Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Ab initio **study of the structure of 1,3-butadiene on a Si(001) surface** KI-JEONG KONG, BEYONG-HWAN RYU, YOUNG-MIN CHOI, JEONG-O LEE, KISEOK AHN, HYUNJU CHANG — By employing *ab initio* total-energy calculations we have studied the adsorption of 1,3-butadiene molecule on a dimer-reconstructed Si(001) surface. We have found that the [4+2] products are thermodynamically more stable than the [2+2] products. There are basically two kinds of [4+2] products: (i) the well-known on-top di-σ configuration over a single dimer and (ii) end-bridge configurations occupying two successive dimers in the same dimer row. In [EB] configuration at one ML coverage, 1,3-butadiene molecules at opposite end of dimer bond together to form cubane (C_8H_8)-like square geometry with one hydrogen atom at each apex, which is stabilized by the full compensation of dangling bonds and converting two π-bonds to two σ-bonds. The staggered end-bridge (s-[EB]) is also stable by strain release. By comparing the simulated STM images and experimental ones, we pointed out that the [EB] configuration shows similar feature to that attributed as [2+2] configuration in previous experiments. The calculated core-level shifts(CLS) of C 1s orbital show little difference between peak from interface C atom bonded directly to silicon and that from surface C atom with unsaturated double bond.

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Date submitted: 07 Dec 2004 Electronic form version 1.4