Why is Operando Crucial for the Future of Surface Science?

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Climate change concerns have spurred a growing interest in developing environmentally friendly technologies for energy generation (i.e. green H_2 from water splitting) and to re-utilize CO_2 in thermal catalysis applications where it is reacted with green H_2 to produce liquid fuels. Moreover, the electrochemical reduction of CO_2 (CO_2RR) into value-added chemicals offers an additional possibility to store renewable energy into chemical bonds. Thus, efficient, selective and durable catalysts must be developed. Nonetheless, in order to tailor the chemical reactivity of nanocatalysts, fundamental understanding of their structure and surface composition under reaction conditions must be obtained. Surface science characterization methods are key to gain such insight, however, such methods must be applied under operando conditions, since even morphologically and chemically well-defined pre-catalysts will be susceptible to drastic modifications during catalysis. Even more, such changes might be reversible when the applied external stimulus (pressure, temperature, electrical potential, chemical environment) is removed, leading to misleading information on the nature of the active sites when only pre-natal and post-mortem characterization data are available.

This talk will provide examples of the operando evolution of catalysts employed in the thermal and electrocatalytic reduction of CO_2 as well as the oxygen evolution reaction (OER) using model pre-catalysts ranging from nanoparticles (Cu NPs, CuZn NPs, Cu_2O cubes, ZnO@Cu_2O cubic NPs, CoO_x NPs), to thin films ($Co_{1+\delta}Fe_{2-\delta}O_4$) and single crystals [Cu(100),(111), Ga/Cu(111),(100)]. Some of the aspects that will be discussed here include the understanding of the active state formation, and the correlation between the dynamically evolving structure and composition of the working catalysts and their catalytic performance. Our studies are expected to open up new routes for the reutilization of CO_2 through its direct conversion into industrially valuable chemicals and fuels and a more efficient green hydrogen production.