

Supplementary information for

Highly efficient bismuth substitution induced A-site ordered layered perovskite electrode for symmetrical solid oxide fuel cells

Yang Yang^{a, b}, Zhengpeng Chen^c, Mingfei Li^c, Muming Rao^c, Fangjun Jin^a, Yihan
Ling^{*a}, Peizhong Feng^{*a}, Shaorong Wang^b

^a School of Materials Science and Physics, China University of Mining and
Technology, Xuzhou 221116, P. R. China

^b School of Chemical Engineering and Technology, China University of Mining and
Technology, Xuzhou 221116, P. R. China

^c Guangdong Energy Group Science and Technology Research Institute Co. Ltd,
Guangzhou 510000, China

[*] Corresponding Author:

Yihan Ling, Peizhong Feng

School of Materials Science and Engineering,
China University of Mining and Technology,
Xuzhou 221116, P.R. China

E-mail address: lyhyy@cumt.edu.cn

lyhyy@mail.ustc.edu.cn

Details for the calculation of oxygen vacancy formation energy

Spin-polarized density functional theory (DFT) calculation was used to study the effect of Bi doping on oxygen vacancy formation energy. The theoretical calculation is based on the Materials Studio software package, and is carried out using pseudopotential and plane wave basis set. The generalized gradient functional PBE functional in density functional theory (DFT) is chosen as the exchange correlation energy. U values for both the d-orbitals of Mn and the f-orbitals of Pr set at 3.0 and 6.0 eV, respectively, and the cutoff for kinetic energy at 630 eV. The tolerance for self-consistency was selected to be 1.0×10^{-5} eV per atom, 0.03 eV Å⁻¹ for force, 0.05 GPa for maximum stress, and 0.001 Å for the maximum displacement. The primitive cells of L-PBM and L-Bi-PBM were Pr₄Ba₄Mn₈O₂₃ and Pr₃Bi₁Ba₄Mn₈O₂₃. The oxygen vacancy formation energy was calculated according to:

$$\Delta E_{\text{vac}} = E(\text{defect}) - E(\text{perfect}) + 0.5E(\text{O}_2, \text{g}) \quad (1)$$

where ΔE_{vac} is oxygen vacancy formation energy, $E(\text{defect})$ is the total energy of the non-stoichiometric structure, $E(\text{perfect})$ is the total energy of stoichiometric structures, and $E(\text{O}_2, \text{g})$ is the total energy of a triplet O₂ molecule.

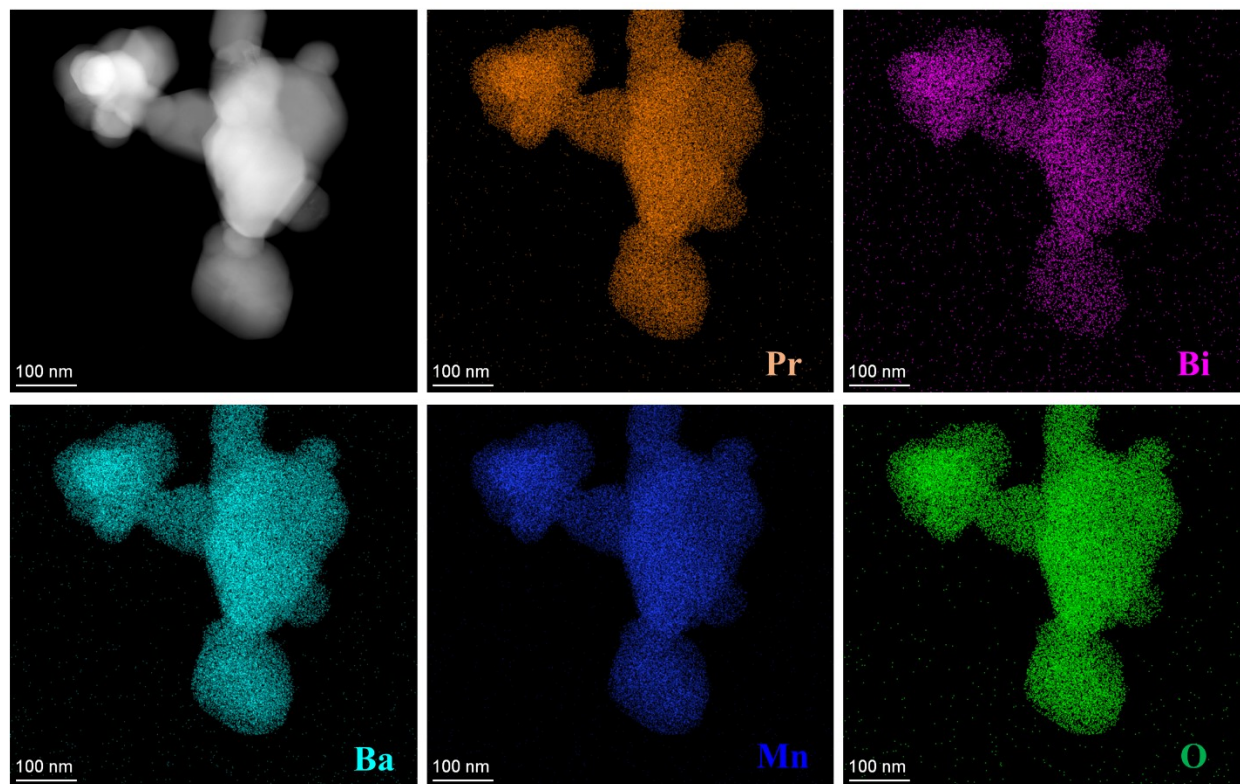


Fig. S1 HADDF and mapping result of the Bi-PBM electrode powder prepared in air.

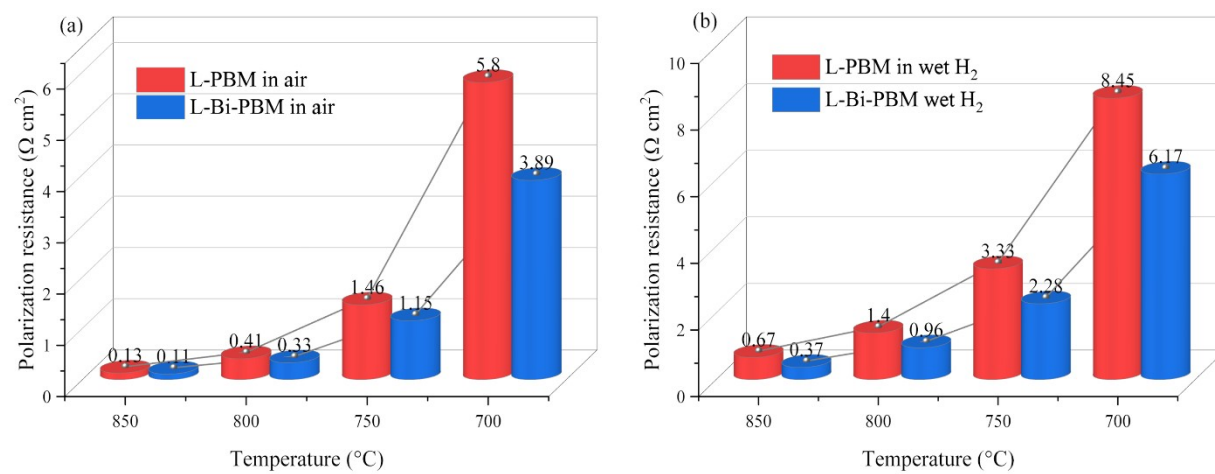


Fig. S2 Polarization resistance of L-PBM and L-Bi-PBM obtained at different temperature.

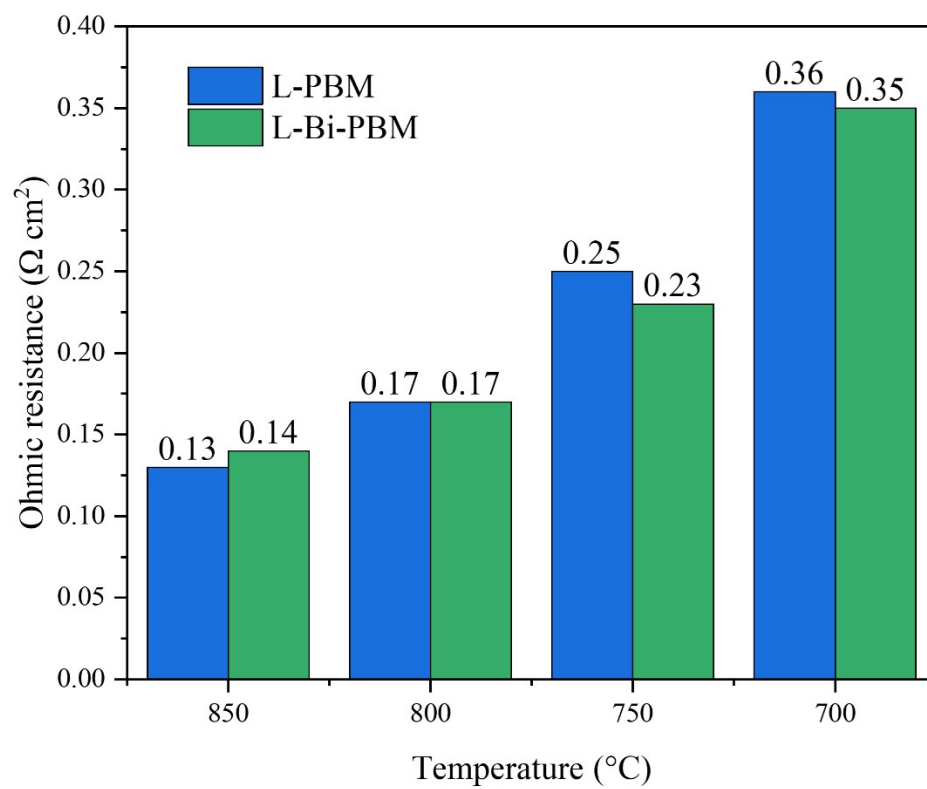


Fig. S3 Ohmic resistance of L-PBM and L-Bi-PBM at different temperature.

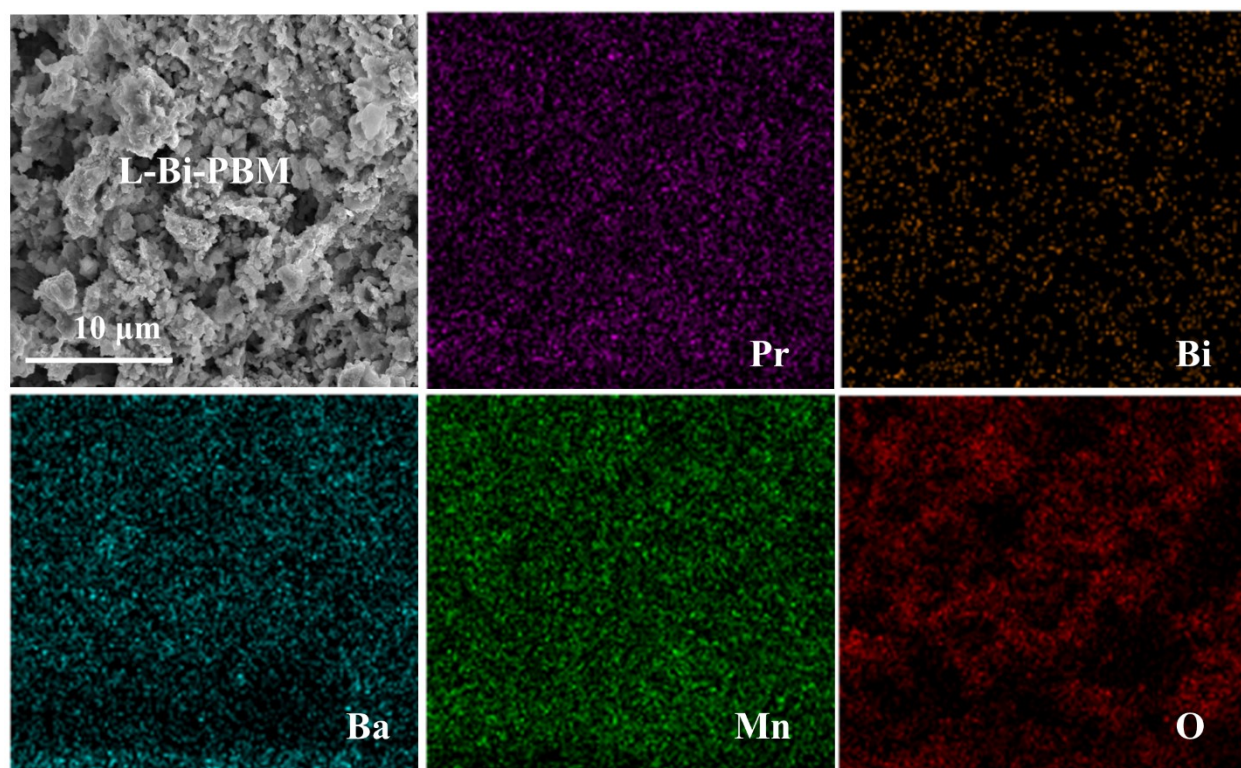


Fig. S4 EDS mapping results of L-Bi-PBM electrode after stability test

Table 1 The comparison of polarization resistances with the reported electrodes

Electrode	Electrolyte	Temperature (°C)	R _p (air, Ω cm ²)	R _p (H ₂ , Ω cm ²)	Ref.
PrBaMn _{1.5} Fe _{0.5} O _{5+δ}	LSGM	800	0.22	0.68	1
SmBaMn ₂ O _{5+δ}	LSGM	850	0.13	0.57	2
Pr-PrBaMn ₂ O _{5+δ}	LSGM	800	0.016	0.20	3
SmBaMn _{1.9} Mg _{0.1} O _{5+δ}	LSGM	900	0.073	0.263	4
La _{0.75} Sr _{0.25} Cr _{0.5} Mn _{0.5} O _{3-δ}	YSZ	900	0.35	0.3	5
Pr _{0.7} Ca _{0.3} Cr _{0.6} Mn _{0.4} O _{3-δ}	YSZ	800	4	30	6
La _{0.8} Sr _{0.2} FeO _{3-δ}	YSZ	800	0.31	0.58	7
Sr ₂ Fe _{1.5} Mo _{0.5} O _{6-δ}	LSGM	800	0.24	0.27	8
La _{0.4} Sr _{1.6} MnO _{4±δ}	LSGM	800	0.87	2.07	9
GdBaFe ₂ O _{5+δ}	LSGM	800	0.073	1.911	10
PrBaMn ₂ O _{5+δ}	ScSZ	850	0.13	0.67	This work
Pr _{1.8} Bi _{0.2} BaMn ₂ O _{5+δ}		850	0.11	0.37	

References:

- 1 L. Zhao, K. F. Chen, Y. X. Liu and B. B. He, J Power Sources, 2017, **342**, 313-319.
- 2 Y. Zhang, H. L. Zhao, Z. H. Du, K. Swierczek and Y. Y. Li, Chem Mater, 2019, **31**, 3784-3793.
- 3 Y. H. Gu, Y. L. Zhang, Y. F. Zheng, H. Chen, L. Ge and L. C. Guo, Appl Catal B-Environ, 2019, **257**, 117868.
- 4 Y. Zhang, B. Z. Zhang, H. L. Zhao, K. Swierczek, Z. H. Du, Y. Y. Li, L. Xu and H. Li, Catal Today, 2021, **364**, 80-88.

- 5 D. M. Bastidas, S. W. Tao and J. T. S. Irvine, *J Mater Chem*, 2006, **16**, 1603-1605.
- 6 A. El-Himri, D. Marrero-Lopez, J. C. Ruiz-Morales, J. Pena-Martinez and P. Nunez, *J Power Sources*, 2009, **188**, 230-237.
- 7 D. Tian, B. Lin, Y. Yang, Y. H. Chen, X. Y. Lu, Z. G. Wang, W. Liu and E. Traversa, *Electrochim Acta*, 2016, **208**, 318-324.
- 8 Q. A. Liu, X. H. Dong, G. L. Xiao, F. Zhao and F. L. Chen, *Adv Mater*, 2010, **22**, 5478-5482.

