STRUCTURE OF PURE Si–Si, Ge–Ge, AND MIXED Si–Ge ADDIMERS ON Si(001) SURFACE

T.V. Afanasieva, A.A. Greenchuck, I.P. Koval, M.G. Nakhodkin

Taras Shevchenko National University of Kyiv
(*64, Volodymyrs'ka Str., Kyiv 01601, Ukraine; e-mail: greenchuckaa@gmail.com*)

S u m m a r y

The adsorption of Ge on the Si(001) surface has been studied using *ab initio* quantum chemical (QM) and combined quantum-chemical–molecular-mechanical (QM/MM) cluster calculations. Multiconfigurational self-consistent field calculations that took the configuration interaction into account were performed to examine the geometric and electronic structures of pure Si–Si, Ge–Ge, and mixed Si–Ge addimers on the Si(001) surface. All addimers were found to possess a biradical character, being not tilted with respect to the surface. The bond lengths in Si–Si, Ge–Ge, and Si–Ge addimers were determined to equal 2.35, 2.45, and 2.41 Å, respectively. The formation of pure Ge–Ge addimers on the Si(001) surface was found to be more beneficial energetically than that of mixed Si–Ge addimers. The natural orbital occupation numbers (NOONs) of antibonding orbitals in Si–Si, Ge–Ge, and mixed Si–Ge addimer structures on the Si(001) surface were calculated to be 0.56, 0.65, and 0.66, respectively. The NOONs of antibonding orbitals for surface dimers was found to be 0.35. The biradical character was more pronounced in the addimer case. The influence of a voltage applied to an STM tip on the NOONs of antibonding orbitals in pure Si–Si and mixed Si–Ge addimers on the Si(001) surface has been analyzed. Under the action of the tip voltage, the multiplicity of a pure Ge–Ge addimer was observed to change from the singlet to the triplet one.