Atomic scale simulations with machine learning techniques of electrochemical processes for hydrogen production

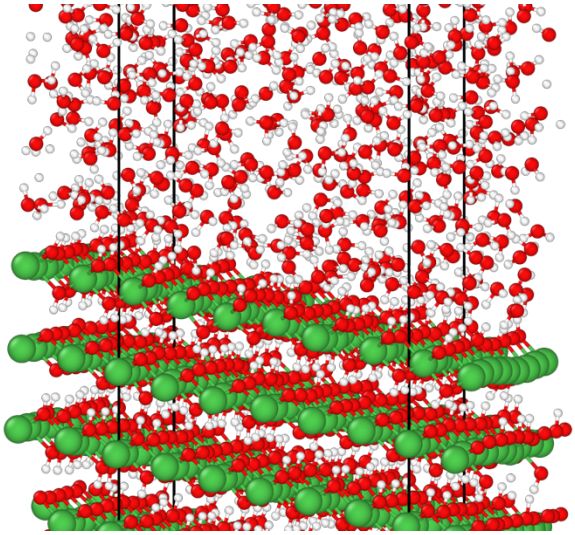

Figure 1: Model of the interface between the β-NiOOH electrocatalyst and liquid water

This project supports the transition to sustainable energy by advancing the understanding of Fe- and Co-doped NiOOH catalysts, a key material for green hydrogen production through alkaline water electrolysis. The focus is on unraveling the structural complexity of the interface and the role of charge accumulation in enhancing the catalytic performance of the oxygen evolution reaction (OER), a crucial but inefficient step in water electrolysis. Recent experimental and theoretical evidence link charge buildup to enhanced catalytic activity. This is a key property that our group contributed to establish [1-3] and that traditional studies often fail to account for. This project builds on these findings by systematically examining the surface thermodynamics of doped NiOOH under realistic electrochemical conditions and exploring how charge accumulation influences the material's performance.

To address the complexity of catalyst surfaces beyond the spatial and temporal limitations of DFT, we will develop and validate a reactive machine learning force field (ML-FF) to enable large-scale simulations of these systems, targeting the kinetics of the oxygen evolution reaction (OER) mechanisms. We will use a combination of simulation techniques (DFT, molecular dynamics with ML-FFs, enhanced sampling methods) to model reactivity and to correlate it to structural and electronic properties. This project is part of a long-standing collaboration with our experimental partners at the Fritz Haber Institute in Berlin, Germany.

References

[1] H. N. Nong et al., *Key role of chemistry versus bias in electrocatalytic oxygen evolution*, Nature 587, 408–413 (2020)

[2] G. Righi et al., *On the origin of multihole oxygen evolution in hematite photoanodes*, Nature Catalysis 5, 888–899 (2022)

[3] T. Jones. D. Teschner, S. Piccinin, *Towards realistic models of the electrocatalytic oxygen evolution reaction*, Chemical Reviews 124, 15, 9136–9223 (2024)