

## TAILORING THE PROPERTIES OF A-SITE SUBSTITUTED $\text{Ba}_{1-x}\text{Gd}_{0.8}\text{La}_{0.2+x}\text{Co}_2\text{O}_{6-\delta}$

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The double perovskite  $\text{BaGd}_{0.8}\text{La}_{0.2}\text{Co}_2\text{O}_{6-\delta}$  (BGLC) shows excellent performance as oxygen electrode for Proton Ceramic Fuel Cells (PCFCs) and electrolyzer cells (PCEC), with polarization resistances in wet oxygen of 0.04 and 10  $\Omega\text{cm}^2$  at 650 and 350 °C, respectively [1]. Compared with other reported PCFC cathodes [2], BGLC performs better both at high and low temperature. The excellent performance of BGLC in proton ceramic cells is rationalized by a suggested partial proton conductivity at intermediate temperatures, supported by significant hydration up to 400°C observed by thermogravimetric studies. However, the chemical stability of BGLC in high steam pressures under PCEC operation remains a concern due to its highly basic A-site. Thus, tailoring the A-site stoichiometry by partial substitution of Ba with La may be a viable route for further optimizing the balance between chemical stability and electrochemical performance.

In the literature we find numerous defect chemical models describing  $\text{REBaCo}_2\text{O}_{5.5+\delta}$ -type double perovskites, but these are typically limited to describing the oxygen non-stoichiometry. Little can be found which relates defect chemistry to electrochemical performance, electrical conductivity or hydration behavior. Thus, this contribution aims to develop a global defect chemical model of the system  $\text{Ba}_{1-x}\text{Gd}_{0.8}\text{La}_{0.2+x}\text{Co}_2\text{O}_{6-\delta}$  ( $x = 0-0.5$ ) by investigating its structural and functional properties as a function of Ba-site substitution. The complex structural behavior of Ba-site substituted BGLC is elucidated by combining synchrotron and neutron diffraction data with high temperature XRD to describe the local Co-O environment and the degree of cation and anion ordering as a function of temperature and  $p\text{O}_2$ . The implications of A-site stoichiometry on proton incorporation are further investigated by thermogravimetric hydration studies supported by neutron powder diffraction of dry and deuterated samples. Finally, these properties are linked to oxygen non-stoichiometry, electrical conductivity and electrochemical performance to develop and validate our general defect chemical model for the system  $\text{Ba}_{1-x}\text{Gd}_{0.8}\text{La}_{0.2+x}\text{Co}_2\text{O}_{6-\delta}$  ( $x = 0-0.5$ ).

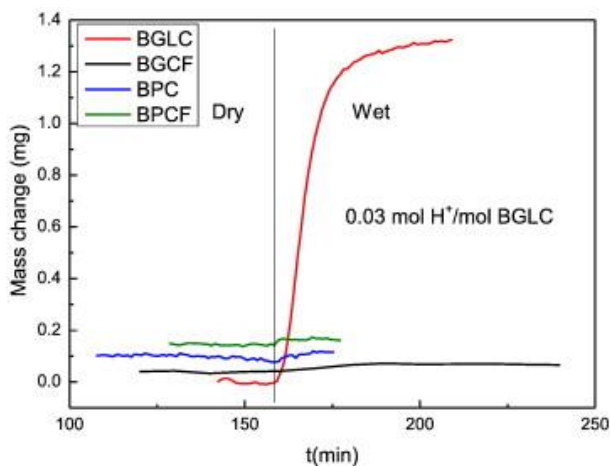


Figure 1 – Hydration of BGLC after isothermal switch from  $p\text{H}_2\text{O} = 3 \cdot 10^{-5}$  to  $p\text{H}_2\text{O} = 0.02 \text{ atm}$  [1]

### REFERENCES:

1. Strandbakke, R., V.A. Cherepanov, A.Y. Zuev, D.S. Tsvetkov, C. Argirusis, G. Sourkouni, S. Prünke, and T. Norby, Gd- and Pr-based double perovskite cobaltites as oxygen electrodes for proton ceramic fuel cells and electrolyser cells. *Solid State Ionics*, 2015. 278: p. 120-132.
2. Dailly, J., S. Fourcade, A. Largeau, F. Mauvy, J.C. Grenier, and M. Marrony, Perovskite and A2MO4-type oxides as new cathode materials for protonic solid oxide fuel cells. *Electrochimica Acta*, 2010. 55(20): p. 5847-5853.