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Ab initio study of silane and disilane adsorption on Si(100)-(2x1) surface MIN HUANG, Department of Materials Science and Engineering, The University of Texas at Dallas, JOHN RANDALL, YVES J. CHABAL, ROBERT M. WALLACE, KYEONGJAE CHO — Silane (SiH_4) and disilane (Si_2H_6) are common precursors for the growth of Si and SiO_2thin films for microelectronic and photovoltaic devices. The adsorption of silane and disilane on Si(100)-(2x1) surface, which are important steps in the growth of Si films in atomic layer epitaxy (ALE), were investigated using density functional theory calculations. The silane molecule dissociates on the Si surface at the intra-dimer site with barrier energy of 0.22 eV. We investigate both Si-Si bond cleavage and Si-H bond cleavage mechanisms for adsorption of Si_2H_6 on Si (100) surface. A Si-H bond cleavage mechanism was found to be more favored than Si-Si bond cleavage mechanism due to the lower barrier energy of 0.04 eV. The lower barrier energy for Si_2H_6 dissociation than that of SiH_4 agrees well with the experimental results showing that Si_2H_6 has higher sticking coefficient than SiH_4on Si surface at 300K. The vibration frequencies of Si_2H_5, SiH_3, SiH_2, SiH resulting from dissociation of silane and disilane 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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