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Reactivity of adatoms with H-terminated Si(111) surface: A first-principles study

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Using the first-principles calculation, we have investigated the reactivity of adatoms with various valencies on the H/Si(111) surface, which is useful in understanding the initial stage of epitaxial growth. The reaction properties of the adatoms with substrate are significantly different respect to their valencies. For examples, the adatoms in group IV (C, Si, Ge), V (P), and VI (S) are stabilized with substitutional adsorption, where the adatoms make direct bonds with the substrate with breaking a H-substrate bond. On the other hand, in the adsorption of the alkali metal (Na), the simple metal (Al), and the nobel metal (Ag), the energy barriers are needed to break the H-Si bonds and thus, the substitutional adsorption does not take place. When a 3d transition metal (TM) adatom approach to the substrate, the H atom can break the Si-H bond without energy barrier. Furthermore, some kinds of TMs (Sc, Ti) are also stabilized with substitutional adsorption. The physical origins for the different reactivity of adatoms with different valencies as well as mechanism for the substitutional adsorption would be presented.