Atomic Layer Process (ALP) for Metal Oxide Thin Films: Enhancing Selectivity and Inhibitors' Role

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The precise deposition of metal oxide thin films onto various substrates without additional patterning is essential for advanced semiconductor patterning. Area-selective atomic layer deposition (AS-ALD) offers a promising solution, enabling selective deposition and preventing unwanted coverage. Small molecular inhibitors (SMIs) with aliphatic alkyl chains, like DMA-TMS, TMPS, and Hacac, are widely studied for AS-ALD, enabling precise control on nanometer-scale patterns. However, research on SMIs with aromatic blocking groups is limited. This study explores the chemical and physical passivation abilities of four Si-based SMIs with phenyl ligands: TCPS, MDCPS, CDMPS, and DCDPS. DFT calculations reveal that TCPS, MDCPS, and CDMPS prefer exothermic adsorption reactions on SiO2 surfaces, leading to a significant increase in water contact angle (3-40°), confirming successful passivation. Monte Carlo simulations showed that MDCPS (91% surface coverage) exhibited superior passivation and selectivity, surpassing aliphatic SMIs like DMA-TMS. These findings demonstrate the advantages of aromatic SMIs for semiconductor applications.

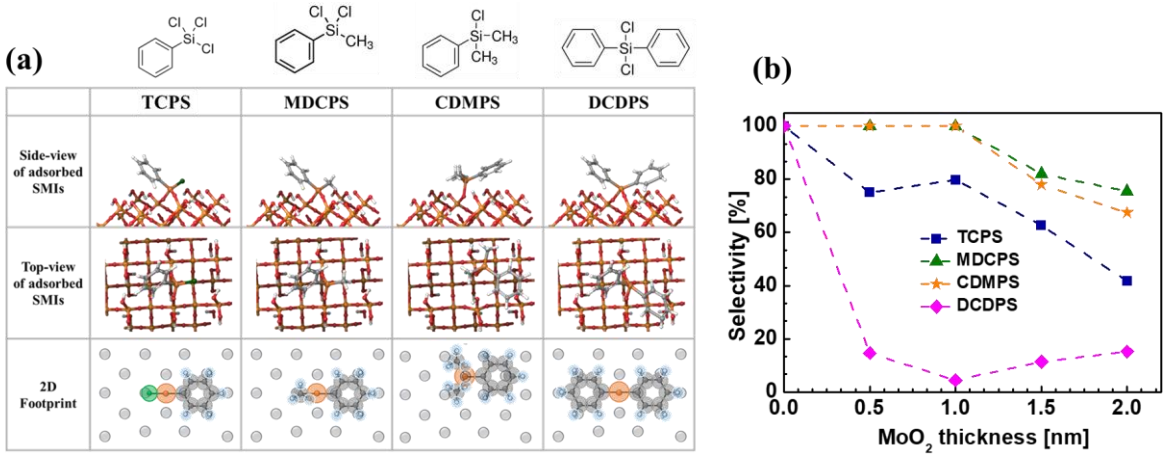

Fig. 1. (a) The adsorption structures of aromatic SMIs on SiO_2 surfaces based on the number of reactive groups. (b) The selectivity of ASALD MoO_2 on SiO_2, depending on various inhibitors