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Quantum chemical studies of geometries and STM images of acetylene adsorbed on Ge (001)

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Ab initio MO and DFT methods are used to study the structure of the 2x1 reconstruction of the Ge(001) surface using cluster models and allowing subsurface relaxations. The dimer formation force strongly affects down to the fourth-layer atoms, while fifth - to deeper layer atoms relax only slightly. The formation of asymmetric dimers is characterized by a dimer bond length of 2.48A. Several cluster models have been tested to build a reasonable representation of the c(4x2) Ge (001) surface. Using a cluster model with two dimers, adsorption of one and two acetylene molecules on the surface has been tested. For the most stable geometry, the CC bond becomes essentially a double bond and the Ge dimer bonds are not cleaved. Overlapping and combining HOMO and HOMO-1 of many clusters, we are able to produce patterns which qualitatively correlate with scanning tunneling microscopy(STM) image of c(4x2), p(2x2) Ge (001) surfaces and C2H2 adsorption configuration on the Ge (001) surface.