A Look through the Operando Glass:
First-Principles Based Multiscale Modeling of Working Catalysts

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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 multiscale modeling turns out to be a major challenge.

I will introduce corresponding approaches and discuss their current capabilities and limitations, using oxide formation in the context of oxidation catalysis as a showcase.