Adsorbates and surface screening at the Ferroelectric Oxide Surfaces: A Synchrotron Ambient Pressure X-ray Photoelectron Spectroscopy (XPS) Study.

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Ferroelectric materials show strong electric fields at the surface. These electric fields can be screened by different mechanisms, namely intrinsic, such as charge carriers or defects, or extrinsic, mainly adsorbates, that play a crucial role in the stabilization of polarization domains. In this sense, when considering a ferroelectric material, the electrostatic interactions between the surface and adsorbates are a critical aspect for the polarization dynamics. In these materials, understanding the interplay between ferroelectric phase stability, screening and atomistic processes at the surface is a key to control low-dimensional ferroelectricity as it has been proven in different PFM experiments [1]. Among the adsorbates in ambient conditions, water molecules due to its ubiquitous presence and its polar nature play a critical role. Despite its influence has been demonstrated to strongly affect PFM [2] and ferroelectric polarization dynamics, little is known about the water induced electrochemical reactions at the surface of ferroelectric materials for different environmental conditions.

Ambient Pressure X-ray photoelectron spectroscopy (AP-XPS) has proved as a powerful tool to study the interface of oxide surfaces in the past [3]. Using this technique, we studied the composition of the surface of ferroelectric single crystals and thin films at the line CIRCE in ALBA. In this contribution we will show our measurements on $LiNbO_3$[4], $Pb(Zr,Ti)O_3$, $BaTiO_3$ and $BiFeO_3$ in different controlled water atmospheres. We were able to identify the presence and measure the thickness of molecularly absorbed water, OH groups and the formation of carbonates for different conditions of pressure (humidity), temperature and polarization state. Results can be used to explain PFM results in the literature when working in ambient conditions.

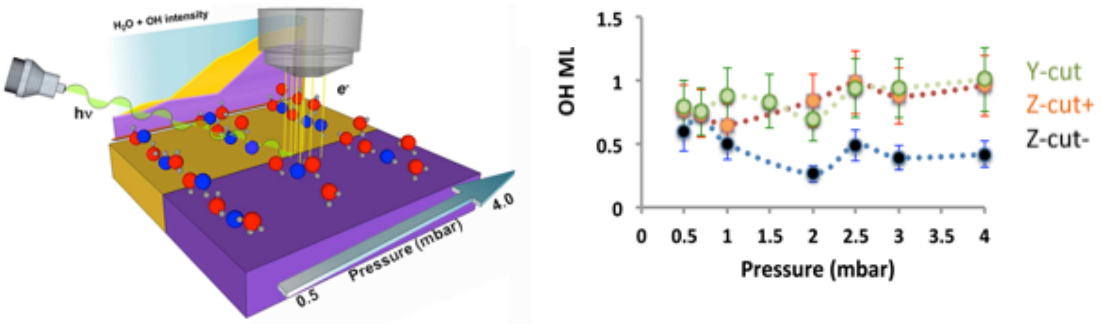

Figure: Left: Scheme of AP-XPS measures. Right: OH thickness (in monolayers) as a function of water pressure on different surfaces of a $LiNbO_3$ crystal [3].

References

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