

# Ulrich Aschauer

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**Tuesday, 24<sup>th</sup> October 2023, 16:00 s.t.**

TU Wien, Institut für Angewandte Physik, E134  
1040 Wien, Wiedner Hauptstraße 8-10  
Yellow Tower „B“, 5th floor, SEM.R. DB gelb 05 B



**The seminar will be also held as a zoom Meeting**

<https://tuwien.zoom.us/j/96062751637?pwd=ZkRUWnlkUFFZb2pEdm55ZzFteTBNdz09>

Meeting ID: 960 6275 1637

Password: 9ANd8XWj

## **OER on oxide and oxynitride surfaces: effect of orientation, cation leaching and dimer formation**

Development of novel photocatalyst materials does not only rely on finding materials with suitable bulk properties (band gap, carrier mobility, band edges) but also on a detailed understanding of their surface structure and chemistry under photocatalytic application conditions. For structurally or chemically complex materials, the surface structure is particularly difficult to anticipate from intuition alone. Density functional theory (DFT) calculations in combination with thermodynamic models can be used to predict surface structures under application conditions and the resulting oxygen-evolution reaction (OER) chemistry. In this talk, I will highlight case studies for structurally complex materials in the form of perovskite-derived layered oxides of the class  $A_2B_2O_7$  and chemically complex perovskite oxynitrides that are commonly synthesized starting from these layered materials.

For the layered oxides, our calculations predict surface restructuring by cation leaching on the catalytically relevant surface, which has a detrimental effect on the catalytic activity. Consequently, strategies mitigating this dissolution need to be implemented. For oxynitrides our results show that the degree of anion order, which is controlled by the synthesis conditions, will affect the particle shape and therefore also the photocatalytic activity, rendering this material class more tunable than oxides. Finally, I will show how a particular dimer structure of the OER reaction intermediates commonly forms on oxynitride surfaces. The effect of this dimer on the catalytic reaction profile will be generalized by investigating this reaction intermediate across a wide range of oxides.

All interested colleagues are welcome to this seminar lecture (45 min. presentation followed by discussion).

Friedrich Aumayr  
(LVA-Leiter)

Ulrike Diebold  
(Seminar Chair)