

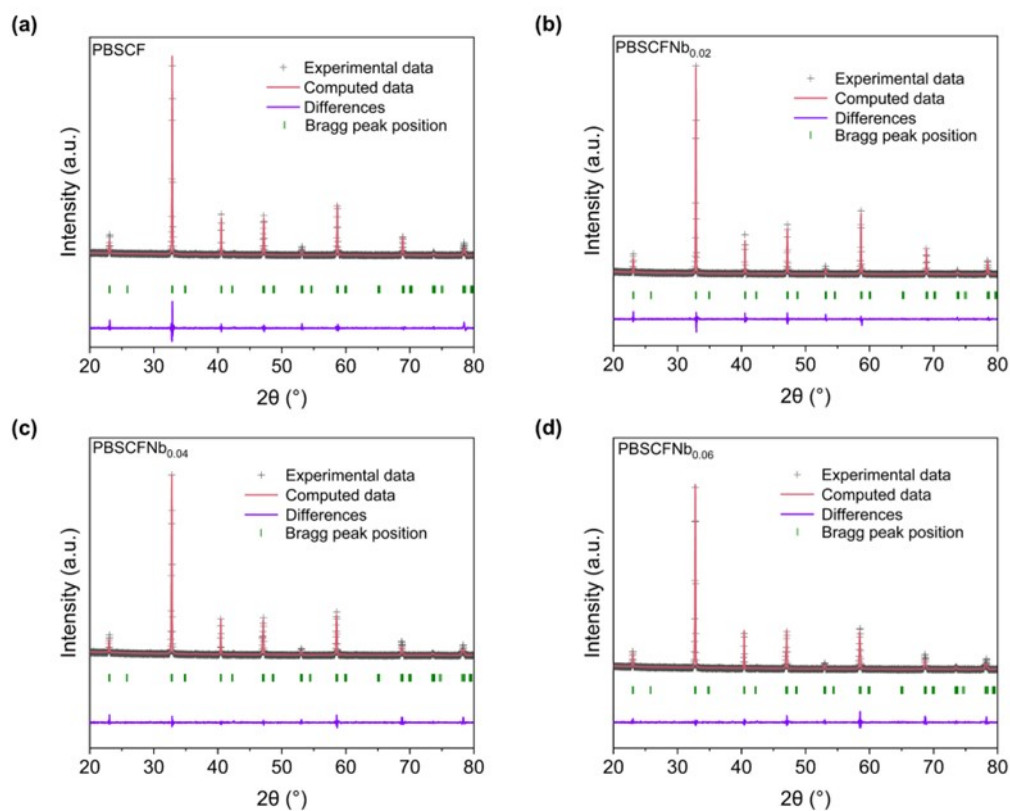


Fig. S1 XRD refined results of PBSCFNb_x

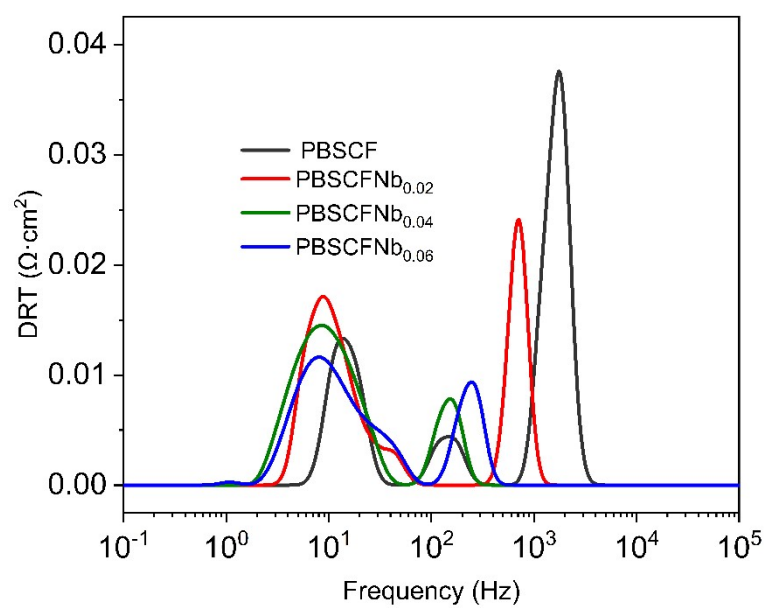


Fig. S2 DRT curve of PBSCFNb_x at 800 °C

Table S1 Rietveld refined results

PBSCFNb _x	Space group	a	c	V	X ²	<i>R</i> _{wp} (%)	<i>R</i> _p (%)
x=0	P4/mmm	3.851183	7.71949	114.399	2.50	9.51	7.01
x=0.02	P4/mmm	3.853876	7.71735	114.493	2.41	9.67	6.55
x=0.04	P4/mmm	3.865034	7.71074	115.187	2.05	8.77	6.30
x=0.06	P4/mmm	3.868033	7.70239	115.465	2.11	9.31	6.75

Table S2 Elements concentration of PBSCFNb_{0.04}

element	O	Fe	Co	Sr	Nb	Ba	Pr	total
atom ratio	52.39	5.64	16.38	4.90	0.62	4.30	15.76	100.00

Table S3 Calculation results of tolerance factor t

PBSCFNb _x	x=0	x=0.02	x=0.04	x=0.06
t	1.0723	1.0718	1.0713	1.0708

Table S4 Average TEC(K⁻¹) of PBSCFNb_x at 30–750 °C

PBSCFNb _x	x=0	x=0.02	x=0.04	x=0.06	SDC
dL/L ₀	21.1×10 ⁻⁶	20.5×10 ⁻⁶	18.8×10 ⁻⁶	18.0×10 ⁻⁶	12.7×10 ⁻⁶

Table S5 Ratio of $O_{vacancy}$, Fe^{4+} , Pr^{4+} and Co^{4+} in $PBSCFNb_x$

Sample	$O_{vacancy}$ (%)	Fe^{4+} (%)	Pr^{4+} (%)	Co^{4+} (%)
x=0	20.35	15.15	57.11	4.77
x=0.02	17.82	13.45	56.93	4.69
x=0.04	15.97	7.71	55.89	3.81
x=0.06	13.27	3.03	51.17	3.4

Table S6 Oxygen vacancy quantitative analysis of PBSCFNb_x

PBSCFNb _x	x=0	x=0.02	x=0.04	x=0.06
spins	6.936e ⁺¹⁶	5.836e ⁺¹⁶	4.967e ⁺¹⁶	3.539e ⁺¹⁶

Table S7 Errors due to conductivity fitting

PBSCFNb _x	300°C	350°C	400°C	450°C	500°C	550°C
x=0	1.0481E-6	1.56947E-6	1.48261E-6	2.75818E-6	1.89455E-6	2.26897E-6
x=0.02	1.5424E-6	1.53887E-6	1.61908E-6	1.71947E-6	1.27881E-6	2.26644E-6
x=0.04	2.0435E-6	2.05724E-6	1.40423E-6	1.87842E-6	1.58091E-6	2.28574E-6
x=0.06	1.9865E-6	2.26841E-6	3.76589E-6	2.89852E-6	2.16582E-6	1.66824E-6
PBSCFNb _x	600°C	650°C	700°C	750°C	800°C	
x=0	2.14735E-6	3.16783E-6	2.04719E-6	1.78297E-6	4.37207E-6	
x=0.02	2.53803E-6	4.04398E-6	3.72458E-6	2.61783E-6	3.09006E-6	
x=0.04	3.74828E-6	2.88653E-6	3.35606E-6	4.39818E-6	2.03599E-6	
x=0.06	1.43852E-6	2.58864E-6	3.59243E-6	1.82648E-6	3.48359E-6	

Table S8 Errors due to ASR fitting

PBSCF	600°C	650°C	700°C	750°C	800°C
R_s	0.093689	0.0034867	0.0007828	0.0010823	0.00026022
R_{HF}	0.052807	0.030961	0.0015762	0.0015048	0.00055807
R_{LF}	0.043867	0.033986	0.0010548	0.00064827	0.00046443
$CPE1$	0.2427	0.067855	0.01695	0.029668	0.017087
$CPE2$	0.054728	0.22258	0.19151	0.053696	0.031776

PBSCFNb _{0.02}	600°C	650°C	700°C	750°C	800°C
R_s	0.0004214	0.0004649	0.0004774	0.0007677	0.0008685
R_{HF}	0.0005580	0.0097706	0.0055752	0.0042472	0.0021552
R_{LF}	0.014292	0.0081027	0.0045054	0.0032687	0.0019189
$CPE1$	0.030839	0.058085	0.087142	0.16098	0.14056
$CPE2$	0.045943	0.040034	0.030864	0.026693	0.025825

PBSCFNb _{0.04}	600°C	650°C	700°C	750°C	800°C
R_s	0.0026098	0.0012762	0.0005391	0.0005258	0.0010412
R_{HF}	0.0323	0.016725	0.0055925	0.0046462	0.0042847
R_{LF}	0.028292	0.013755	0.004323	0.0037573	0.0030557
$CPE1$	0.28622	0.14157	0.072183	0.097786	0.18049
$CPE2$	0.068335	0.068843	0.049149	0.049227	0.043454

PBSCFNb _{0.06}	600°C	650°C	700°C	750°C	800°C
R_s	0.0005060	0.0004975	0.0003103	0.0002972	0.0001886
R_{HF}	0.0019265	0.0017064	0.0008287	0.0005678	0.0002939
R_{LF}	0.0015623	0.013849	0.0007189	0.0004323	0.0001745
$CPE1$	0.011539	0.018077	0.017163	0.020156	0.01366
$CPE2$	0.084732	0.048115	0.021378	0.013797	0.0056939