning tunneling microscopy (STM) and the \textit{ab initio} pseudopotential calculations. An NH\(_3\) molecule had been known to spontaneously dissociate into NH\(_2\) and H and form the so-called on-dimer configuration (OD). In OD, NH\(_2\) and H bond with two Si atoms of one Si dimer. However, our study shows that there exist two distinct configurations of NH\(_3\)/Si(001). One is the existing model of OD, which is found to be the lowest energy state. The other is identified to be an inter-dimer configuration (ID), where NH\(_2\) and H adsorb at two Si atoms at the same side of two adjacent dimers along the dimer row. The simulated STM images of OD and ID are in good agreement with experimental observations, proving the existence of two distinct adsorption configurations of NH\(_3\)/Si(001).

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