

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- σ 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 π -bonds to σ -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 tunneling microscope (STM) image, which is in good agreement with the experimental data.