Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Structural and Na-ion conduction characteristics of $Na_3PS_xSe_{4-x}$

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Supporting Information

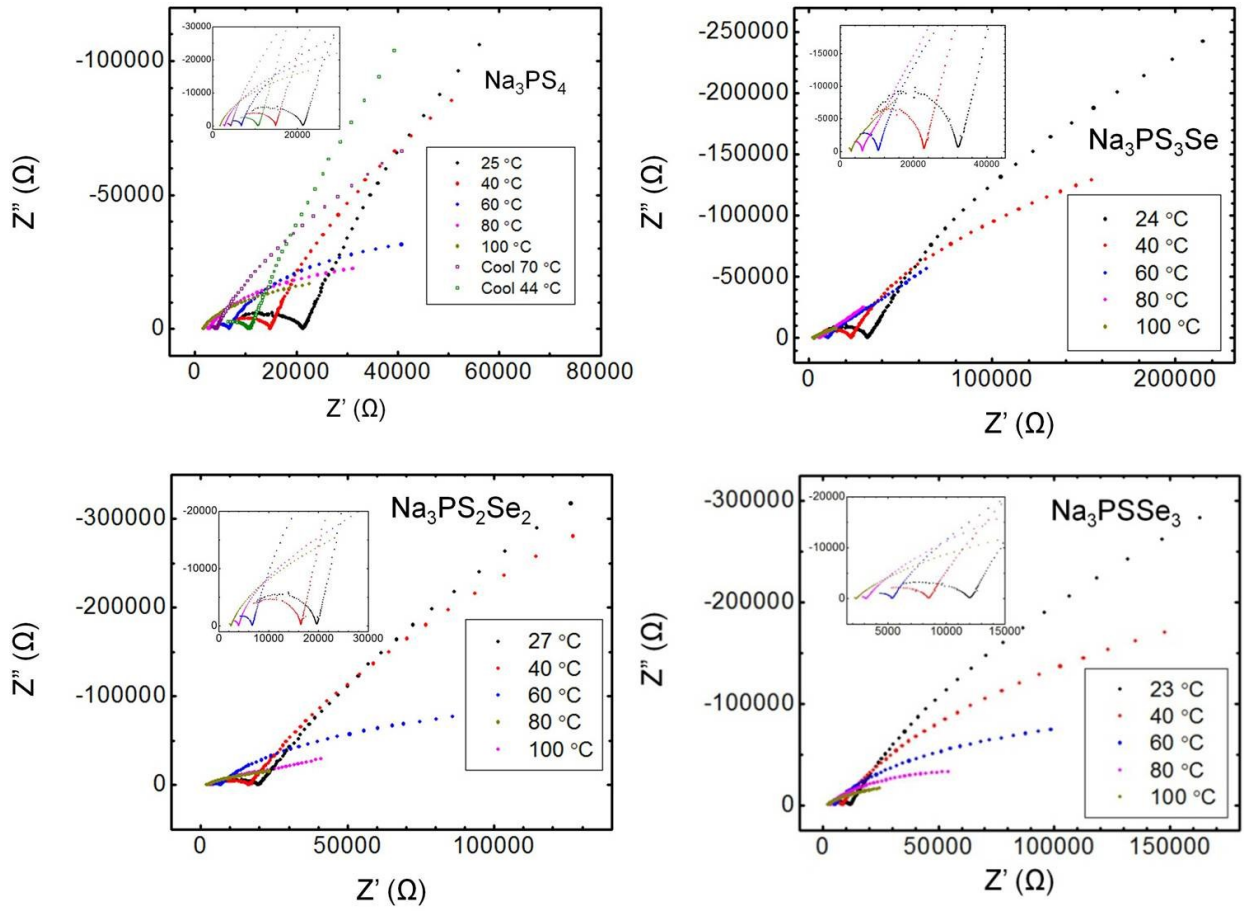

Figure S1. Variable-temperature impedance spectra for Na_3PS_4, Na_3PS_3Se, $Na_3PS_2Se_2$ and Na_3PSSe_3.

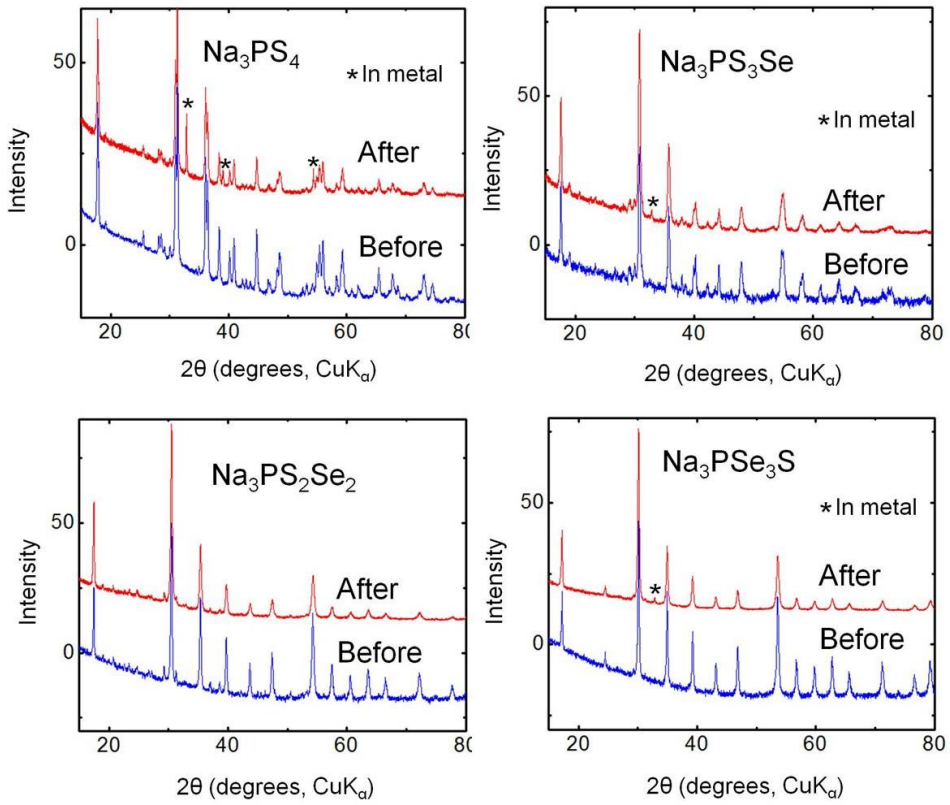

Figure S2. Diffraction patterns of Na_3PS_4, Na_3PS_3Se, $Na_3PS_2Se_2$ and Na_3PSSe_3, which were collected before and after the variable-temperature measurements.

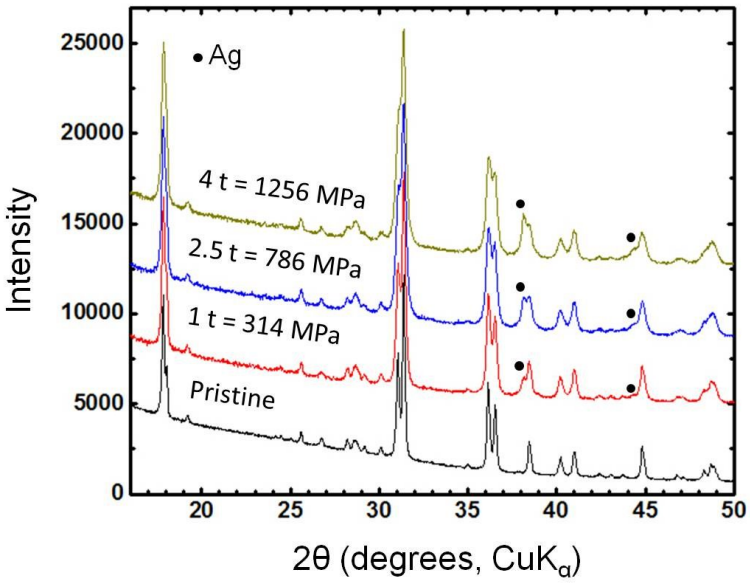

Figure S3. Diffraction patterns of the Na_3PS_4 powder samples which were pressed at different pressures. Ag impurity is present, since Ag paste was used as blocking electrodes for the impedance measurements.

Table S1. Crystallographic data for Na_3PS_3Se based on the Rietveld refinement of the synchrotron X-ray data

Radiation	Synchrotron X-ray (11BM, APS)
Crystal system	Tetragonal
Space group	*P-42$_1$c* (#114)
Lattice parameters	$a = b = 7.06428(4)$ Å $c = 7.13193(6)$ Å
Cell volume	355.912(5)Å^3
Density (calculated)	2.56686 g/cm^3
λ	0.413991 Å
R_{wp}	8.614%
R_{Bragg}	3.609%
χ^2	1.377

Table S2. Atomic site information for Na_3PS_3Se

Atom	Wyck.	*x/a*	*y/b*	*z/c*	Occ.	B_{iso} (Å^2)
Na1	4d	0	0.5	0.0507(3)	1	5.07(6)
Na2	2b	0	0	0.5	1	5.3(1)
P	2a	0	0	0	1	1.43(3)
S/Se	8e	0.1851(1)	0.1607(1)	0.1689(1)	S = 0.75 Se = 0.25	4.96(5)

Table S3. Crystallographic data for $Na_3PS_2Se_2$ based on the Rietveld refinement of the synchrotron X-ray data

Radiation	Synchrotron X-ray (11BM, APS)
Crystal system	Cubic
Space group	*I-43m* (#217)
Lattice parameters	$a = b = c = 7.15665(3)$Å
Cell volume	366.547(5)Å^3
Density (calculated)	2.91725 g/cm^3
λ	0.413991 Å
R_{wp}	9.131%
R_{Bragg}	2.712%
χ^2	1.321

Table S4. Atomic site information for $Na_3PS_2Se_2$

Atom	Wyck.	*x/a*	*y/b*	*z/c*	Occ.	B_{iso} (Å^2)
Na	6b	0	0.5	0.5	1	6.24(5)
P	2a	0	0	0	1	1.28(3)
S/Se	8c	0.17299(4)	0.17299(4)	0.17299(4)	S = 0.5 Se = 0.5	2.14(1)

Table S5. Crystallographic data for Na_3PSSe_3 based on the Rietveld refinement of the synchrotron X-ray data

Radiation	Synchrotron X-ray (11BM, APS)
Crystal system	Cubic
Space group	*I-43m* (#217)
Lattice parameters	$a = b = c = 7.24079(3)$Å
Cell volume	379.628(4)Å^3
Density (calculated)	3.22693 g/cm^3
λ	0.413991 Å
R_{wp}	8.890%
R_{Bragg}	2.842%
χ^2	1.371

Table S6. Atomic site information for Na_3PSSe_3

Atom	Wyck.	*x/a*	*y/b*	*z/c*	Occ.	B_{iso} (Å^2)
Na	6b	0	0.5	0.5	1	5.83(4)
P	2a	0	0	0	1	1.38(3)
S/Se	8c	0.17422(3)	0.17422(3)	0.17422(3)	S = 0.25 Se = 0.75	2.45(1)