Supporting Information

A Room-Temperature Chloride-Conducting Metal-organic Crystal $[Al(DMSO)_6]Cl_3$ for Potential Solid-State Chloride-Shuttle Batteries

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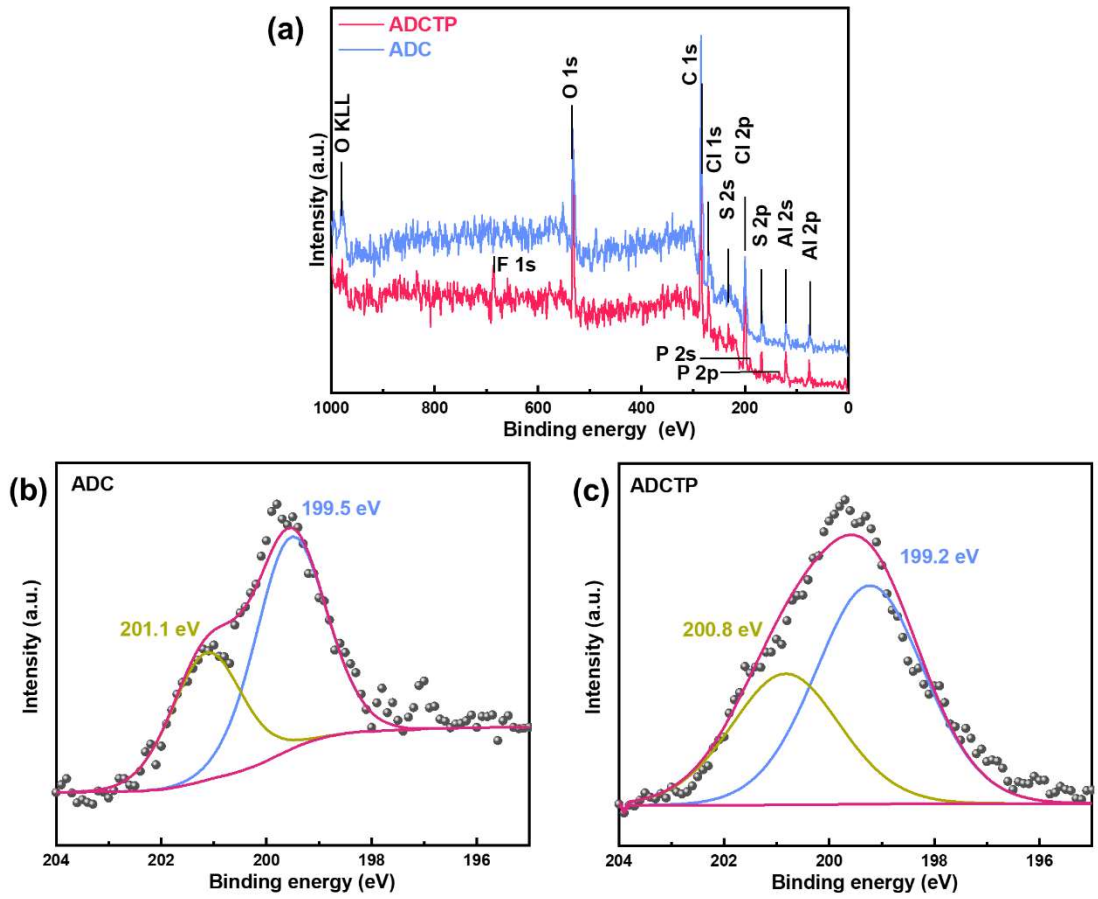

Figure S1 (a)Total XPS survey of ADC and ADCTP, Cl 2p of (b) ADC and (c) ADCTP.

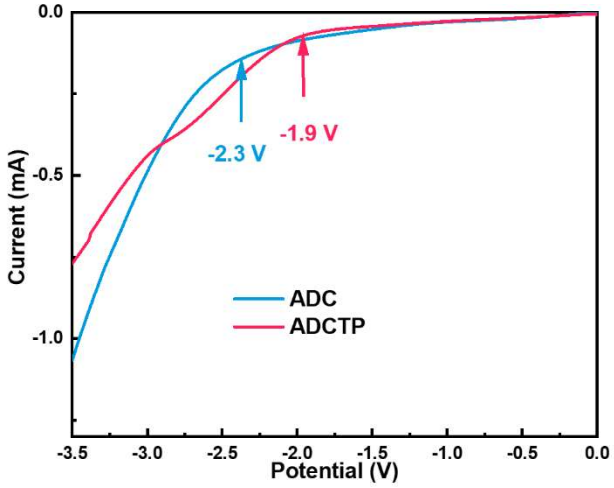

Figure S2 Cathodic linear sweep voltammetry (LSV, scan rate of 0.2 mV s^{-1}) of ADC and ADCTP in the range of 0 - −3.5 V.

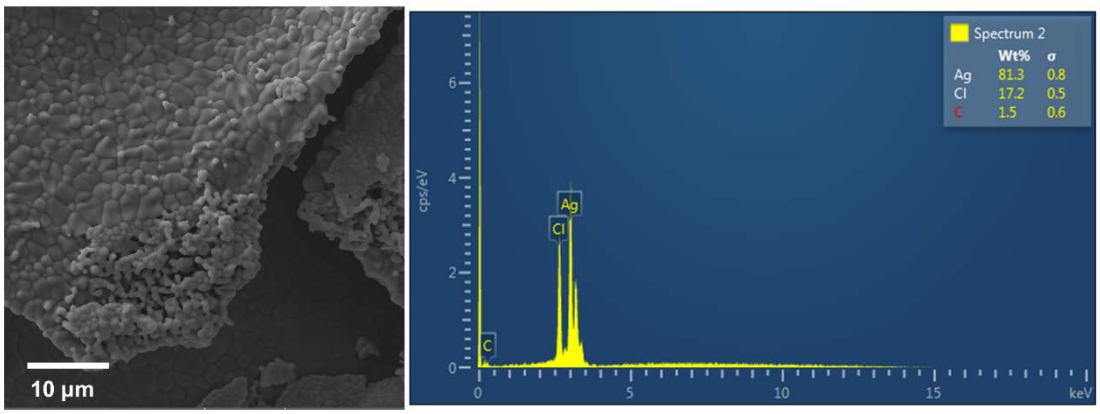

Figure S3. SEM and EDS spectrum of Ag-AgCl electrode materials.

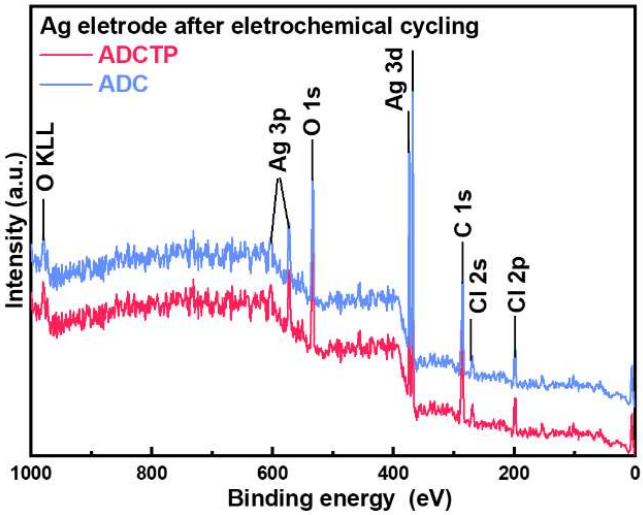

Figure S4 Total XPS survey of Ag electrodes after initially electrochemical chlorination in ADC and ADCTP electrolyte systems.

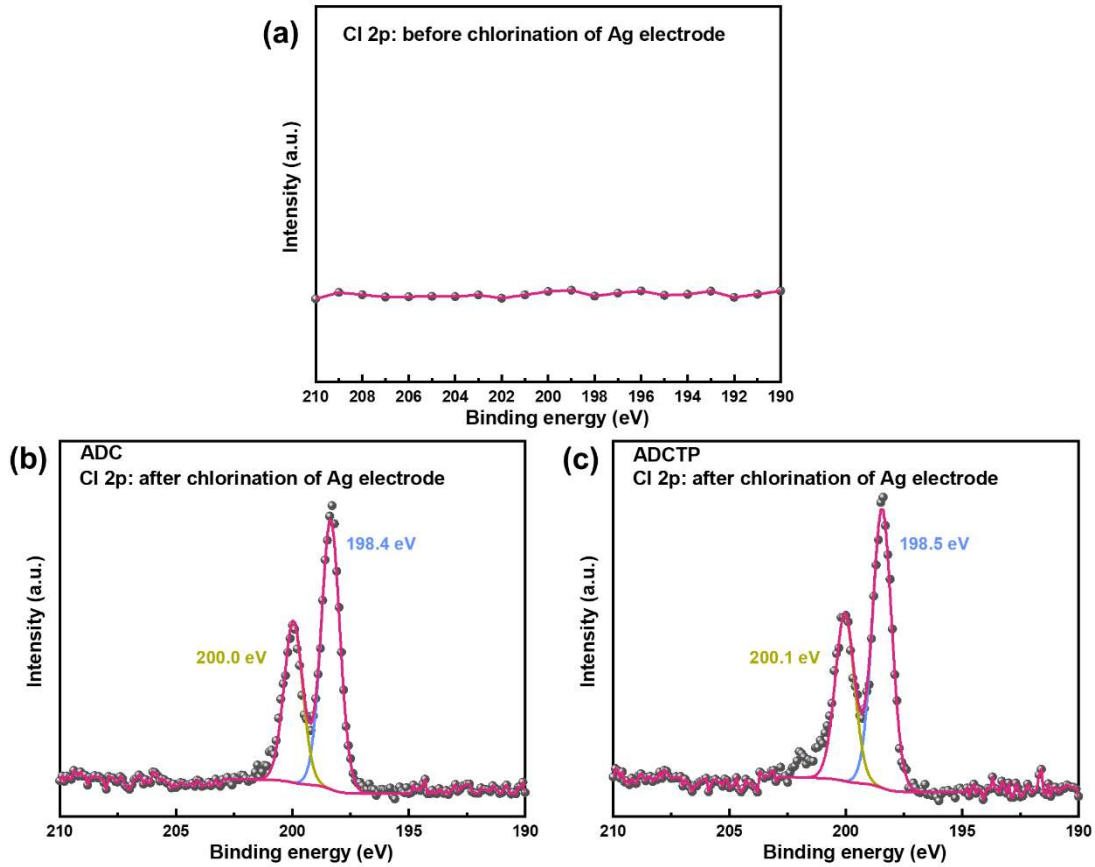

Figure S5 (a) XPS spectrum of Cl 2p for Ag electrode before chlorination, XPS spectrum of Cl 2p for Ag electrode after chlorination in (b) ADC and (c) ADCTP.

Table S1 Crystal parameters of R-3H $Al(DMSO)_6Cl_3$ phases in ACD and $TBAPF_6$ composited ACDTP samples gained *via* Rietveld XRD refinement.

Samples			ADC	ADCTP
Lattice parameter	R-3H phase	a value (Å)	10.3792	10.3734
		b value (Å)	10.3792	10.3734
		c value (Å)	22.4656	22.4659
		volume ($Å^3$)	2095.9340	2093.5990
Reliability factors	*R*wp		8.51%	6.70%
	*R*p		6.66%	5.18%
	χ^2		1.592	1.654

Table S2 The list of FTIR band positions of $Al(DMSO)_6Cl_3$ and $Al(DMSO)_6Cl_3$-10wt%$TBAPF_6$ at room temperature. (vw - very weak, w - weak, sh - shoulder, m - medium, st - strong, vst - very strong, br - broad, ν - stretching, δ - bending, ρ - rocking)[1]

Frequencies (cm^{-1})		Assignments	Frequencies (cm^{-1})		Assignments
ADC	ADCTP		ADC	ADCTP	
2994st	2994st	$\nu_{as(CH)}$	1006m	1006m	$\nu_{s(SO)}$
2984st	2984st	$\nu_{as(CH)}$	958m	959m	$\rho_{r(CH3)}$
2962st	2962st	$\nu_{as(CH)}$)	930vw	929vw	$\rho_{r(CH3)}$
2899vst	2899vst	$\nu_{s(CH)}$)	-	880st	$\nu_{s(PF)}$
2820w	2820w	$\nu_{s(CH)}$	-	850vst	$\nu_{s(PF)}$
1440wv	1440wv	$\delta_{as(HCH)}$)	-	838vst	$\nu_{s(PF)}$
1422m	1422m	$\delta_{as(HCH)}$	728st	728st	$\nu_{as(CS)}$
1331vw	1332vw	$\delta_{s(HCH)}$	696vst	696vst	$\nu_{as(CS)}$
1307vw	1307vw	$\delta_{s(HCH)}$	544st	544st	ν_{AlO}
1063vw	1063vw	$\nu_{s(SO)}$	527st	527st	ν_{AlO}

Table S3 The temperature-dependent bulk impedance and ionic conductivity evaluated from EIS

Temperature (K)		293	308	323	338	353
Bulk resistance (Ω)	ADC	2084	1354	820	313	144
	ADCTP	225	180	133	101	71
σ (S cm^{-1})	ADC	2.172E-5	3.343E-5	5.520E-5	1.446E-4	3.143E-4
	ADCTP	2.012E-4	2.515E-4	3.403E-4	4.482E-4	6.376E-4

Figure S6 Photographs of sealable SEM holder for sample transfer.

Figure S7 Photographs of sealable XRD holder.

[1] a) N. Górska, E. Mikuli, *Vib. Spectrosc* **2016**, 86, 253; b) K. D. Fulfer, D. G. Kuroda, *PCCP* **2018**, 20, 22710; c) A. Migdał-Mikuli, N. Górska, E. Szostak, *J. Therm. Anal. Calorim.* **2007**, 90, 223.