Ab initio study of the adsorption silane and disilane on Si(100)-(2x1) surface

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Silane (SiH_4) and disilane (Si_2H_6) are common precursors for the growth of Si and SiO_2 thin films which are used for solar energy cells, microelectronic and photovoltaic devices. The adsorption of silane and disilane on Si(100)-(2x1) clean surface were investigated using density functional theory calculations. The silane molecule dissociates on the Si (100) surface with barrier energy of 0.22 eV with respective to silane gas. We investigate the dissociation of Si_2H_6 through both Si-Si bond cleavage and Si-H bond cleavage on Si (100) surface. The Si-H bond cleavage mechanism with barrier energy of 0.04 eV was found to be more favored than the Si-Si bond cleavage mechanism with barrier energy of 0.71 eV with respective to the disilane gas. Based on the calculated barrier energies, the sticking coefficient ratio: $s(Si_2H_6)/s(SiH_4)$ was estimated to be ≈2800 at 300 K, which is consistent with the experiment results [1]. The vibration frequencies of species such as Si_2H_5, SiH_3, SiH_2, SiH resulting from dissociation of silane and disilane on Si surface were calculated and compared with experimental results available. The simulation results will facilitate the controlled ALE for atomically precise manufacturing applications.

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