

## [SP-04]

# Double dative bonding configuration: Pyrimidine on Ge(100)

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The Ge(100) surface was exposed to pyrimidine molecules at 300 K and the STM images of the pyrimidine adsorbed surfaces were recorded in real time. The oval shaped-bright spots are observed in the filled-state STM images and assigned to adsorbed pyrimidine molecules. We note that the pyrimidine molecules do not reside on top of the Ge dimers but induce the buckling of neighboring bare Ge dimers. The STM images suggest that pyrimidine molecules adsorb on the down-Ge atoms of the buckled Ge dimers by Ge-N dative bonding.<sup>(1)</sup> With the exposure of pyrimidine increased up to 0.25 ML, the well-ordered phase of  $c(4 \times 2)$  is formed. The ordered  $c(4 \times 2)$  structure indicates that pyrimidine molecules adsorb on every other dimer due to steric hindrance. Theoretically calculated STM images show that the lone-pair electrons of two N atoms in the pyrimidine molecule form two Ge-N dative bonds with the down-Ge atoms of neighboring Ge dimer rows to give the most stable configuration and the adsorbed pyrimidine molecule is tilted to the Ge surface.\* At 0.50 ML, bright but fuzzy zigzag lines are observed, which suggests that incoming pyrimidine molecules adsorb on the down-Ge atoms of every dimer in a zigzag way with less steric hindrance. In this way, the  $p(2 \times 2)$  structure is formed along the dimer row.

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[참고문헌]

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