INTERACTION OF AN OXYGEN MOLECULE WITH THE Si(001)2 × 1 SURFACE. INFLUENCE OF THE INITIAL SURFACE CHARGE

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S u m m a r y

The adsorption process of an oxygen molecule on the top of a dimer row on the Si(001)2 × 1 surface is investigated by the semiempirical MNDO-PM3 method. Adsorption of an oxygen molecule on the clean Si(001)2 × 1 surface, surface charged with elementary $Q = -1e$ charge, and silicon surface with an Bi adsorbed atom is examined. The activation energies for oxygen dissociation on Si(001)2 × 1 are equal 0.88, 0.85, 0.45, and 0.51 eV for the singlet and triplet system states, state with elementary charge, and for the silicon surface with an adsorbed Bi atom, respectively. The influence of initial charge on the dissociation process of an oxygen molecule is discussed. The probability of oxidation is shown to depend on the initial charge presence on the Si(001)2 × 1 surface.