

실리콘 표면의 1,3-부타디엔 분자의 흡착 구조에 관한 제일 원리 연구  
 Ab initio study of the adsorption structure of 1,3-butadiene on a Si(001) surface

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By employing *ab initio* total-energy calculations we have studied the adsorption of 1,3-butadiene molecule ( $C_4H_6$ ) on a dimer-reconstructed Si(001) surface. We have found that the [4+2] products are thermodynamically more stable than the [2+2] products. Two kinds of stable [4+2] products are found: (i) the well-known on-top di-sigma configuration over a single dimer and (ii) end-bridge ([EB]) configuration occupying two successive dimers in the same dimer row. In [EB] configuration at one mono layer (ML) coverage, 1,3-butadiene molecules at opposite end of dimer combine together to form cubane ( $C_8H_8$ )-like square geometry with one hydrogen atom at each apex, which is stabilized by converting remaining pi-bonds to sigma-bonds. The calculated core-level shifts (CLS) of C 1s orbital in stable configurations show little difference between peaks from interface C atom bonded directly to silicon surface and those from surface C atom with unsaturated double bond. We have also simulated the scanning tunnelling microscope (STM) image, which is in good agreement with experimental STM data.