

Electronic support information

Sillén-Aurivillius phase bismuth niobium oxychloride, $\text{Bi}_4\text{NbO}_8\text{Cl}$, as a New Oxide Ion Conductor

Maksymilian Kluczny³, Jun Tae Song^{1,2}, Taner Akbay⁴, Eiki Niwa¹, Atsushi Takagaki^{1,2}, and Tatsumi Ishihara^{1,2,3*}

¹) International Institute for Carbon Neutral Energy Research (WPI-I2CNER), Kyushu University, Motooka 744, Nishiku, Fukuoka, 819-0395, Japan

²) Department of Applied Chemistry, Faculty of Engineering, Kyushu University, Motooka 744, Nishiku, Fukuoka, 819-0395, Japan

³) Department of Automotive Sciences, Graduate School of Integrated Frontier Sciences, Kyushu University, Motooka 744, Nishiku, Fukuoka, 819-0395, Japan

⁴) Department of Materials Science and Nanotechnology Engineering, Yeditepe University, Turkey

* corresponding author

Table S1. List of used dopants

SrCO ₃	99.99%	Kishida Chemical
BaCO ₃	99.99%	Wako
CaCO ₃	99.99%	Wako
La ₂ O ₃	99.99%	Kishida Chemical
SnO ₂	99.9%	Kishida Chemical
ZrO ₂	99.9%	Kishida Chemical
Al ₂ O ₃	99.9%	Kojundo Chemical
Ga ₂ O ₃	99.99%	Kojundo Chemical
Er ₂ O ₃	99.9%	Kojundo Chemical
MoO ₃	99.9%	Kishida Chemical

Table S2 Density and composition of prepared samples

Composition	Calcination conditions	Density (% of theoretical)
Bi ₄ NbO ₈ Cl	800°C, 20h	60.3%
Bi _{3.85} Sr _{0.15} NbO ₈ Cl	800°C, 20h	62.1%
Bi _{3.8} Sr _{0.2} NbO ₈ Cl	800°C, 20h	60.7%
Bi _{3.9} Sr _{0.1} NbO ₈ Cl (2-step synthesis)	900°C, 20h	77%
Bi _{3.9} Sr _{0.1} NbO ₈ Cl (2 step synthesis)	900°C, 48h	96.3%

Table S3 Refined structural parameters of $\text{Bi}_{4-x}\text{M}_x\text{O}_{8-\delta}\text{Cl}$ samples using XRD data collected at room temperature.

	None	La 10mol%	Sn 2.5mol%	Ba 2.5mol%	Sr 2.5mol%	Sr 3.75mol%	Sr 5mol%
Space group	$P2_1cn$	$P2_1cn$	$P2_1cn$	$P2_1cn$	$P2_1cn$	$P2_1cn$	$P2_1cn$
a (Å)	5.4721(18)	5.4683(13)	5.4714(18)	5.483(2)	5.4731(11)	5.4750(16)	5.4781(11)
b (Å)	5.4771(17)	5.4805(15)	5.4743(17)	5.480(2)	5.4744(11)	5.4745(15)	5.4775(10)
c (Å)	28.673(10)	28.609(6)	28.656(10)	28.758(14)	28.627(6)	28.753(8)	28.739(6)
V (Å ³)	859.365(33)	857.383(64)	858.306(95)	864.087(2)	857.720(4)	861.952(11)	862.350(84)
R_{wp}	35.66	30.28	29.56	31.28	28.71	23.21	23.36
R_p	26.29	20.27	22.34	23.10	20.87	16.57	16.28
R_e	11.00	9.65	10.16	10.40	4.85	8.18	9.43
S	3.2406	9.8425	2.9092	3.0076	5.9213	2.8385	2.4766

Table S4 Impedance fitting parameters

	R1 / Ohm	R2 / Ohm	R3 / Ohm	R4 / Ohm
873 K	104.4	34.12	447	74.41
823K	148.2	105.7	1034	159.8
773K	175.8	238.1	2266	836.4
723K	200.2	969.3	5313	7949
673K	214.9	2656	11983	30792

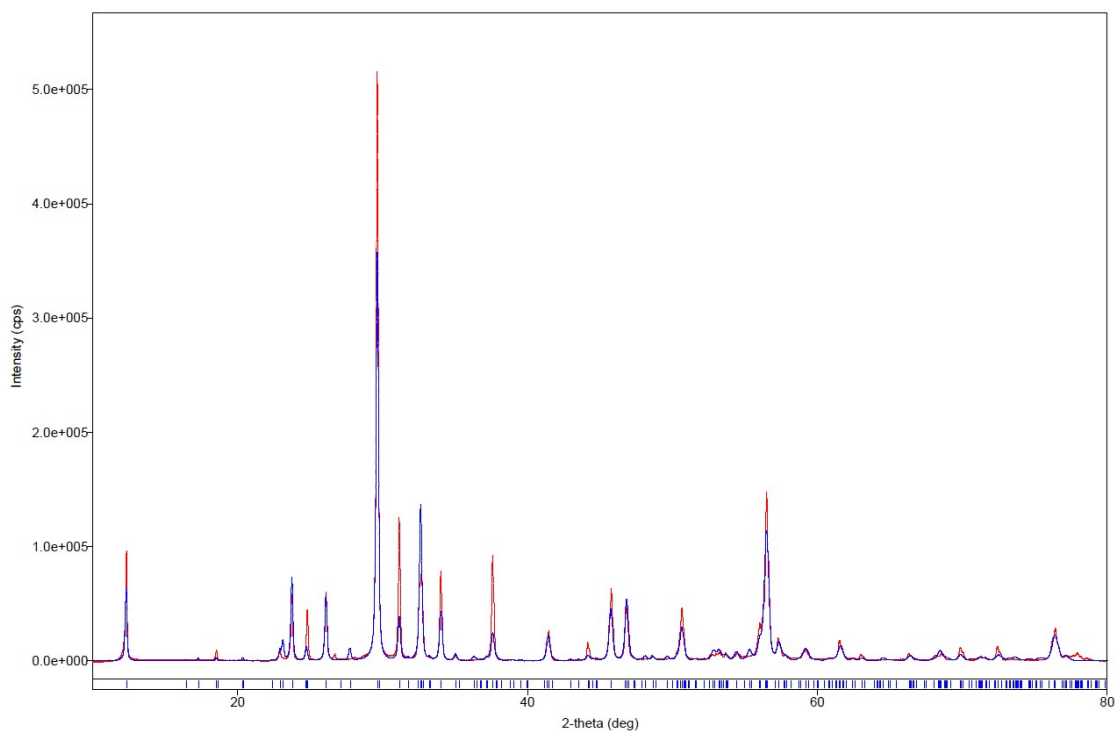


Figure S1 Measured and refinement XRD patterns of $\text{Bi}_{3.9}\text{Sr}_{0.1}\text{NbO}_{8-\delta}\text{Cl}$. Red line is measurement and blue line is fitted results of XRD pattern.

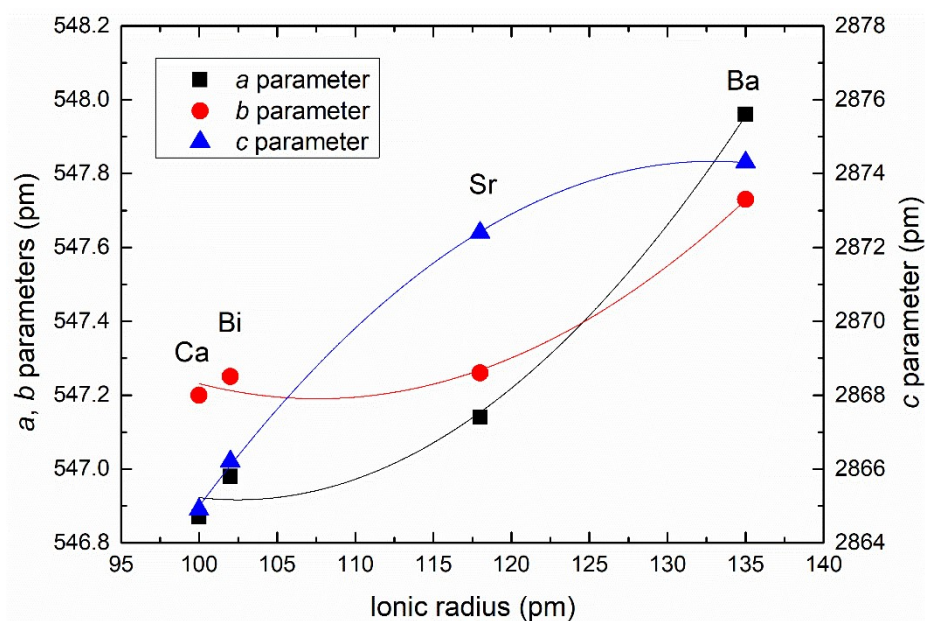


Figure S2, Lattice parameter as a function of ionic radius of dopant M in $\text{Bi}_{4-x}\text{M}_x\text{NbO}_8\text{Cl}$

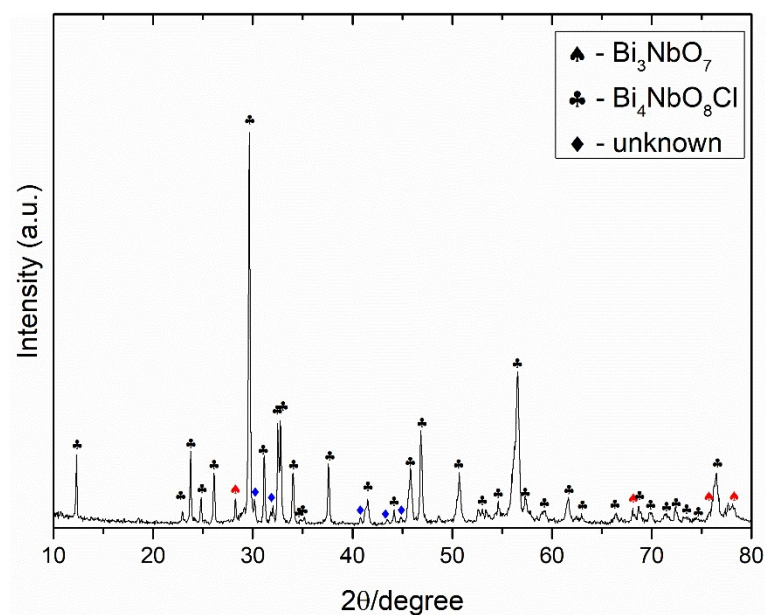


Figure S3(a) XRD patter of $\text{Bi}_4\text{NbO}_8\text{Cl}$ after P_{O_2} measurement

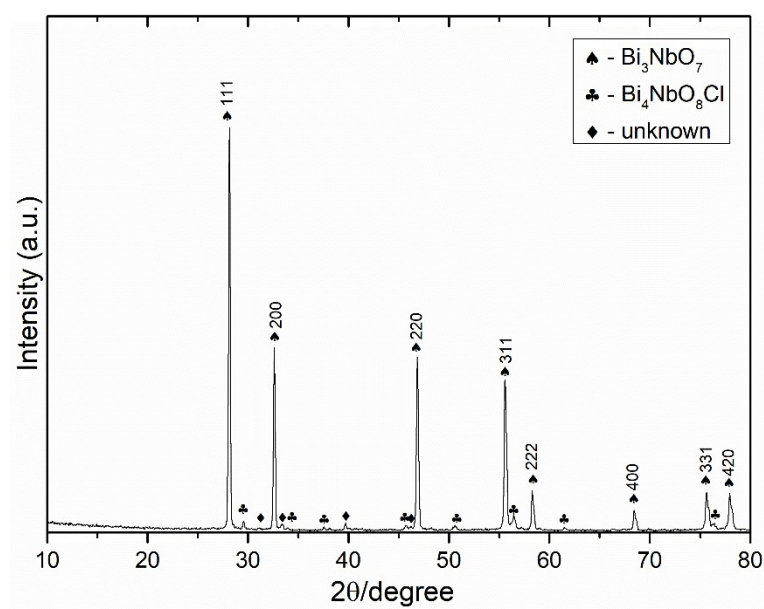


Figure S3(b) XRD patterns of $\text{Bi}_{3.8}\text{Sr}_{0.2}\text{NbO}_{8-\delta}\text{Cl}$ after P_{O_2} measurement.

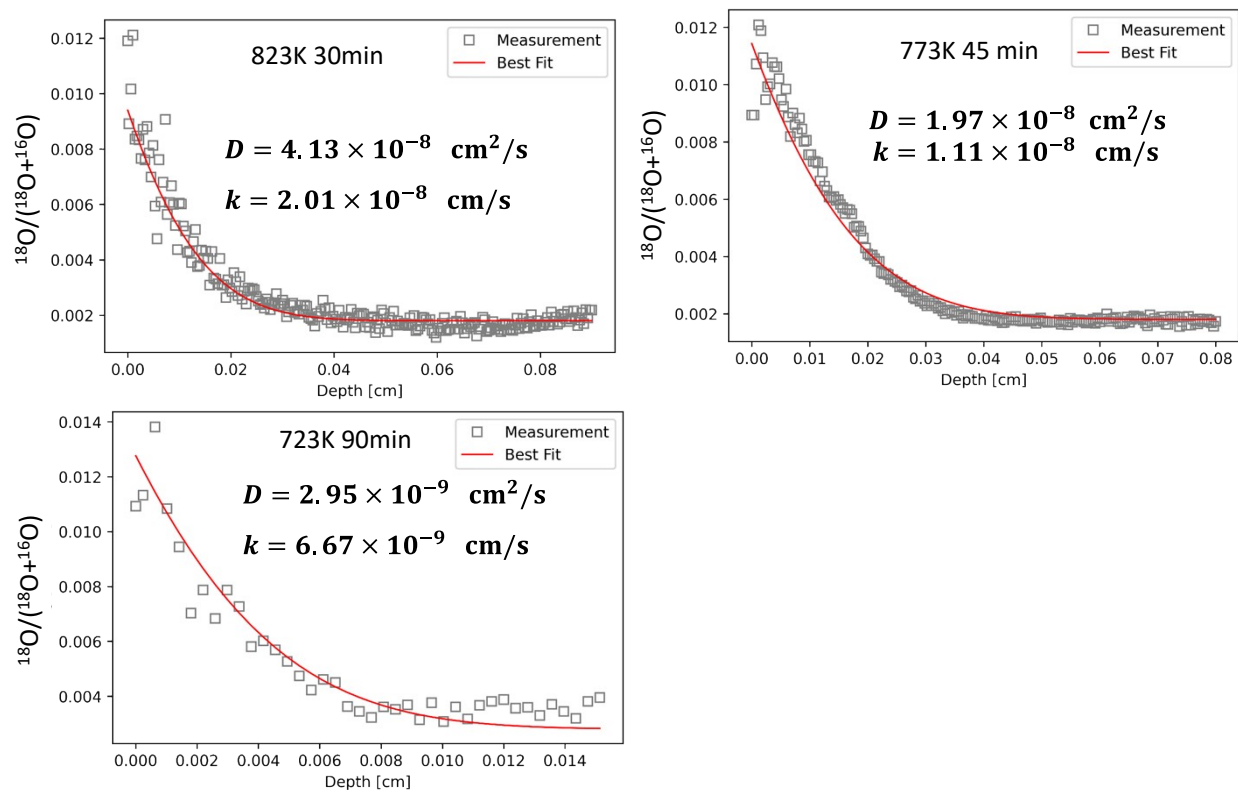


Figure S4. ^{18}O diffusion profiles and fitted results on $\text{Bi}_{3.9}\text{Sr}_{0.1}\text{NbO}_{8-\delta}\text{Cl}$.