ADSORPTION OF V GROUP METALS AND OXYGEN ON SILICON SURFACE Si(001)2× 1. 2. INTERACTION OF ATOMIC OXYGEN WITH As/Si(001) SURFACE

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An influence of atomic oxygen on the As/Si(001) surface is investigated by the MNDO- 3 semiempirical method. The potential energy surface for atomic oxygen adsorbed on the ideal As/Si(001) surface is calculated. There are found three equilibrium binding sites for atomic oxygen adsorption with formation of As¯O¯As, As¯O¯Si and Si¯O¯Si bridge structures. The formation of the last structure is the most energetically favourable. Trench-like defects, which are formed by missing rows of an As dimer on the As/Si(001) surface are simulated. First, an oxygen atom forms the Si¯O¯Si bridge structure with top silicon atoms in the trench and then forms the Si¯O¯Si bridge structures under the top Si layer.