Abstract Submitted
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First-principles study of the self-organization mechanism of NH_3 on Si(001)[1] YONG-SUNG KIM, HANCHUL KIM, Korea Research Institute of Standards and Science — We have investigated the self-organization of NH_3 molecules on the Si(001) surface using the first-principles pseudopotential calculations. In order to find out the adsorption pathways and understand the mechanism of self-organization, we have calculated the potential energy surfaces of an incoming NH_3 molecule with one pre-adsorbed NH_3 molecule. Based on the results, we propose a kinetic process model of NH_3 self-organization: (i) the incoming molecules are attracted towards the pre-adsorbed molecules due to the H-bonding interaction. (ii) By forming the H-bond with the pre-adsorbed molecule, an incoming molecule can achieve physisorption states. (iii) Subsequently, the physisorbed NH_3 molecule is attracted to adjacent "down" Si atoms to complete the molecular adsorption process. (iv) Finally, the adsorbed NH_3 dissociates into NH_2 and H fragments. The resultant self-organized pattern is in accordance with recent STM experiments. However, it is in stark contrast with the energetically favored pattern that is characterized by H-bond formation between the dissociated fragments. This indicates that the self-organization of NH_3 on Si(001) is governed by the kinetics rather than the energetics.

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