Mo-doping allows high performance for a perovskite cathode applied in proton-conducting solid oxide fuel cells

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Experimental section

$Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_{3-\delta}$ (BSCF) and $Ba_{0.5}Sr_{0.5}Co_{0.7}Fe_{0.2}Mo_{0.1}O_{3-\delta}$ (BSCFMo) powders were synthesized by a wet chemical route,[1] using $Ba(NO_3)_3$, $Sr(NO_3)_2$, $Co(NO_3)_3$, $Fe(NO_3)_3$ and $(NH_4)_6Mo_7O_{24}$ as the starting materials in an aqueous solution. Both BSCF and BSCFMo powders were calcined at 1000 ^oC for 3 h to get a pure phase. The phase purity of these powders was examined by X-ray diffraction (XRD, Rigaku Ultima IV). The morphology and elemental distribution of BSCFMo powder were analyzed by scanning transmission electron microscopy (STEM, JEM-2100F). X-ray photoelectron spectroscopy (XPS) analysis of both BSCF and BSCFMo powders was conducted on a Thermo Fisher ESCALAB 250Xi spectrometer using an AlKα (1486.6 eV) radiation source.

The performance of the BSCFMo cathode was evaluated on the $BaZr_{0.1}Ce_{0.7}Y_{0.2}O_{3-\delta}$ (BZCY). Anode supported Ni-BCZY/BCZY half cells were prepared and the preparation details can be found in our previous reports. BSCFMo-BCZY composite cathode was deposited on the sintered BCZY electrolyte surface, followed by a calcination at 900 ^oC for 10 min in a microwave sintering furnace. Then, the cell was tested in the fuel cell testing condition using H2 as the fuel and the electrochemical performance of the cell was recorded using an electrochemistry workstation (Squidstat Plus, Admiral Instrument). For comparison, the cell using the BSCF cathode was fabricated and tested in the same procedure.

Theoretical calculations were performed with the first principle method, using the VASP (Vienna ab initio simulation package) software and the calculation details can be found in our previous studies.[2, 3]

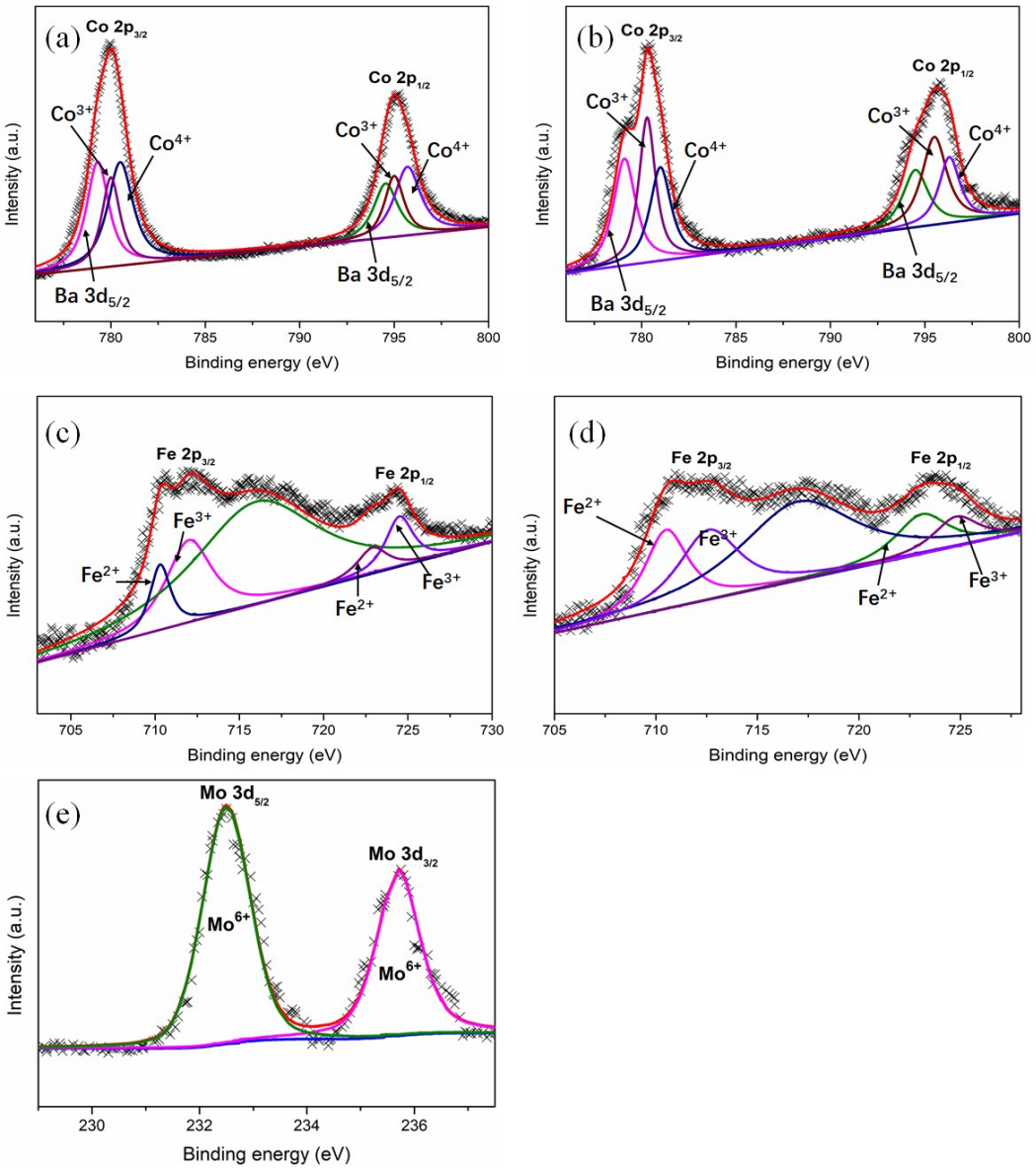

Figure S1. XPS spectra of (a) Co 2p and Ba 3d in BSCF, (b) Co 2p and Ba 3d in BSCFMo, (c) Fe 2p in BSCF, (d) Fe 2p in BSCFMo, (e) Mo 3d in BSCFMo.

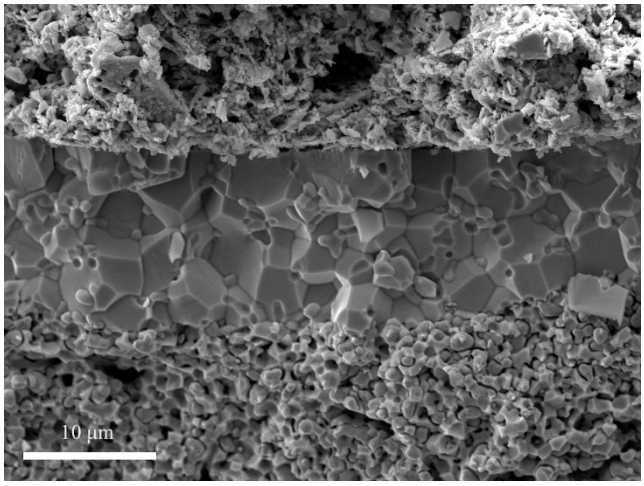

Figure S2. SEM image for the BSCF cell after testing.

Reference

1. Y. P. Xia, Z. Z. Jin, H. Q. Wang, Z. Gong, H. L. Lv, R. R. Peng, W. Liu and L. Bi, *J Mater Chem A*, 2019, **7**, 16136-16148.
2. X. Xu, H. Q. Wang, J. M. Ma, W. Y. Liu, X. F. Wang, M. Fronzi and L. Bi, *J Mater Chem A*, 2019, **7**, 18792-18798.
3. X. Xu, H. Q. Wang, M. Fronzi, X. F. Wang, L. Bi and E. Traversa, *J Mater Chem A*, 2019, **7**, 20624-20632.