

# Localizing Adsorption and Deprotonation Sites of Water on SrTiO<sub>3</sub> by X-ray Standing Wave Excited Photoelectron Spectroscopy (XSW-XPS)

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Development of efficient catalysts is one of the main routes leading to a sustainable future, both environmentally and economically. In the field of solar energy conversion, oxide semiconductors attract attention owing to their photocatalytic properties and stability under oxidizing conditions. Promising candidates on this route are perovskites, a class of compounds with ABO<sub>3</sub> chemical structure. Extreme flexibility of their chemical structure allows substitution of A and B atoms providing a handle to control surface and bulk material properties. We investigated water adsorption onto the (001) surface of SrTiO<sub>3</sub>, a prototypical perovskite, shown to be catalytically active towards hydrolysis [1].

Thorough understanding of such catalytic processes requires chemically sensitive structural information about the species at the interface. To obtain this information from H<sub>2</sub>O/SrTiO<sub>3</sub>(001) interface we combined chemical sensitivity of X-ray Photoelectron Spectroscopy with structural resolution using X-ray Standing Wave (XSW) excitation yielding identification of bonding sites of chemical species with sub-angstrom precision [2]. As a result, we have localized bonding sites of water and hydroxyls as well as identified several different species of the latter.

The results of the measurements show that the oxygen of the water (at 100 K) has a 3.5 eV higher binding energy ( $E_b$ ) than the bulk SrTiO<sub>3</sub> oxygen, is located 3.5 Å above the surface plane and in-plane disordered. This water layer coexists with at least two types of loosely bound interfacial hydroxyls (2.4 eV higher  $E_b$ ), which desorb together with the H<sub>2</sub>O. A third type of hydroxyl is stable at room temperature, with the oxygen 2.3 Å above the surface plane. The disordered water layer as well as different hydroxyls could not have been resolved by surface x-ray diffraction [3].

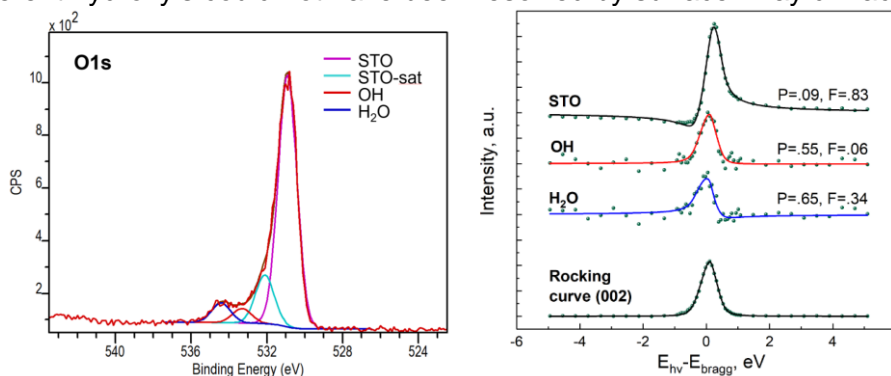


Figure 1. (left) O 1s photoelectron spectrum and fit to the components for water on SrTiO<sub>3</sub>(001). (right) X-ray standing wave results (symbols) and the fit to the data for three oxygen components: bulk oxygen, OH and H<sub>2</sub>O for the (002) reflection. Symbols represent the integral photoelectron yield of each component at the corresponding energy.

## References:

[1] J. G. Mavroides, J. A. Kafalas, and D. F. Kolesar *Appl. Phys. Lett.* **28**, 241 (1976)

[2] Ed. J.Zegenhagen and A. Kazimirov *The X-Ray Standing Wave Technique* (2013) ISBN: 978-981-277-900-7

[3] H. Hussain, X. Torrelles, P. Rajput, M. Nicotra, G. Thornton, and J. Zegenhagen *J. Phys. Chem. C* **118**, 10980-10988 (2014)