

Determining Structure-Activity Relationships in Oxide Derived Cu—Sn Catalysts During CO₂ Electroreduction Using X-Ray Spectroscopy

Laura C. Pardo Pérez , Alexander Arndt, Sasho Stojkovikj, Ibbi Y. Ahmet, Joshua T. Arens, Federico Dattila, Robert Wendt, Ana Guilherme Buzanich, Martin Radtke ... [See all authors](#) 

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Abstract

The development of earth-abundant catalysts for selective electrochemical CO₂ conversion is a central challenge. Cu—Sn bimetallic catalysts can yield selective CO₂ reduction toward either CO or formate. This study presents oxide-derived Cu—Sn catalysts tunable for either product and seeks to understand the synergistic effects between Cu and Sn causing these selectivity trends. The materials undergo significant transformations under CO₂ reduction conditions, and their dynamic bulk and surface structures are revealed by correlating observations from multiple methods—X-ray absorption spectroscopy for in situ study, and quasi in situ X-ray photoelectron spectroscopy for surface sensitivity. For both types of catalysts, Cu transforms to metallic Cu⁰ under reaction conditions. However, the Sn speciation and content differ significantly between the catalyst types: the CO-selective catalysts exhibit a surface Sn content of 13 at. % predominantly present as oxidized Sn, while the formate-selective catalysts display an Sn content of ≈70 at. % consisting of both metallic Sn⁰ and Sn oxide species. Density functional theory simulations suggest that Sn^{δ+} sites weaken CO adsorption, thereby enhancing CO selectivity, while Sn⁰ sites hinder H adsorption and promote formate production. This study reveals the complex dependence of catalyst structure, composition, and speciation with electrochemical bias in bimetallic Cu catalysts.