

The functionality of heterointerfacial sites using area selective atomic layer deposition

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Background

Heterointerfaces are a sub-class of defects arising from atomic mismatches across material boundaries. These coordinatively unsaturated sites modulate the electronic and geometric structure of catalysts to facilitate specific reactive adsorption, activation, and transformation of reactant molecules.¹ In electronic devices the critical heterointerfaces are “buried” between the layers,² whereas for catalysts, the reaction performance can depend on both the buried interfaces (i.e. metal support interactions) and on the exposed heterointerfacial (defect) sites, interacting with substrate and product molecules, see **Scheme 1**.

Results and discussion

In the current work, we use a bottom-up area selective atomic layer deposition (AS-ALD) to form supported thin layer raft-like oxides. To facilitate the AS geometry, we developed a new approach, which uses NaCl nanocrystals as masking domains during the ALD process. This unique approach allows us to apply this methodology onto silicon wafers and on different surface area particulate silica support materials. The HRSEM-EDS (Energy Dispersive Spectroscopy) mapping in **Figure 1** shows an example of a well-defined multilayer structure, formed following the sequential deposition of TiO₂ (≈20 nm) and subsequently Al₂O₃ (≈20 nm) layers onto an NaCl-mask before and after mask removal. Leveraging on the strength of AS-ALD we study the structure, binding energy, strain and more of the exposed heterointerface, aiming to decouple those from the exposed basal plan and bulk effects. We compare our AS-ALD materials to materials obtained using a top-down deposition of thin nanosheets of layer double hydroxides. All materials are extensively characterized using XPS, DRIFT-IR, HRSEM and HRTEM, grazing angle-WAXS and probe molecules TPD-MS. The functionality of the heterointerfacial sites is tested using Aldol type condensation reactions for the conversion of biomass derived platform molecules as a target and probe reaction.

References

- (1) Xie, C., et al., ACS Catal. 2020, 10 (19).
- (2) Christensen, D. V., et al., APL Materials 2018, 7 (1), 013101.

