

# Atomistic Studies of the Electrode-Electrolyte Interface

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Fundamental understanding of processes at the electrode-electrolyte interface is crucial to develop optimized materials for sustainable energy production. In this talk, I will present two examples highlighting the importance of atomistic studies on model catalytic surfaces to reveal structure-function relationships in electrocatalytic systems.

First, I will introduce our customized experimental setup, which enables comprehensive structural, chemical, and electrochemical characterization on the same sample. This setup facilitates the transfer of the electrode from an ultra-high vacuum, suitable for surface science tools, to an electrochemical cell in inert atmosphere. Using this approach, we investigated potential-induced changes on Au(111) surfaces in acidic media. Chemical changes were monitored using ex-situ X-ray photoemission spectroscopy, providing insights into its electrochemical response, including oxide formation at the onset of the oxygen evolution reaction. Furthermore, we discuss the impact of different electrolyte anions on surface electro-oxidation.

Secondly, I will provide an overview of the local properties of point defects in transition metal dichalcogenides semiconductors ( $\text{MX}_2$ , M=transition metal, X=chalcogen), proposed as active sites for the hydrogen evolution reaction. Employing 4K scanning tunneling microscopy, spectroscopy, and non-contact atomic force microscopy, we achieved atomic-scale correlation between morphology and electronic properties of various types of structural defects in  $\text{MoSe}_2$  and  $\text{WS}_2$  monolayers. Our investigations revealed that substitutional oxygen, which suppresses deep in-gap states associated with chalcogen vacancies, predominates as the point defect in these semiconductors [1, 2]. These findings unveil the crucial role of local properties in determining the material's functionality for hydrogen production, which eventually govern the actual reaction mechanism.

[1] Barja *et al.*, Nat. Comm. **10**, 3382 (2019)

[2] Schuler *et al.*, PRL **123**, 076801 (2019)