Learning from fundamental surface science for atomic layer deposition – an *ab initio* endeavour

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Atomic Layer Deposition (ALD) emerges as an important technique in addressing the evolving complexities of microelectronics fabrication, offering the potential of atomically precise material construction. But as every practitioner of the method knows, the reality is much more complex and many physical and chemical effects have to be considered, tested and investigated to arrive at the goal of a targeted materials synthesis. A current forefront challenge is achieving area-selective ALD (AS-ALD), aiming for selective material growth on target surfaces, with small molecule inhibitors (SMIs) presenting a promising strategy to prevent deposition on non-growth areas.

The nature of the process requires an in-depth understanding of the underlying surface chemistry as well as a mechanistic understanding of the adsorption and decomposition reactions that can happen in the SMI as well as the ALD process steps. Our latest research shines a light on SMI-based AS-ALD, offering insights into experimental results and pushing the boundaries toward predictive computational analysis.[5–8]

At its core, ALD is governed by surface chemistry principles, allowing extrapolations from fundamental studies on molecular-surface interactions, often performed in more experimentally controlled settings. Extensive research into the reactivity of organic adsorbates on semiconductor surfaces has unearthed key reaction mechanisms, bridging insights reactivity known from molecular chemistry.[1,2] For metal surfaces, while a local view on chemical bonding may fall short, the interplay with organic adsorbates is still within reach of computational approaches. Our findings include investigations into the stability of the longest known acene chain on Cu(111)[3] and the behavior of non-alternant aromatic compounds on metallic substrates.[4]

The presentation concludes with our first steps towards understanding N-heterocyclic carbenes on metal surfaces.