

# Correlating atomic scale structure and activity of model catalysts for Oxygen Evolution Reaction

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Water splitting into hydrogen and oxygen is a clean, sustainable and fossil-free route to production of hydrogen gas, the ultimate clean energy carrier (figure 1). The oxygen evolution reaction (OER) is considered the limiting half-reaction in the overall process, due to its complex kinetics and large overpotential [1]. To develop new materials with optimized catalytic properties is one of the most crucial challenges towards a more sustainable way of clean and renewable energy sources. In order to achieve this long-standing goal, atomistic understanding of the processes taking place at the electrode-electrolyte interface is demanded. Here we provide structural, chemical and electrochemical characterization on exactly the same sample. Our customized experimental set up allows for transferring the catalyst from ultra high vacuum (UHV) conditions to an electrochemical cell in a controlled atmosphere. This optimized approach enables the direct correlation between the surface properties at the microscopic scale, - composition and structure-, and the macroscopic response of the catalyst.

Ruthenium oxides are promising earth-abundant catalysts for the OER in both, alkaline and acidic electrolyte. We explore different oxidation states of Ru surfaces, grown using two different methodologies under UHV conditions: direct oxidation of the metallic surface and molecular beam epitaxy of thin films of the oxide [2]. In situ structural and chemical characterization of the prepared Ru-oxides are carried out by Low Energy Electron Diffraction (LEED) and X-Ray Photoemission spectroscopy (XPS). The oxide surfaces previously characterized under UHV conditions are then transferred under controlled atmospheric conditions into the electrochemical cell for the electrochemical test. After the electrochemical measurements, the sample is transferred back to the UHV system in order to identify potential changes induced by the electrochemical process.

## References

- [1] N. B. Halck, V. Petrykin, P. Krtil, and J. Rossmeisl, *Phys. Chem. Chem. Phys.*, **16**(27),13682–13688 (2014)  
[2] B. Herd, J. C. Goritzka, and H. Over, *J. Phys. Chem*, **117**, 15148-15154 (2013)

## Figures

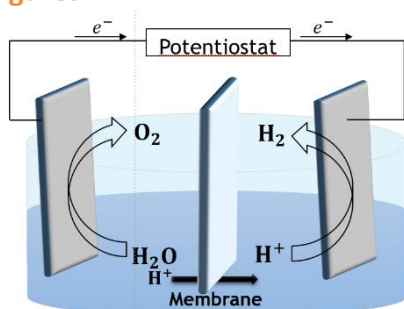


Figure 1. Scheme of an electrochemical cell with hydrogen evolution reaction and oxygen evolution reaction.