Scandium-doped manganate anode for a proton-conducting solid oxide steam electrolyzer

Lizhen Gan, a Lingting Ye, a Mingzhou Liu, a Shanwen Tao, c Kui Xie b *

a School of Mechanical and Automotive Engineering, Hefei University of Technology, No.193 Tunxi Road, Hefei, Anhui 230009, China.
b Key Lab of Design & Assembly of Functional Nanostructure, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, China.
c School of Engineering, University of Warwick, Coventry, CV4 7AL, United Kingdom.
*Corresponding: kxie@fjirsm.ac.cn; Tel/Fax: 0086-591-63179173

Fig.S1 Equivalent circuit diagram used to model the impedance data. The Rs is series resistance while the Rp is the electrode polarization resistance.

Fig.S2 Structure and schematic of the proton conducting solid oxide electrolyser. (a) a schematic figure of a 2-mm-thick electrolyte supported single cell with a configuration of LSM-BCZYZ/BCZYZ/BCZYZ-LSCM, here the LSM-BCZYZ is a composite anode while the LSCM-BCZYZ is a composite cathode; (b) a testing schematic figure for the high temperature test for steam electrolysis, here the cell is tested in two electrode mode.

In this part, the solid oxide electrolyser is an 2-mm-thick BCZYZ electrolyte supported configuration. The electrode area is 1 cm$^2$ in symmetric position. The BCZYZ and electrode powder are in a weight ratio of 35:65. The electrode thickness is around 15 μm.
Fig. S3 HR-TEM images of LSM (a) and LSMS0.05 (b).

Fig. S4 (a) XPS result of Mn (a1), O (b1) in the oxidized LSM; Mn (a2), O (b2) in the reduced LSM.

Fig. S5 The defect reactions for the doping of Sc in LSM lattice. In this work, the Mn is normally a mixed state with +4 and +3 in B site. The first reaction is for Mn$^{3+}$ while the second is for the reaction of Mn$^{4+}$. If the oxygen vacancy combines with oxygen, the hole will be generated as charge carrier.

$$\begin{align*}
\text{Sc}_2O_3 + \text{Mo}_{O_{\text{Sc}}} & \rightarrow 2\text{Sc}_{2}\text{O}_{\text{A}} + 3O_{\text{O}} \\
\text{Sc}_2O_3 + \text{MoO}_{\text{Sc}} & \rightarrow 2\text{Sc}_{2}\text{O}_{\text{A}} + 1/2V_{\text{O}}^{\text{w}} + 3O_{\text{O}} \\
& \rightarrow O_{\text{O}}^{\text{w}} + h^0
\end{align*}$$

Fig. S6 TGA test of oxidized LSM (a) in 5%H$_2$/Ar from 20 °C to 800 °C (5 °C·min$^{-1}$) to determine the oxygen nonstoichiometry.

TGA is a common method to determine the nonstoichiometry of oxide materials. In this work, the \( \text{La}_{0.8}\text{Sr}_{0.2}\text{MnO}_3 \) has assumed to be a chemical formula of \( \text{La}_{0.8}\text{Sr}_{0.2}\text{MnO}_{3.00} \) as a reference to compare
the oxygen loss. In this figure, the weight loss is 3.96% which indicates the oxygen loss. Therefore, the oxygen loss per $\text{La}_{0.8}\text{Sr}_{0.2}\text{MnO}_3$ is $3.96\% \times \left[138.9 \times 0.8 + 87.62 \times 0.2 + 54.94 \times 1 + 16.00 \times 3\right] / 16.00 = 0.54$

Fig. S7 Cross sectional FESEM images of the solid oxide symmetric cell with the (a) LSM composite electrode and (b) LSMS$_{0.05}$ composite electrode.

Fig.S8 (a) The FESEM image of composite anode based on LSMS$_{0.05}$-BCZYZ in air; (b) EDS maps of composite anodes based on LSMS$_{0.05}$-BCZYZ in air.