Decoding Atomic-Level Transformations and Active Sites for Next-Generation Electrocatalysts

The global transition to **sustainable energy** has emphasized the need for efficient hydrogen production, with **water electrolysis** emerging as a key technology. This process splits water into oxygen and hydrogen, producing a ***clean energy carrier*** crucial for reducing greenhouse gas emissions. However, the oxygen evolution reaction (OER)—a critical step in water splitting—faces significant challenges due to its sluggish kinetics and high energy requirements. **Transition metal oxides (TMOs)**, such as iron, cobalt, and nickel oxides, are promising OER catalysts because of their ***abundance, stability, and catalytic activity***. Their catalytic performance is closely linked to their **electronic properties** and **surface structure**, which undergo complex changes during OER due to **surface reconstructions**, **phase transitions**, and alterations in **oxidation states**. Currently, the dynamic structural and electronic evolutions of these materials under realistic OER operating conditions remain poorly understood, primarily due to the lack of analytical techniques capable of **real-time atomic-scale** observations. This knowledge gap limits the rational design of efficient and durable catalysts.

The DeCOD€ project aims to address these challenges through an **innovative, interdisciplinary approach** that combines advanced instrumentation, precise material synthesis, and real-time atomic-scale investigations under operational conditions. To achieve the project's objectives, advanced ***in situ*** and ***operando*** techniques will be employed, including **electrochemical scanning tunneling microscopy (EC-STM)** integrated with **ultra-high vacuum (UHV)** material synthesis, enabling direct observation of structural and electronic transformations in TMOs during the OER. Our innovative EC-STM system, developed within the project, incorporates a **custom-built flow cell** to mitigate the gas bubbles formation, integration of **high-speed electronics** for **video-rate imaging**, and an **automated tip coater (ATC)** for reproducible and stable imaging. These advancements overcome the limitations of existing techniques, enabling direct observation of transient phenomena such as the ***active sites formation***, ***surface restructuring***, and ***defect dynamics under realistic operating conditions***.

The project will utilize well-defined TMO model systems synthesized under UHV with precise control of **composition**, **structure**, and **morphology**. These materials will be comprehensively characterized using techniques such as **X-ray photoelectron spectroscopy (XPS)**, **low-energy electron diffraction (LEED)** and **ultraviolet photoelectron spectroscopy (UPS)**. Advanced statistical data analysis workflow, will process large datasets to correlate *atomic-scale changes with catalytic performance*, **bridging the gap between microscopic observations and macroscopic metrics.**

Within the framework of this project, we will seek answers to four fundamental questions in electrocatalysis: ***(1)*** *What are the active and stable phases during the OER?* ***(2)*** *How do surface structure modifications, including defects and doping, influence catalytic activity?* ***(3)*** *How do oxidation state transitions affect electronic structures and their catalytic behavior?* ***(4)*** *How can the insights gained inform the rational design of efficient and cost-effective catalysts?* By answering these questions, we aim to uncover mechanisms driving TMO catalytic performance and establish structure–activity relationships that will inform the design of **next-generation catalysts**.

The project's novel approach lies in the comprehensive, **real-time investigation of the dynamic behavior of TMOs during OER**. By combining **atomic-scale imaging** with **advanced data analysis**, we aim to move beyond traditional empirical methods in catalyst development. The expected outcomes include groundbreaking discoveries regarding catalyst behavior, facilitating the development of TMO-based catalysts with enhanced ***efficiency, stability, and scalability***. By reducing dependence on precious metals and utilizing widely available TMOs, the results align with global policies supporting the transition to **clean energy technologies.**

Beyond its direct contribution to OER research, the project will introduce groundbreaking methodological innovations in **electrochemical surface science.** The findings will be applicable to other catalytic systems, such as carbon dioxide reduction and fuel cells, opening new avenues for clean energy technologies.