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Site-specific CO₂ adsorption and surface oxidation of Cu catalysts at near-ambient pressure

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Cu-based catalysts are a cornerstone of technological efforts to build sustainable energy cycles. They show promising activity towards CO₂ reduction, in heterogeneous as well as electrocatalytic reaction pathways. The ability of the Cu surface to adsorb CO₂ in a chemisorbed state and accommodate oxygen atoms is favourable to breaking the stable C=O double bond - the first and most important step towards catalytic conversion into, e.g. methanol.

Therefore, understanding the chemical composition of the catalyst surface *in situ* is essential to unraveling the underlying reaction mechanism.

Crystalline Cu surfaces are frequently used as model catalysts for fundamental studies on this reaction. At pressures > 0.01 mbar, they have been found to catalyze CO₂ dissociation. Atomic sites with lower coordination, such as steps (7-fold) and kinks (6-fold), may increase catalytic activity but the role of these active sites has not been studied comprehensively. Most previous studies have only considered a few, typically high symmetry, Cu surfaces.

In the work presented here, we employ a curved model catalyst with variable surface structure to investigate CO₂ adsorption and dissociation at near-ambient pressures. Using XPS to characterize different reactant and product species, we study the reaction on the highly symmetric (111) surface, as well as increasingly corrugated surfaces. We follow the reaction from onset to saturation, covering a wide pressure and temperature range.

We observe how the coverage of competing surface species evolves over time, as CO₂ adsorbs into both physisorbed and chemisorbed states and eventually dissociates into CO gas and atomically adsorbed O. Gradual surface oxidation prevents further CO₂ adsorption and leads to eventual saturation of the surface. The step-density dependent differences are quantified by kinetic modelling.

In this talk, I will discuss how the different surface sites (terraces, steps, kinks) control the chemical composition of the *surface coverage* as well as the *kinetics* of the reaction in different ways and reveal new insights into the reaction mechanism.

if "Other", please specify:

I apply for a travel grant

Yes

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