ADSORPTION OF MOLECULAR OXYGEN ONTO $Si_{1-x}Ge_x$/Si(001) SURFACE

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S u m m a r y

On the basis of *ab initio* calculations, the adsorption of O_2 molecules onto a $Si_{1-x}Ge_x$/Si(001) surface has been considered at a qualitative level, and stable adsorption configurations of molecular oxygen have been determined. The O_2 molecule was found to be chemisorbed without dissociation onto the $Si_{1-x}Ge_x$/Si(001) surface. In the case where the $Si_{1-x}Ge_x$/Si(001) surface is presented by pure Si–Si or mixed Si–Ge ad-dimers, the adsorption of O_2 molecules was found to be barrierless. In the case where the surface is presented by pure Ge–Ge ad-dimers, the chemisorption barrier was found to be lower than 0.1 eV. The adsorption of O_2 molecule on the $Si_{1-x}Ge_x$/Si(001) surface is accompanied by a change of the spin state of the system from the triplet to the singlet one and by a reduction of the surface chemical reactivity.