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Non-Covalent Interactions and Thermal Effects in the Quest for Selective Atomic Layer Deposition JONATHAN WONG, TAEWON SUH, KA UN LAO, JAMES R. ENGSTROM, ROBERT A. DISTASIO JR., Cornell Univ, DISTASIO GROUP/ENGSTROM GROUP COLLABORATION — In the manufacturing of nanoscale devices, the Atomic Layer Deposition (ALD) process has several desirable characteristics that allow aluminum oxide films to be grown (on dielectric or metallic substrates) with a precise thickness and intricate three-dimensional features. Furthermore, the gas-phase synthetic nature of ALD is very compatible with present manufacturing lines. However, the ALD process lacks control over substrate selectivity at the exceedingly small length scales required for the manufacturing of high-density transistor units that would extend the applicability of Moore's law. In this work, we utilized van der Waals (vdW) inclusive density functional theory (DFT) and high-level quantum chemical methods to study substrate selectivity in this process via the formation of Lewis acid-base complexes (or adducts) with the trimethylaluminum ALD precursor. We will demonstrate how non-covalent interactions and thermal effects modify both the kinetics and thermodynamics of the ALD process. In this context, we will also discuss several promising yet unexplored avenues towards increasing the efficiency of the ALD process and obtaining substrate selectivity.

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