The structure and local dynamics of proton-conducting oxides

Francesco Giannici[1], Alessandro Longo[2], Antonino Martorana[1]

[1] Dipartimento di Chimica Inorganica e Analitica "Stanislao Cannizzaro", Università di Palermo, Italy

[2] CNR-ISMN, Palermo, Italy

Proton-conducting oxides operating at intermediate temperatures (400-700 ℃) are among the most sought-after of materials in modern electrochemical technology: their prospected applications include fuel cells, hydrogen purifiers, chemical reactors, and sensors. [1] To date, low chemical stability and low overall conductivity prevent their widespread application. After nearly 20 years of research efforts on trivalent-doped II-IV perovskites such as Y:$BaCeO_3$, other types of structures have been proposed recently, opening plentiful opportunities for the solid-state chemist. Synchrotron radiation techniques give unprecedented insights on the critical points that control the properties of proton-conducting oxides, and they are an essential guide for computational simulations, as well as for the interpretation of dynamical (EIS, IR, QENS) and thermochemical (TGA) data.

The **first part** of the presentation contains an overview of the local structure analysis in various doped $BaCeO_3$ and $BaZrO_3$ perovskites, achieved through EXAFS measurements on Zr, Y, In, Ba, Ce and Gd, to clarify the peculiar role of the dopant, the segregation in grain boundaries, and the interactions with other lattice defects. Local structure analysis provides evidence that each different dopant shows unique behavior, and that the ionic radius is not useful to outline an effective doping strategy of perovskites. The high dopant solubility, the high symmetry around the doped site, and the low local disorder, are all detrimental for the proton conductivity. [2-6]

The **second part** is devoted to alternative structures based on tetrahedral units, such as rare-earth niobates and gallates. A full case study will be discussed, as an example of the use of three complementary synchrotron radiation techniques (EXAFS, in situ and high-resolution XRD) to unravel the complex structural features of $La_{1-x}Ba_{1+x}GaO_4$, and their interplay with the proton bonding and conductivity. [7]

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[2] - A. Longo et al. - *Chem. Mater.* **18** (2006) 5782
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