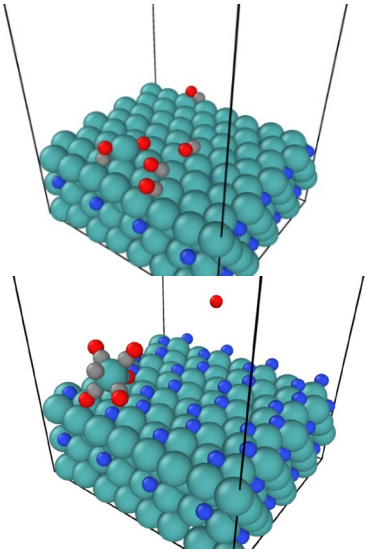

Fig. 1. Adsorption behavior of $Mo(CO)_6$ on Mo_2N surfaces with and without exposed N.
Top: Mo_2N surface without exposed N atoms. Bottom: Mo_2N surface with exposed N atoms. The optimized/MD snapshots show a clear termination dependence: on the N-free surface, $Mo(CO)_6$ readily undergoes dissociative adsorption, creating surface-bound Mo species that can initiate film growth. In contrast, when surface N atoms are exposed, $Mo(CO)_6$ adsorption is strongly suppressed and dissociation is not observed under the same conditions, indicating that N-rich termination passivates the reactive sites and inhibits precursor uptake.

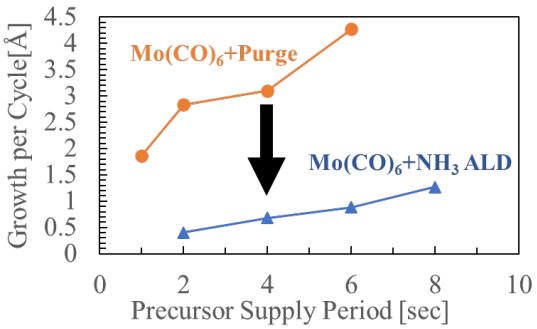

Fig. 2. Suppression of GPC by adding NH_3 into the $Mo(CO)_6$ + purge cycle.
Growth per cycle (GPC) is plotted as a function of $Mo(CO)_6$ dose time. Within the examined time window, the $Mo(CO)_6$-only sequence ($Mo(CO)_6$ + purge) does not exhibit a clear saturation behavior that would indicate an ALD half-cycle. When NH_3 is introduced (alternating $Mo(CO)_6/NH_3$ exposure), the GPC is consistently reduced by nearly one order of magnitude across the same dose-time range, demonstrating that NH_3 effectively suppresses $Mo(CO)_6$-driven growth, likely via surface nitridation and reduced precursor uptake.