566c Chemical Mechanisms of Contamination in Atomic Layer Deposition of Hfo¬2

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Atomistic mechanisms for atomic layer deposition of HfO2 using metal chloride and metal organic precursors was investigated using density functional theory. In addition to the ligand exchange mechanisms which we have previously calculated, we have explored various mechanisms which lead to contamination of the films with atoms from the precursor ligands. We have used DFT based transition state theory to predict the relative rates of contaminant incorporation with various precursors and have also predicted the rates of incorporation at the initial Si or SiO2 interfaces on which HfO2 is often deposited. Our results correctly predict the contrasting trends of Cl and C contamination as a function of temperature in films grown with HfCl4 and Hf methylamides and the relative contamination at the semiconductor high-K interface versus HfO2.