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QUANTUM–CHEMICAL MODELING OF THE INTERACTION OF ARSENIC ATOM WITH VACANCY DEFECTS ON THE SIO2/SI(100) SURFACE

Quantum–chemical calculations of the properties of a As atom implanted SiO2/Si(100) interface are presented. For simulation of physicochemical properties and estimation of surfaces energy parameters semiempirical method of quantum-chemical modeling PM7 realized on MOPAC software package has been used. Dependencies of the total energy of a As atom cluster system on the location of As atom in oxygen and silicon vacancies are calculated, along with the geometric and electronic characteristics of the equilibrium cluster states with implanted arsenic atoms.

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