Unlocking nickel's potential: New study reveals how to use single atoms to turn CO_2 into valuable chemical resources

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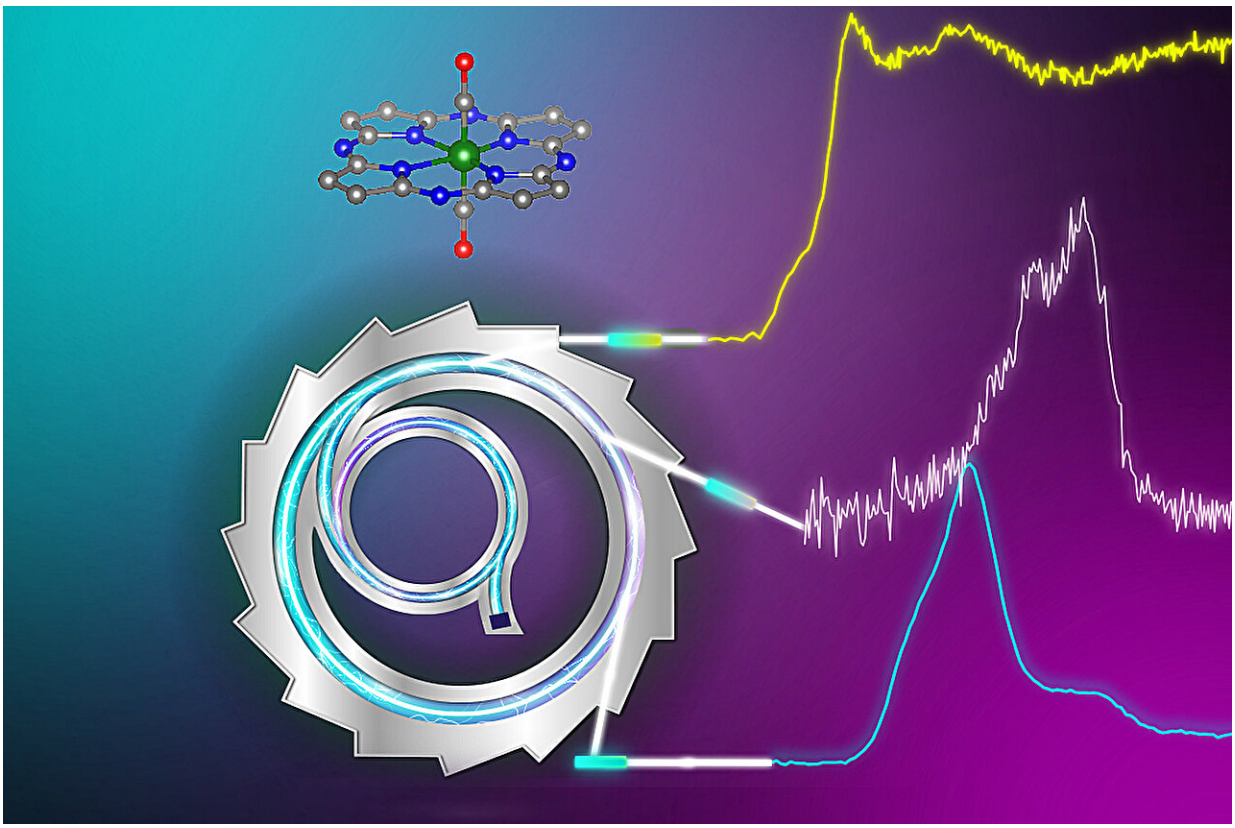

Credit: FHI

Nickel and nitrogen co-doped carbon (Ni-N-C) catalysts have shown exceptional performance in converting CO_2 into CO, a valuable

chemical feedstock. However, the exact working mechanism of these catalysts has remained elusive—until now.

The study "Unveiling the Adsorbate Configurations in Ni Single Atom Catalysts during CO_2 Electrocatalytic Reduction using Operando XAS, XES and Machine Learning" provides direct experimental insights into the nature of adsorbates (molecules that stick to the catalyst's surface) forming at the nickel sites and the evolving structure of the active sites during the CO_2 reduction reaction (CO_2RR). The work is published in the journal *Physical Review Letters*.

The research team employed advanced techniques like operando hard X-ray absorption spectroscopy (XAS) and valence-to-core X-ray emission spectroscopy (vtc-XES) to observe the catalysts in action. These advanced methods, combined with machine learning and density functional theory, allowed the team to map out the local atomic and electronic structure of the catalysts in unprecedented detail. This work illustrates the power of a multi-technique operando characterization approach combined with machine learning and modeling to extract in depth mechanistic insight.

Understanding how nickel-based catalysts interact with CO_2 at the atomic level is crucial for their rational design aiming to improve their efficiency and selectivity. This knowledge can lead to the development of more effective and long-lived catalysts, making the CO_2 reduction process more viable for industrial applications.

Essentially, this research helps pave the way for turning CO_2, a greenhouse gas, into valuable resources like carbon monoxide (CO), which can be used in various industrial processes, including those where it can be combined with green hydrogen from water electrolysis for the synthesis of high order hydrocarbons.

Imagine trying to bake a perfect cake without knowing how the ingredients interact in the oven and how the cake rises or eventually gets burnt during the baking. In the oven analogy, one can see through a window and use the visual information to make changes in the temperature and baking time.

The present study is like having a high-tech camera that lets you see exactly how the ingredients mix and change as they bake, allowing you to tweak the recipe (and/or oven conditions) while you are baking for the best results. Similarly, by understanding how CO_2 interacts with nickel catalysts, scientists can fine-tune the process to generate the desired products more efficiently.

This study not only enhances our understanding of nickel-based catalysts but also sets the stage for future advancements in CO_2 reduction technologies. By providing a detailed picture of how these catalysts work, the research opens up new possibilities for designing even more efficient systems for converting CO_2 into valuable products.

More information: Andrea Martini et al, Adsorbate Configurations in Ni Single-Atom Catalysts during CO_2 Electrocatalytic Reduction Unveiled by Operando XAS, XES, and Machine Learning, *Physical Review Letters* (2024). DOI: 10.1103/PhysRevLett.133.228001

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