Supplementary Information

Oxygen permeation and stability of Mo-substituted BSCF membranes

H. Gasparyan\textsuperscript{a}, J. B. Claridge\textsuperscript{a} and M. J. Rosseinsky*\textsuperscript{a}

\textsuperscript{a} Department of Chemistry, University of Liverpool, Liverpool L69 7ZD, United Kingdom.

rossein@liv.ac.uk

\begin{center}
\begin{table}
\begin{tabular}{|l|c|c|}
\hline
Lattice parameters & Refinement parameters \\
\hline
Space group & a, b, c / Å & R_{wp} / % & 14.5 \\
\hline
DP & Fm\bar{3}m & a=7.9857(3) & R_{exp} / % & 13.6 \\
\hline
SP & Pm\bar{3}m & a=3.9787(5) & $\chi^2$ & 1.06 \\
\hline
BaMoO$_4$ & $I\bar{4}1/a$ & a=5.5465(7) c=12.7643(9) & & \\
\hline
\end{tabular}
\end{table}
\end{center}

S1: Pawley refinement (red line) of XRD data for Ba$_{0.5}$Sr$_{0.5}$Co$_{0.5}$Fe$_{0.125}$Mo$_{0.375}$O$_{3-\delta}$ powders (black line) sintered at 1200 °C for 5 hours. Reflection marks refer to SP (black), DP (blue) and BaMoO$_4$ (green a= Å). The gray line represents the difference between calculated and measured data.

S2: Pawley refinement (red line) of XRD data for Ba$_{0.5}$Sr$_{0.5}$Co$_{0.5}$Fe$_{0.125}$Mo$_{0.375}$O$_{3-\delta}$ powders (blue line) sintered at 1250°C for 5 hours. Reflection marks refer to SP (black), DP (blue) and
BaMoO$_4$ (green). The gray line represents the difference between calculated and measured data.

<table>
<thead>
<tr>
<th>Lattice parameters</th>
<th>Refinement parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Space group</td>
<td>a, b, c / Å</td>
</tr>
<tr>
<td>DP Fm3m</td>
<td>a=7.9798(2)</td>
</tr>
<tr>
<td>SP Pm3m</td>
<td>a=3.9793(7)</td>
</tr>
<tr>
<td>BaMoO$_4$ I41/a</td>
<td>a=5.5532(8) c=12.7096(1)</td>
</tr>
</tbody>
</table>

S3: Time dependence of oxygen permeation flux at 750 °C in 100/100 ml/min air/He for 1 mm BSCF, Ba$_{0.5}$Sr$_{0.5}$Co$_{0.78}$Fe$_{0.195}$Mo$_{0.025}$O$_{3-d}$ and Ba$_{0.5}$Sr$_{0.5}$Co$_{0.5}$Fe$_{0.125}$Mo$_{0.375}$O$_{3-d}$ membranes. Ba$_{0.5}$Sr$_{0.5}$Co$_{0.78}$Fe$_{0.195}$Mo$_{0.025}$O$_{3-d}$ membrane was tested for additional 50 hours and is compared with BSCF (experimental data are extrapolated to 250 hours).