O 121: Overview Talk: Karsten Reuter

Time: Friday 13:15–14:00 Location: HE 101

Invited Talk O 121.1 Fri 13:15 HE 101

A look through the operando glass: First-principles based multiscale modeling of working catalysts — •Karsten Reuter — Technische Universität München

Increasingly available data from operando spectroscopies and microscopies point at a much more dynamic behavior of the surface of working catalysts than traditionally assumed. Instead of a catalytic function that is driven by static active sites as they emerge from a crystal lattice truncation of the nominal catalyst bulk material, a highly dynamic picture is suggested with continuous reaction-induced complex (surface) morphological changes at (near-)ambient reaction conditions or an evolving, possibly liquid-like phase behavior due to limited heat dissipation channels. Scrutinizing and complementing this insight through first-principles based modeling turns out to be a major challenge. The electronic structure level needs to be reliably described to maintain predictive quality. Mikrokinetic simulations have to account for the statistical interplay of all elementary processes, while macroscopic flow simulations evaluate the heat and mass transport in the non-ideal reactor geometries employed in the operando measurements. I will introduce corresponding advanced multiscale modeling approaches and discuss their current capabilities and limitations, using oxide formation in the context of oxidation catalysis as a showcase.