Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

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 *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).

[1]This work was supported by the KISTI under 'The sixth Strategic Supercomputing Support Program.

Hanchul Kim
Korea Research Institute of Standards and Science

Date submitted: 16 Jan 2006 Electronic form version 1.4