Seminar announcement

Tuesday, November 11, 2025
1:00 pm
WSI, Seminar room S 101
<u>Exclusively in person</u>

“Operando X-ray spectroscopy of complex oxide electrocatalysts – bridging surface dynamics and water electrolysis performance”

The transition to sustainable energy systems demands electrocatalysts that combine high activity, stability, and elemental abundance for reactions such as the oxygen evolution reaction (OER) in water electrolysis. A key challenge lies in the dynamic restructuring of catalyst surfaces under operational conditions, where the true active phase often diverges from the as-synthesized material. This complexity is further amplified in strongly correlated oxides, such as perovskite heterostructures, where synergistic interactions among multiple transition-metal cations and epitaxial strain effects govern interfacial electronic states.

I will discuss how operando X-ray photoemission (XPS) and X-ray absorption spectroscopy (XAS) enable direct probing of electronic structure, surface composition, and ligand environments during electrocatalysis. Using epitaxial thin films of model systems such as $LaNiO_3$, we decouple the roles of surface termination, oxidation states, and subsurface correlations in OER activity. Atomic-layer-controlled $LaNiO_3$ films reveal that Ni-terminated surfaces exhibit roughly twice the activity of La-terminated analogs, linked to Ni^{2+}/Ni^{3+} redox dynamics and the formation of highly active surface species.[1] In $La_{0.67}Sr_{0.33}MnO_3$, we demonstrated that ferromagnetic ordering below the Curie temperature enhances OER activity,[2] contributing to the rapidly developing field of spin-enhanced catalysis, as outlined in our recent roadmap.[3]

From a materials design perspective, the cocktail effect in high-entropy oxides (HEOs, e.g. $LaCr_{0.2}Mn_{0.2}Fe_{0.2}Co_{0.2}Ni_{0.2}O_{3-\delta}$) is particularly intriguing, as configurational disorder promotes cooperative redox transitions. XPS studies reveal a synergistic interplay of oxidation and reduction among different transition-metal cations during intermediate adsorption, suggesting that neighboring sites jointly optimize catalytic efficiency.[4]

Lastly, I will introduce our new laboratory-based multicolor operando XPS platform for in situ and operando characterization.[5] This tri-color NAP-XPS system, recently established as the NWO-funded national MESA+ operando HAXPES user facility, enables depth-selective studies of solid–liquid, solid–gas, and solid–solid interfaces. Case studies will illustrate how this approach reveals environment- and temperature-dependent redox dynamics—for example, tracking Fe_xO_Y oxidation and reduction, or probing Pt surfaces in liquid electrolytes. This instrument serves as a “sister system” to the e-conversion NAP-XPS at TUM, opening exciting opportunities for collaboration in operando spectroscopy and catalysis research.

1. Baeumer, C. et al. Tuning electrochemically driven surface transformation in atomically flat LaNiO3 thin films for enhanced water electrolysis. Nat Mater 20, 674–682 (2021).
2. van der Minne, E. et al. The effect of intrinsic magnetic order on electrochemical water splitting. Appl Phys Rev 11, 011420 (2024).
3. van der Minne, E. et al. Spin Matters: A Multidisciplinary Roadmap to Understanding Spin Effects in Oxygen Evolution Reaction During Water Electrolysis. Adv Energy Mater 03556, (2025).
4. Kante, M. V et al. A High-Entropy Oxide as High-Activity Electrocatalyst for Water Oxidation. ACS Nano 17, 5329–5339 (2023).
5. van den Bosch, I. C. G. et al. Laboratory-based in situ and operando tricolor x-ray photoelectron spectroscopy. Sci Adv 11, (2025).

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