Supporting Information

Local structure of a highly concentrated NaClO$_4$ aqueous solution-type electrolyte for sodium ion batteries.

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Table S1. Setup details for the EPSR simulation boxes.

Concentration (m)	Water molecules	Na$^+$ cations	ClO$_4^-$ anions	Density / atoms Å^{-3}	Box size length (Å)
1	1000	18	18	0.09877	31.571
5	1000	90	90	0.09535	33.361
10	1000	180	180	0.09177	35.426
13	1000	234	234	0.08991	36.589
17	1000	306	306	0.08792	38.030

Table S2. Potential parameter values used in EPSR modeling for NaClO$_4$ solution.

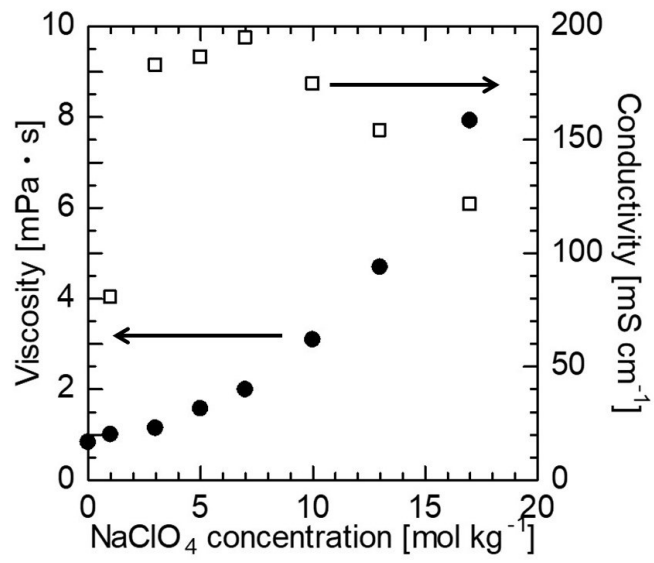|	O$_w$[1]	H[1]	Na[1]	Cl[2]	O$_{Cl}$[2]
ε (kJ mol^{-1})	0.65	0.00	0.514	0.566	0.65
σ (Å)	3.16	0.00	2.29	4.19	3.16
mass	16	2.00	23	35.45	16
charge	-0.8476	0.4238	1.00	1.88	-0.72

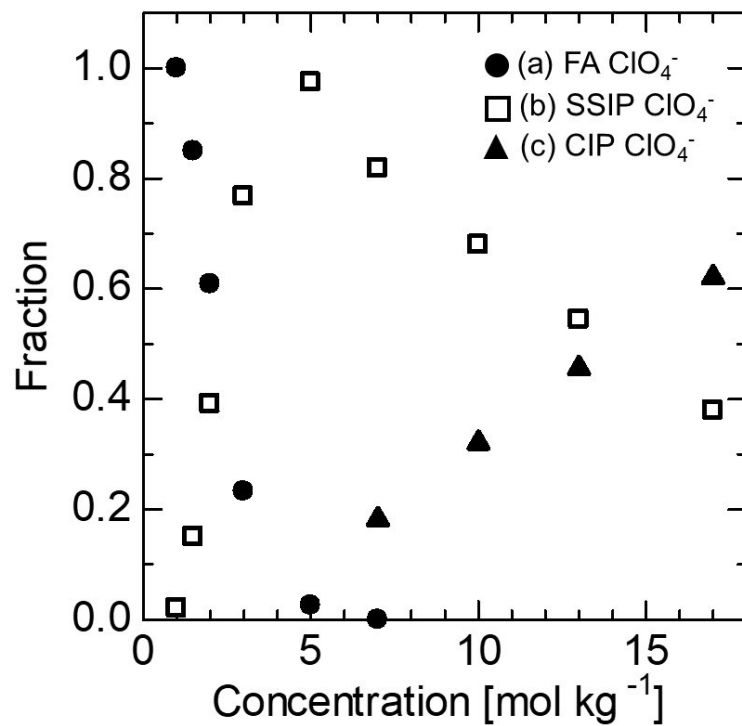Fig. S1 Viscosity and electric conductivity of the $NaClO_4$ aq. electrolytes at various concentrations

Fig. S2 The fraction of each component (FA ClO_4^-, SSIP ClO_4^- and CIP ClO_4^-) in aqueous electrolyte with each $NaClO_4$ salt concentration (1, 3, 5, 7, 10, 13 and 17 m)
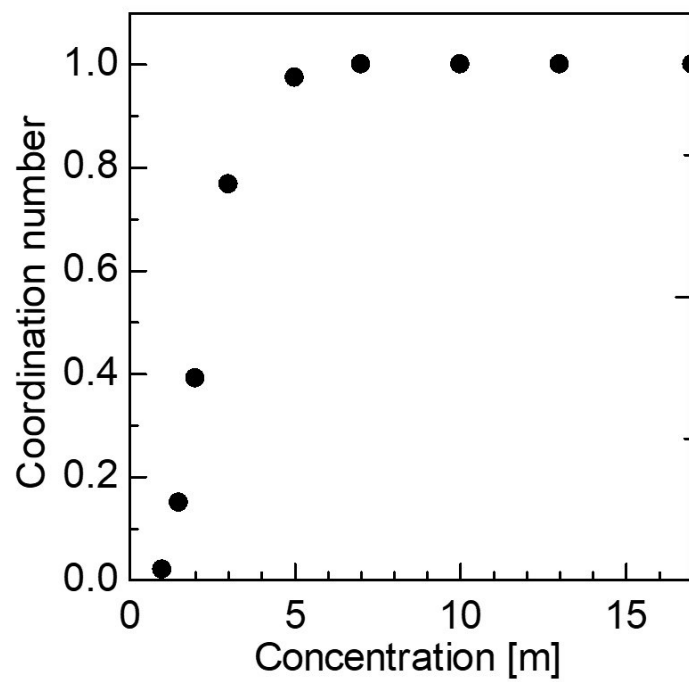
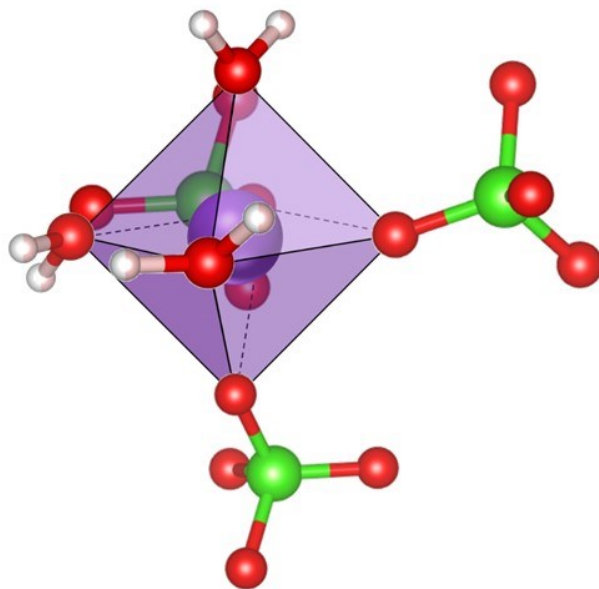Fig. S3 The calculated average coordination number of ClO_4^- ions

Fig. S4 Illustration of the local structure around an Na$^+$ ion in 17 m NaClO$_4$ aqueous electrolyte.
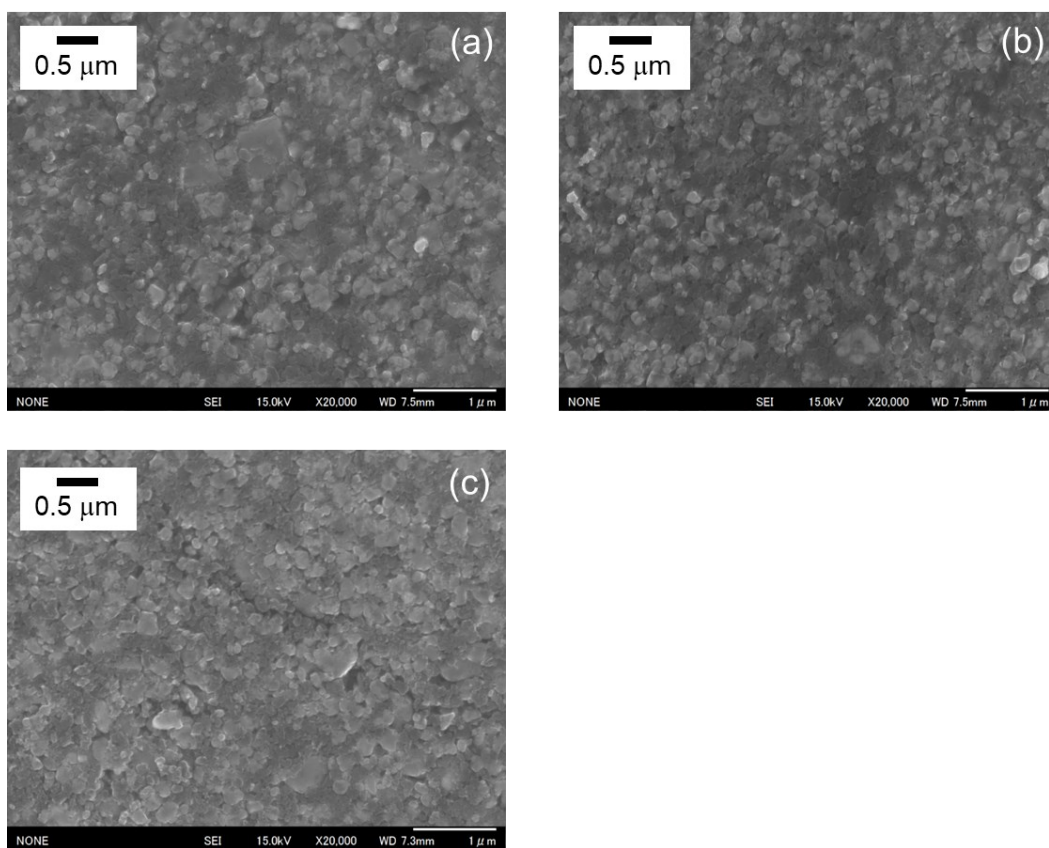
Fig. S5 SEM images of (a) pristine and cycled NTP electrode with (b) 1 m and (c) 17 m NaClO$_4$ aq. electrolytes.
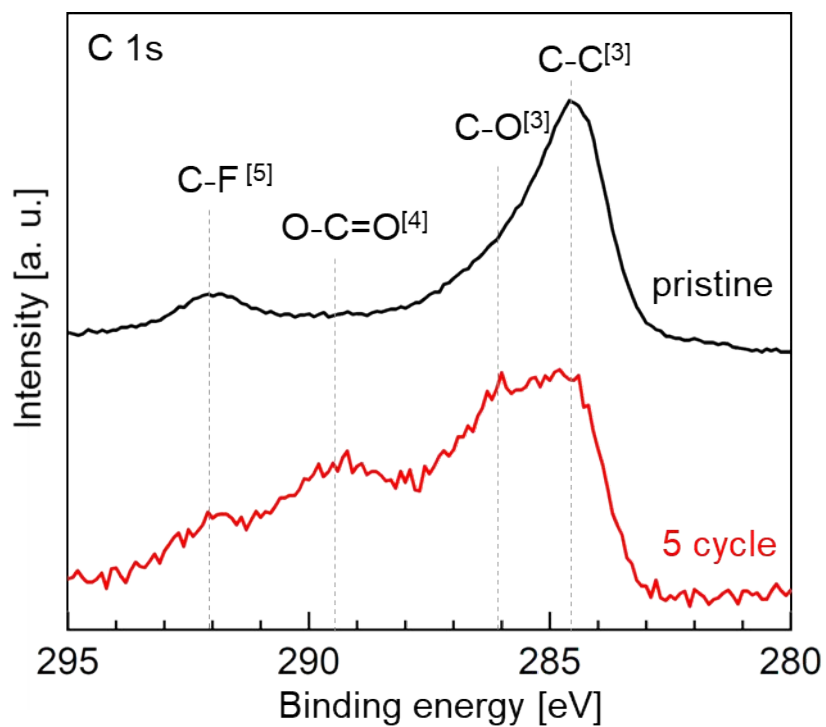
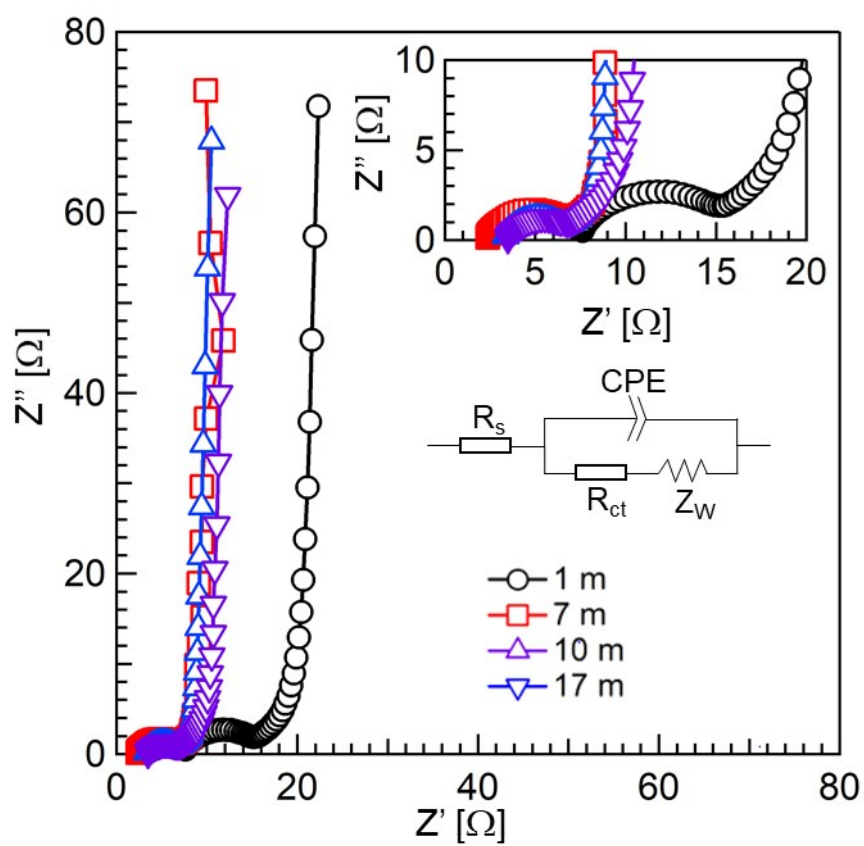Fig. S6 C 1s XPS peaks of NTP electrodes before and after 5 cycles with 17 m $NaClO_4$ aq. electrolyte.

Fig. S7 Nyquist plots of NTP with 1, 7, 10 and 17 m $NaClO_4$ aq. electrolyte. Insets are the magnified spectra and the equivalent circuit.
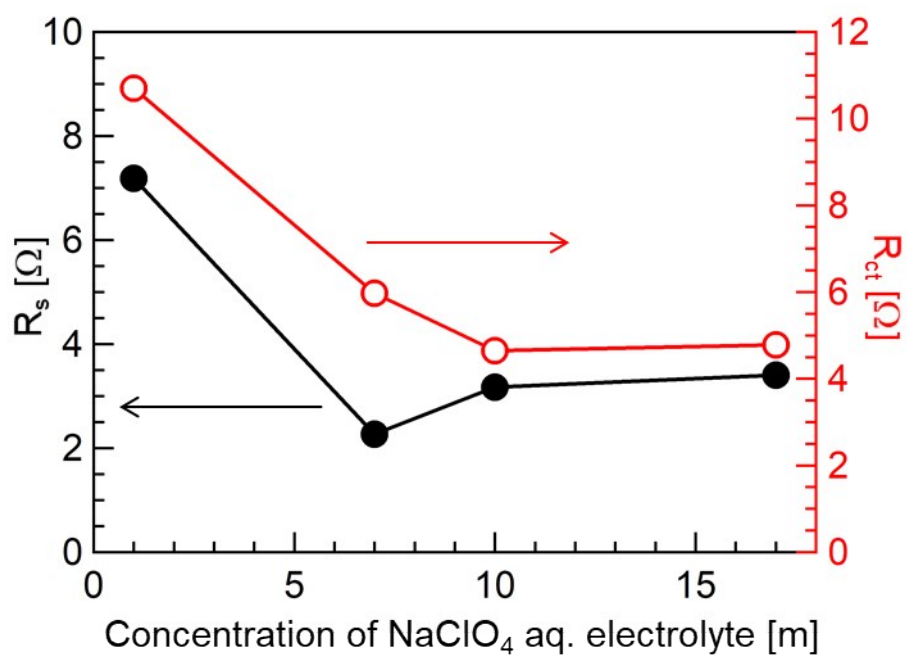
Fig. S8 The calculated R_s and R_{ct} from Nyquist plots in each $NaClO_4$ aq. electrolytes.

Supplementary References

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