The role of surface composition in atomically-defined perovskite catalysts for water electrolysis

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Abstract

The need for highly efficient catalysts to reach a sustainable, clean and renewable energy landscape has led to remarkable improvements and insights in the design rules for (electro-)catalyst materials. Many successful examples employ perovskite-type oxides (ABO_3) because of the large tunability of chemical and electrical properties through the choice of A- and B-site ions, substitutional doping, and the ability to control defect concentrations. Because of inherent differences in surface and bulk properties, further advances in catalyst stability and activity engineering necessitate the derivation of surface-composition-activity relationships in addition to descriptors based on the bulk properties.

Single crystalline surfaces offer the ideal platform to derive such relationships. They enable direct comparison to surfaces investigated in density functional theory (DFT), which are typically limited to a single facet that may or may not be present in catalysts fabricated using traditional routes. Epitaxial thin films allow investigation of perovskite catalysts fabricated with unit-cell precision.[1,2]

In this presentation, I will demonstrate surface-composition-activity relationships in epitaxial $LaNiO_3$ thin films, which are atomically flat both before and after application as electrocatalysts for the oxygen evolution reaction (OER) during water electrolysis, and which possess a controllable surface cationic composition. The surface and sub-surface composition are elucidated using standing wave soft X-ray photoelectron spectroscopy (SW-XPS), a method for achieving greater depth sensitivity in photoemission. We find that for given bulk properties, the surface composition determines the OER activity.

References
1. Weber, M. L. *et al.* Electrolysis of Water at Atomically Tailored Epitaxial Cobaltite Surfaces. *Chem. Mater.* **31**, 2337–2346 (2019).
2. Akbashev, A. R. *et al.* Activation of ultrathin $SrTiO_3$ with subsurface $SrRuO_3$ for the oxygen evolution reaction. *Energy Environ. Sci.* **136**, 1012–1021 (2018).