

STUDY OF THE INTERACTION
OF ATOMS OF THE IV- AND V-TH GROUPS
WITH Si(001) AND Ge(001) SURFACES

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S u m m a r y

Adsorption and diffusion processes of atoms of the IV- (Si, Ge) and V-th (As, Sb, Bi) groups on the Si(001) and Ge(001) surfaces have been simulated, by using quantum chemistry techniques. The mechanism of how the adsorption of elements of the V-th group affects the Si(001) surface is considered. The literature concerning the adsorption of atoms of the V-th group (As, Sb, Bi) and their co-adsorption with oxygen on the Si(001) surface and the diffusion of Bi ad-dimers on the Si(001) surface and Si and Ge ad-dimers on the Ge(001) one is analyzed. The results obtained demonstrate a high capability of quantum chemistry methods to provide the unique information about the interaction between adsorbates and the semiconductor surface.