



	Experiment title: Proton insertion and electronic effects in cathode materials for proton-conducting solid oxide fuel cells	Experiment number: MA-4144
Beamline: ID20	Date of experiment: from: 04/07/18 to: 08/07/18	Date of report:
Shifts: 12	Local contact(s): Chiara Cavallari	<i>Received at ESRF:</i>
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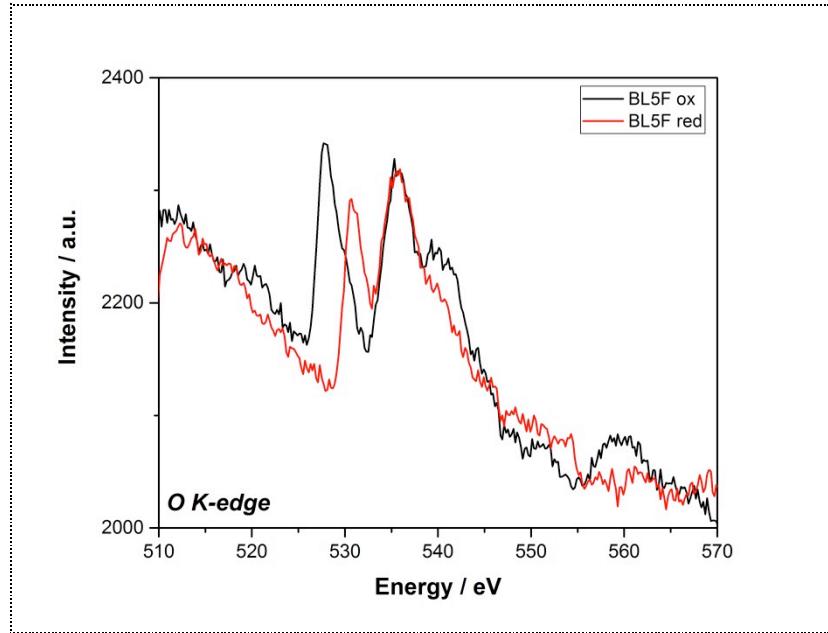
Report:

We performed RXS measurements on materials with the cubic perovskite structure to be used as cathodes in Proton Ceramic Fuel Cell (PCFC). These contain barium and lanthanum in the A-site and iron, yttrium and zinc in the B-site. With these measurements, we measure the low-energy absorption spectrum of the sample directly in the bulk by using inelastic scattering: in this way, we directly probe the oxygen chemical state as a function of iron valence (oxidized and reduced samples) and proton concentration (dry and hydrated samples); together with the EXAFS data taken on BM26A we will obtain a better understanding of the fundamentals of the proton uptake mechanism in order to tune the cathode compositions and properties for reaching higher PCFC performances.

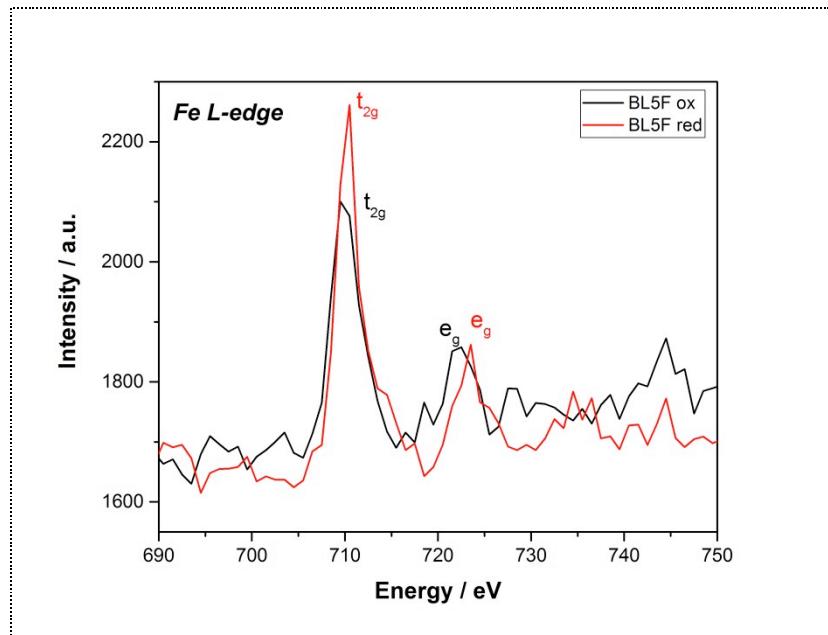
During the same experiment also barium zirconate (BZ) and barium zirconate doped with 17% of Y³⁺ (BZY17, in the dry and hydrated state), used as electrolyte in PCFC, were measured in order to elucidate why the degree of hydration is much lower for cathode compared to electrolyte materials. Relevant spectra at the oxygen K-edge and iron L-edges are reported below.

Ba_{0.95}La_{0.05}FeO_{3-δ} (BL5F) in the oxidized and reduced form

In the plot below, the spectra for BL5F (oxidized and reduced states) at the O K-edge are shown. The main difference is the shift of the first peak of about 3.5 eV, and also the ratio between the two peaks

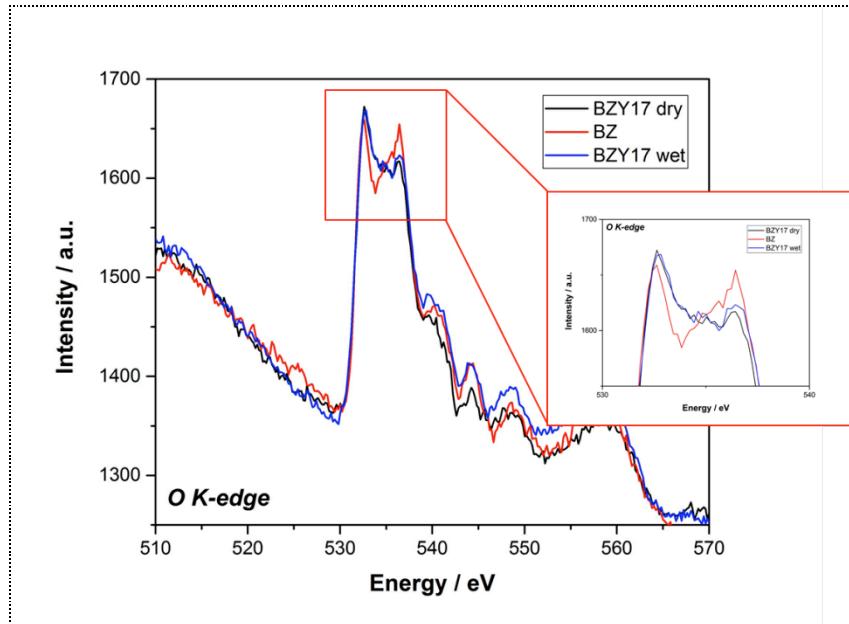


At the iron L-edges, the shift is less pronounced (about 2 eV) and the ratio between the peaks change; in particular in the reduced sample the t_{2g} peak is sharper and more intense in respect to the one of the oxidized sample even if the e_g peaks of the two samples have similar intensity.



BZ, BZY17 (dry) and BZY17 (hydrated)

The plot below shows the comparison of the data acquired for BZ, BZY17 dry and BZY17 wet at the oxygen K-edge. In the inset is evident that the ratio between the two peaks is strongly differs with changing composition (BZ vs. BZY17). The second peak is sharp in BZ and significantly broadened in BZY17, but no remarkable shift in the peaks is observed.



The data analysis using FDMNES is currently underway, to correlate the changes in the spectra with the electronic band structure of the materials.