Supporting Information

Separation of Hydrogen Isotopes using a proton ceramic fuel cell

Meilong Chen,^{ac} Kai Zhao,^{ab} Jun Li,^{ab} Guixiang Lin,^b Dustin Banham,^{ab} Li Du^c and Min Chen *ab

^a School of Materials Science and Energy, Foshan University, Foshan 528000, P.R.China.

^b Guangdong Key Laboratory for Hydrogen Energy Technologies, Foshan 528000, P.R.China.

^c School of Chemistry and Chemical Engineering, South China University of Technology, Guangzhou 510640, P.R.China.

*Corresponding authors. Email address: minchen1981@126.com.



Figure S1 XRD pattern of the BZY powder calcined at 1150 °C for 10 h.



Figure S2 Gibbs free energy change values for the reaction of $H_2(g)+0.5O_2(g) = H_2O(g)$ and $D_2(g)+0.5O_2(g) = D_2O(g)$.

Calculation of Separation Factor Values: The hydrogen/deuterium separation factor (a) can be

calculated using the equations below;

$$\alpha = \left(\frac{[H]}{[D]}\right)_{L} : \left(\frac{[H]}{[D]}\right)_{G}$$
(1)

Where $[H]_L$, $[D]_L$, and $[H]_G$, $[D]_G$ represent the liquid-phase quantities of the isotopes at the cathode and the gasphase isotopes at the anode expressed as concentrations, respectively. In infrared spectroscopy, the isotopic content corresponds to the area of the corresponding peak. Assuming that the peak area of the D₂O is A, the peak area of the HDO is B, and the peak area of the HD is C, the $[D]_L$ and $[H]_L$ concentration can be obtained by the following equation;

$$[D_2O] = [D]_L = \frac{A + B/2}{A + B + C}$$
(2)

$$[H_2O] = [H]_L = \frac{C + B/2}{A + B + C}$$
(3)



Figure S3 Current density of BZY20-based cells tested in a potential static mode under 1:1-H₂+D₂ fuel at 700°C;