Initial nucleation for atomic layer deposition (ALD) of group Ⅲ oxides: a quantum chemical comparative study

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Atomic layer deposition (ALD) enables deposition of ultrathin films with good uniformity. ALD of Al_2O_3 can be easily carried out using trimethylaluminum ($Al(CH_3)_3$) and water. In contrast, it is known that ALD of other group III oxides are very difficult using B, Ga, or In trimethyl precursors with H_2O. In this study, we consider adsorption of the group III trimethyl compounds on a hydroxylated Si(100) surface and their oxidation with water using density functional theory (DFT) calculations. It is observed that molecular adsorption of trimethylaluminum occur with large exothermicity, while adsorption of other metal precursors are weaker. Furthermore, the activation energy for removal of the methyl ligands from the metal atoms is significantly larger for all elements other than Al. In the next reaction, adsorption of H_2O is exothermic on all methyl-terminated surfaces; however, the energy changes are considerably smaller for Ga and In compared to those of B and Al. Moreover, the activation energy for dissociative adsorption of H_2O is smaller than that for the molecular desorption only in the case of Al.