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Spontaneous Reactions of Atomic Hydrogen as a Reactant for Pt Atomic Layer Deposition

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Atomic layer deposition (ALD) of platinum (Pt) and its nanostructures has attracted intensive attention from scientists due to its potential applications in many areas such as microelectronics, sensors, catalysis, energy conversion, storage, and utilization devices. Among various precursors used for Pt ALD, (methylcyclopentadienyl)trimethylplantinum ($MeCpPtMe_3$) is the most common precursor owing to its low sublimation temperature, high thermal stability, and high reactivity towards various reactants including H_2 and O_2 as the most common ones. Herein, we used density functional theory (DFT) to provide insights into the reactions of $MeCpPtMe_3$ with H_2, O_2, and more reactive atomic hydrogen on TiO_2 surface. A complete picture of $MeCpPtMe_3$ and O_2/H_2/H reaction mechanisms, for the first time, are proposed. Interestingly, atomic hydrogen appears to be more effective in the removal of methyl and cyclopentadienyl ligands from $MeCpPtMe_3$ than H_2 or O_2 as a significant energy is required to activate H_2/O_2 molecular dissociation before reacting with the precursor. Our DFT calculation is consistent with the experimental results of successful ALD of Pt on TiO_2 surface using $MeCpPtMe_3$ and atomic hydrogen as a reactant.