

A Catalyst Life and its Circumstances

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Climate change concerns have spurred a growing interest in developing environmentally friendly technologies for green energy generation and storage in the form of chemical bonds. The latter includes green H₂ production from water splitting and the re-utilization of CO₂ via its thermal or electrocatalytic reduction into value-added chemicals and fuels. Moreover, alternative methods for ammonia synthesis either with green H₂ or direct electrocatalytic NH₃ synthesis are also being sought in order to reduce carbon emissions, while providing a transport energy carrier for green hydrogen. In this context, it is thus important to develop low cost, highly efficient and durable catalysts with tunable selectivity. This requires understanding the evolution of their structure and surface/bulk composition under reaction conditions, i.e. while the active sites are being formed or become poisoned leading to their deactivation.

This talk will offer mechanistic insights into the electrocatalytic reduction of CO₂ and nitrate reduction as well as the oxygen evolution reaction using model pre-catalysts ranging from single atoms, size- and shape-controlled nanoparticles, epitaxial thin films to single crystals. I will illustrate the need of a multi-technique *operando* microscopy and spectroscopy approach, when possible combined, to gain understanding into the complex evolution of electrocatalytic materials while at work. Examples will be given on the correlation between their dynamically evolving structure and composition and their activity and selectivity.

These results are expected to open up new routes for the reutilization of CO₂ through its direct conversion into industrially valuable chemicals and fuels such as ethylene, methanol and ethanol, and the generation of green H₂ and ammonia via electrolysis.