Supplementary information

Proton transport enhanced by octahedral distortion and built-in electric field in PMN-TiO_2 heterointerface

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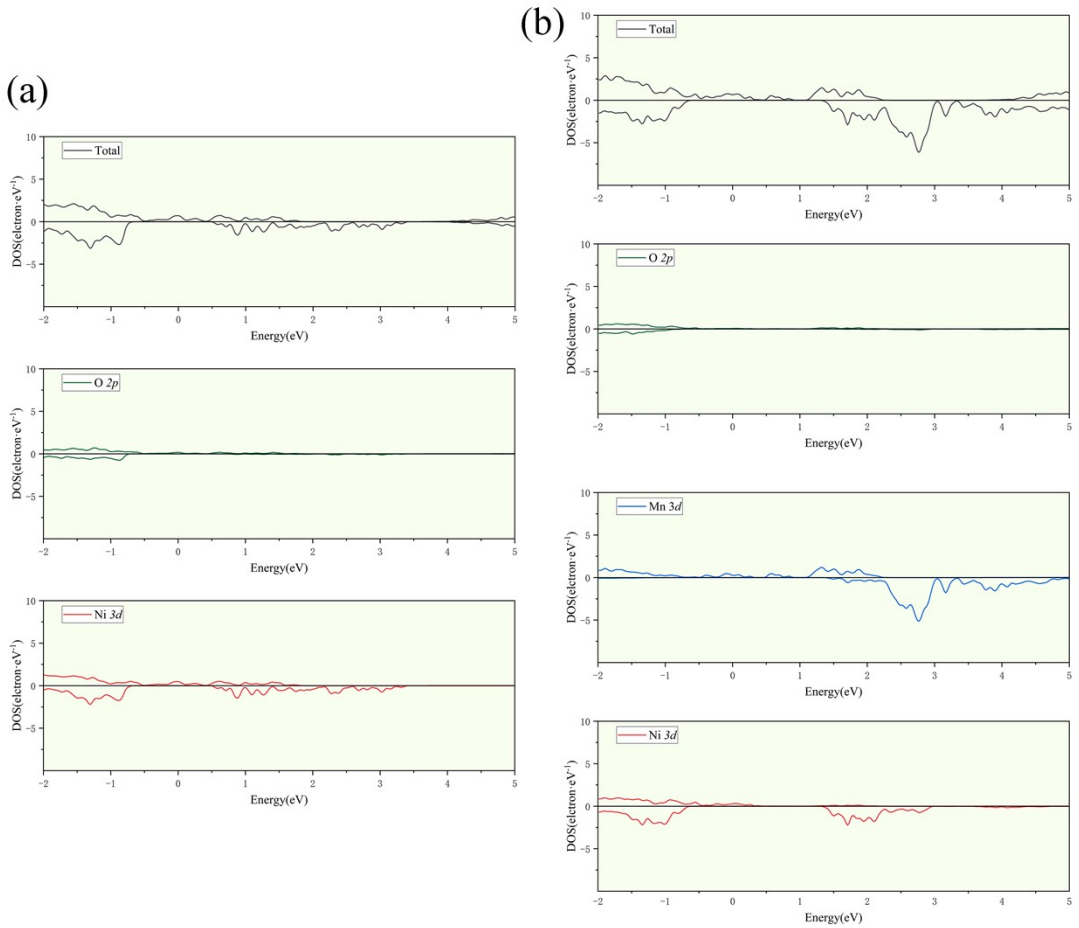
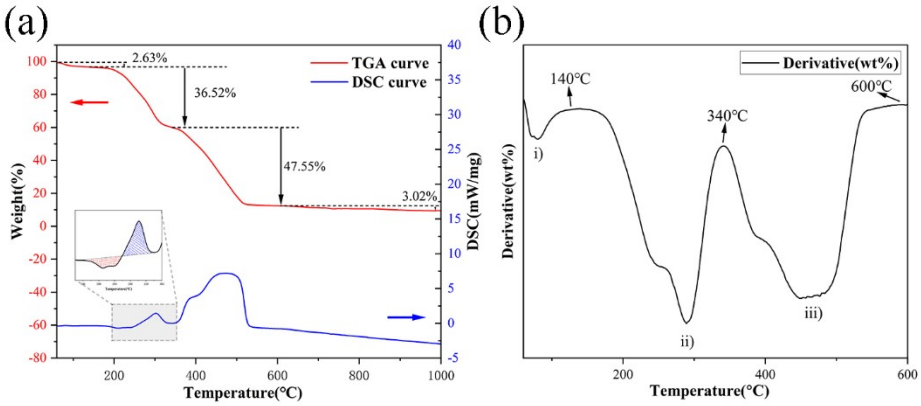
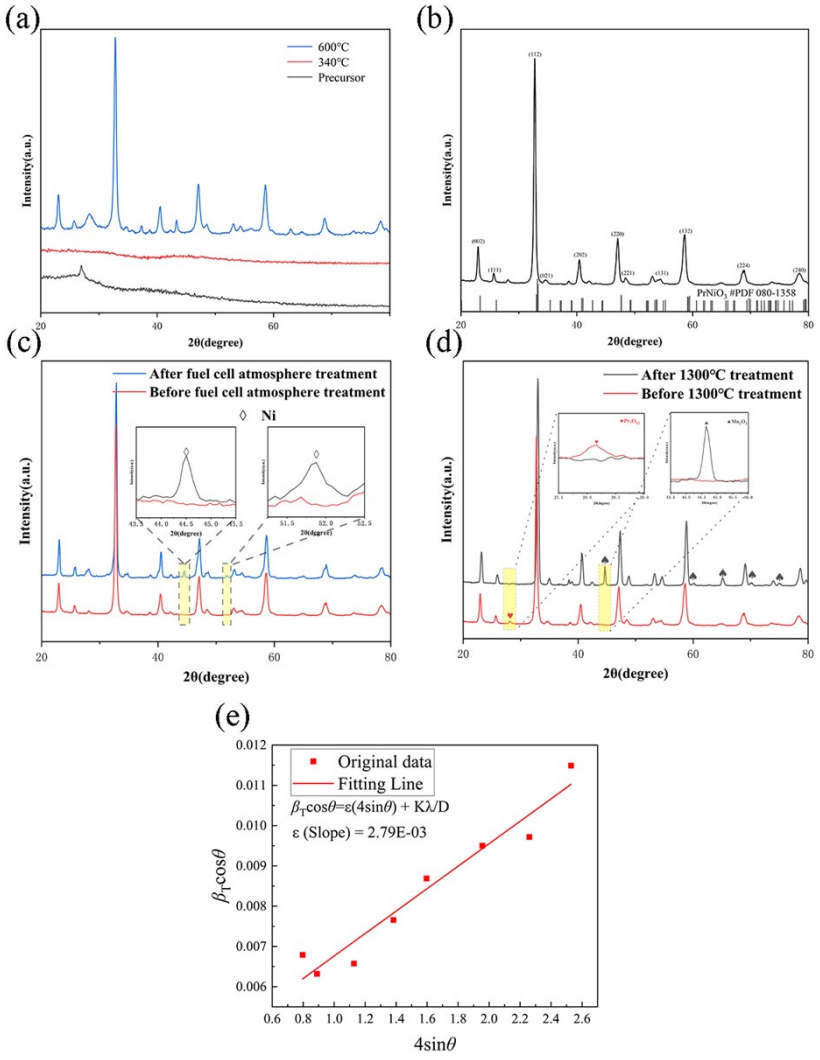


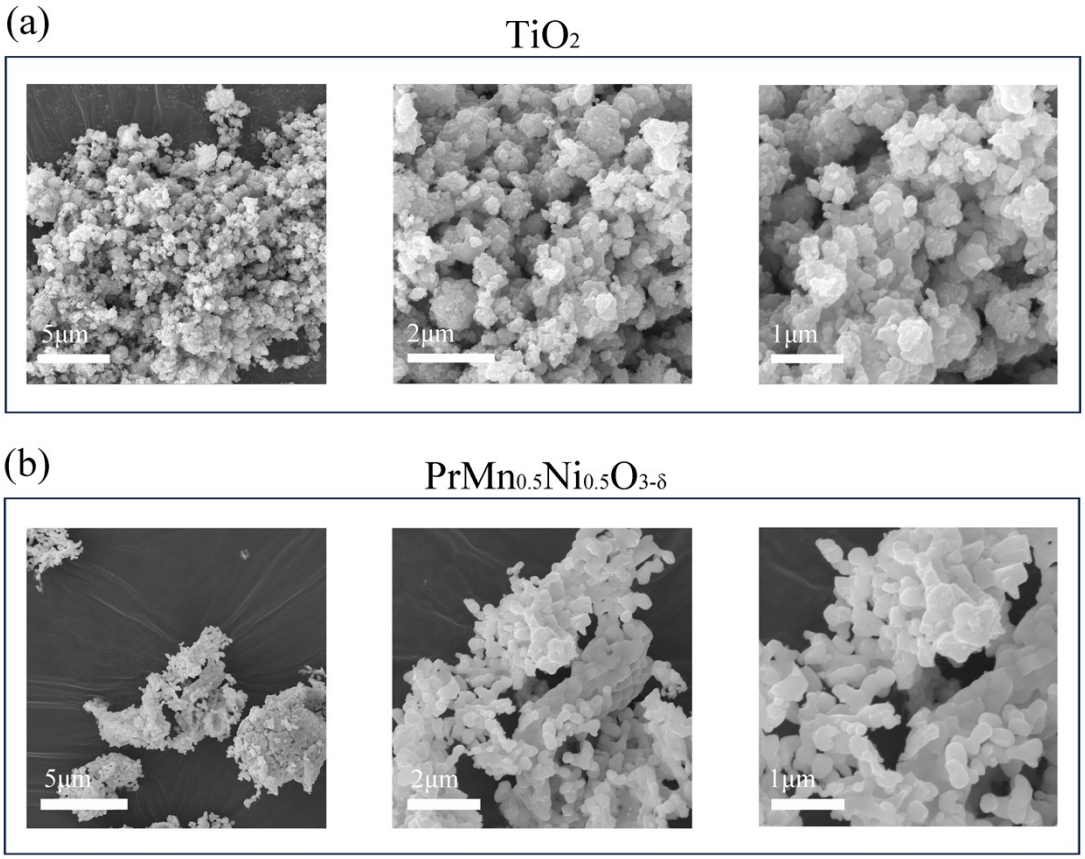
Supplementary Fig. 1 Projected density of states of (a)PNO and (b)PMN



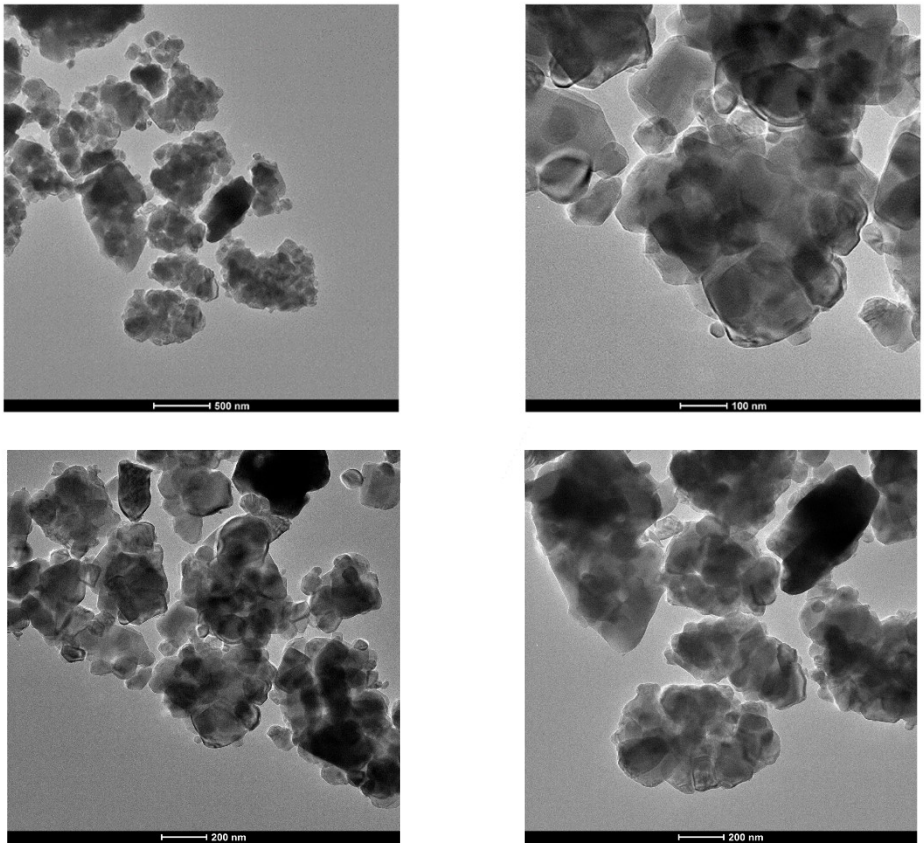
Supplementary Fig. 2 (a) TG analysis (TGA)/DSC curves recorded during the thermal decomposition of PMN precursors. (b) First derivative TGA curves.



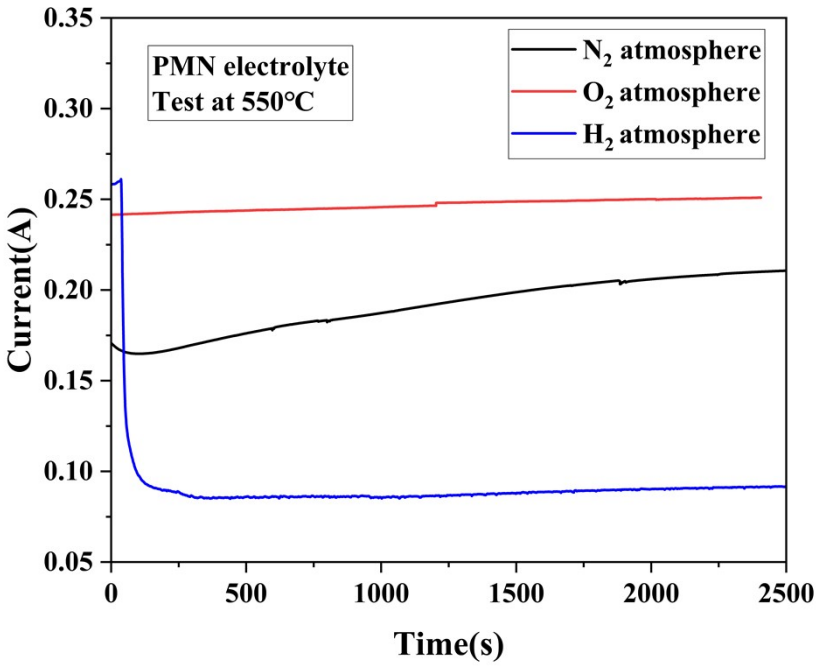
Supplementary Fig. 3 X-ray diffraction patterns (a) precursor, (b) lattice plane of PMN, (c) H_2 treated PMN, (d) high temperature treatment at 1300℃ for 4h and (e) Williamson-Hall plot of PMN.



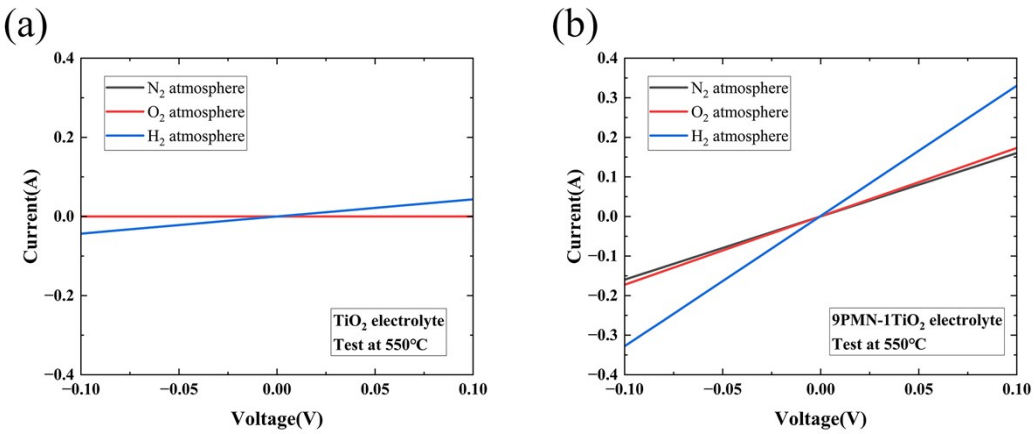
Supplementary Fig. 4 SEM images of (a) $PrMn_{0.5}Ni_{0.5}O_{3-\delta}$ and (b) TiO_2.



Supplementary Fig. 5 TEM images of PMN-TiO_2 composite, showing the interfaces and interact between particles and grains.

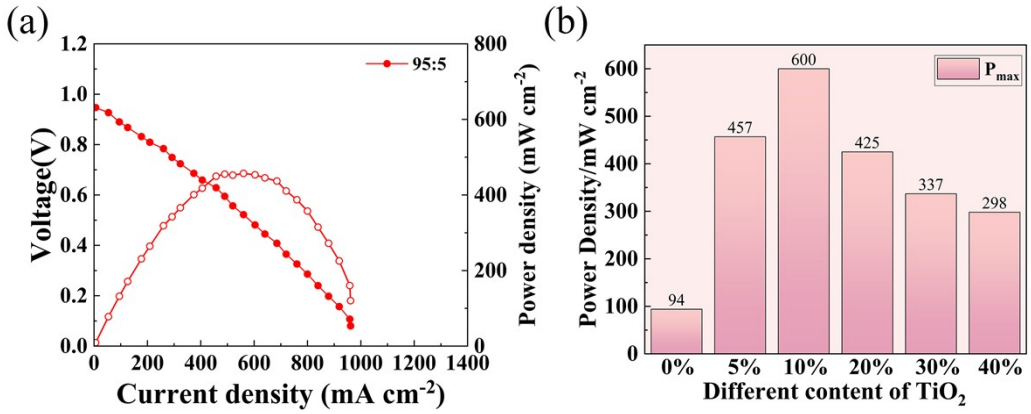


Supplementary Fig. 6 (a)Current-time test of PMN under 0.1V voltage bias.

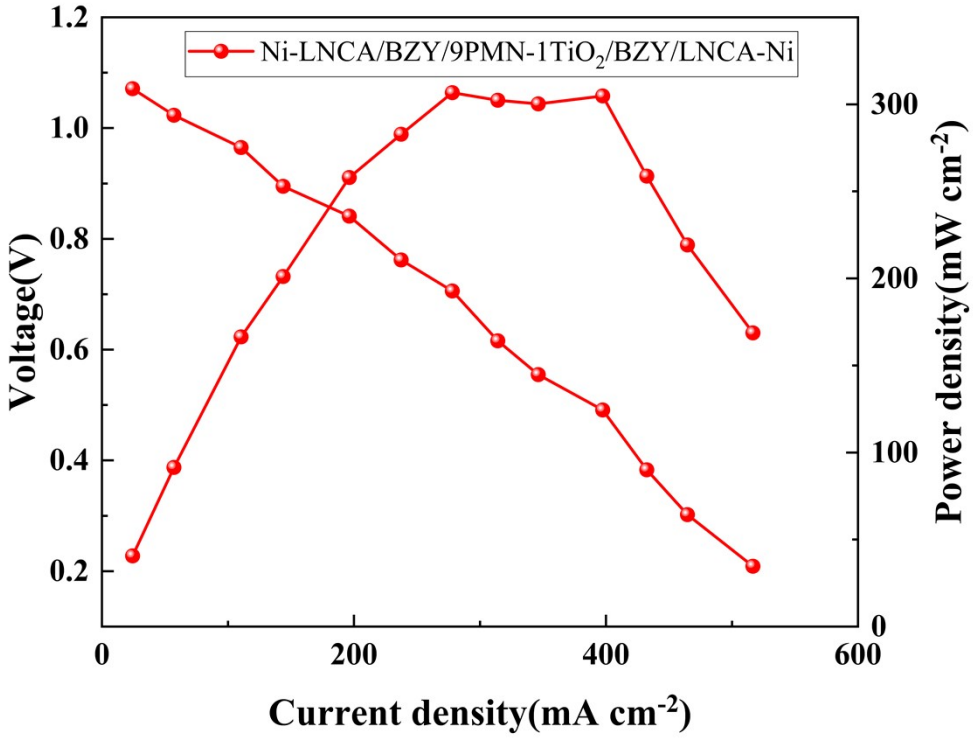


Supplementary Fig. 7 Voltage sweep test after 30 mins atmosphere (N_2, O_2, H_2) treatment of (a)TiO_2 and (b)9PMN-1TiO_2 composite electrolyte from -0.1 V to 0.1 V. Sample coated with Pt on each side for test in O_2 and H_2 atmosphere and coated with Ag on each side for test in N_2 atmosphere.

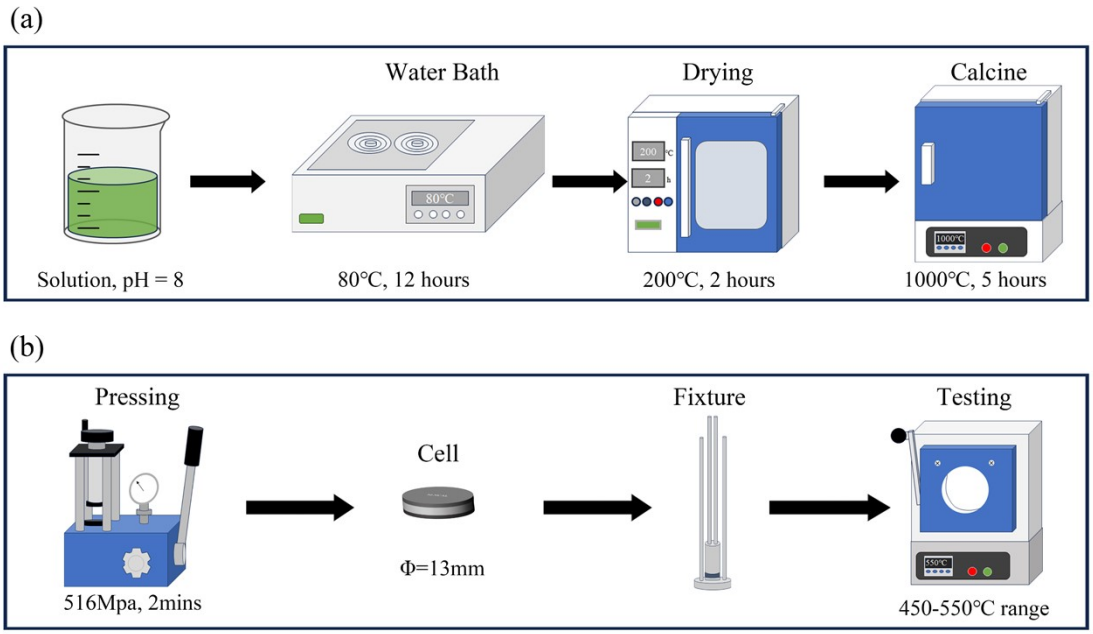
Supplementary Fig. 8 Thickness of PMN, TiO_2 and 9PMN-1TiO_2 electrolyte in DC test.



Supplementary Fig. 9 (a) I-V-P result of 95:5 composite materials electrolyte applying in SOFC. (b) Maximum power density of different content of TiO2.



Supplementary Fig. 10 I-V-P result of Ni/LNCA/BZY/9PMN-1TiO2/BZY/LNCA-Ni fuel cell at 550℃



Supplementary Fig. 11 (a) Sythesis process of PMN powder and (b) fuel cells fabrications, assembling and test.

Supplementary Table 1

The Metal-Oxygen(M-O) bonds distance of $PrNiO_3$ $PrMn_{0.5}Ni_{0.5}O_{3-\delta}$ and PMN-TiO_2 heterostructure, where No.1 to No.6 stand for different M-O bond in octahedron.

$PrNiO_3$						
Distance (Å)	No.1	No.2	No.3	No.4	No.5	No.6
Ni-O	1.94371	1.94371	1.95433	1.95433	1.9426	1.9426
Ni-O Octahedron Distortion factor(Δ): **0.0014%**						
$PrMnO_3$						
Distance (Å)	No.1	No.2	No.3	No.4	No.5	No.6
Mn-O	1.9927	1.9927	1.9752	1.9752	2.0279	2.0279
Mn-O Octahedron Distortion factor(Δ): **0.0121%**						
$PrMn_{0.5}Ni_{0.5}O_{3-\delta}$						
Distance (Å)	No.1	No.2	No.3	No.4	No.5	No.6
Ni-O	2.04781	2.04781	2.07347	2.07347	1.98959	1.98959
Ni-O Octahedron Distortion factor(Δ): **0.0605%**						
Distance (Å)	No.1	No.2	No.3	No.4	No.5	No.6
Mn-O	1.98843	1.98843	1.94492	1.94492	1.94045	1.94045
Mn-O Octahedron Distortion factor(Δ): **0.0239%**						
PMN-TiO_2 Heterostructure						
Distance (Å)	No.1	No.2	No.3	No.4	No.5	No.6
Ni-O	2.07151	2.04045	2.04764	2.14841	2.0984	2.12402
Ni-O Octahedron Distortion factor(Δ): **0.0735%**						
Distance (Å)	No.1	No.2	No.3	No.4	No.5	No.6
Mn-O	1.88058	1.94257	1.95253	1.96495	2.35328	2.24927
Mn-O Octahedron Distortion factor(Δ): **1.5260%**						

Supplementary Table 2

Conductivity results by DC test of PMN, TiO_2, 9PMN-1TiO_2 electrolytes.

Electrolytes	Thickness/cm	**Conductance value/S**			**Conductivity/S cm^{-1}**			
		N_2	O_2	H_2	σ_{e^-}	$\sigma_{O^{2-}}$	σ_{H^+}	σ_{tot}
PMN	0.0983	2.105	2.509	9.16	0.122	0.263	0.018	0.281
TiO_2	0.1276	2.85E-06	2.16E-06	4.34E-01	2.15E-07	2.15E-07	8.64E-02	8.64E-02
9PMN-1TiO_2 Composite	0.0815	1.696	1.722	3.249	0.082	0.138	0.332	0.470