

Supporting Information

Phase Behaviors and Ion Transport Properties of $\text{LiN}(\text{SO}_2\text{CF}_3)_2/\text{Sulfone}$ Binary Mixtures

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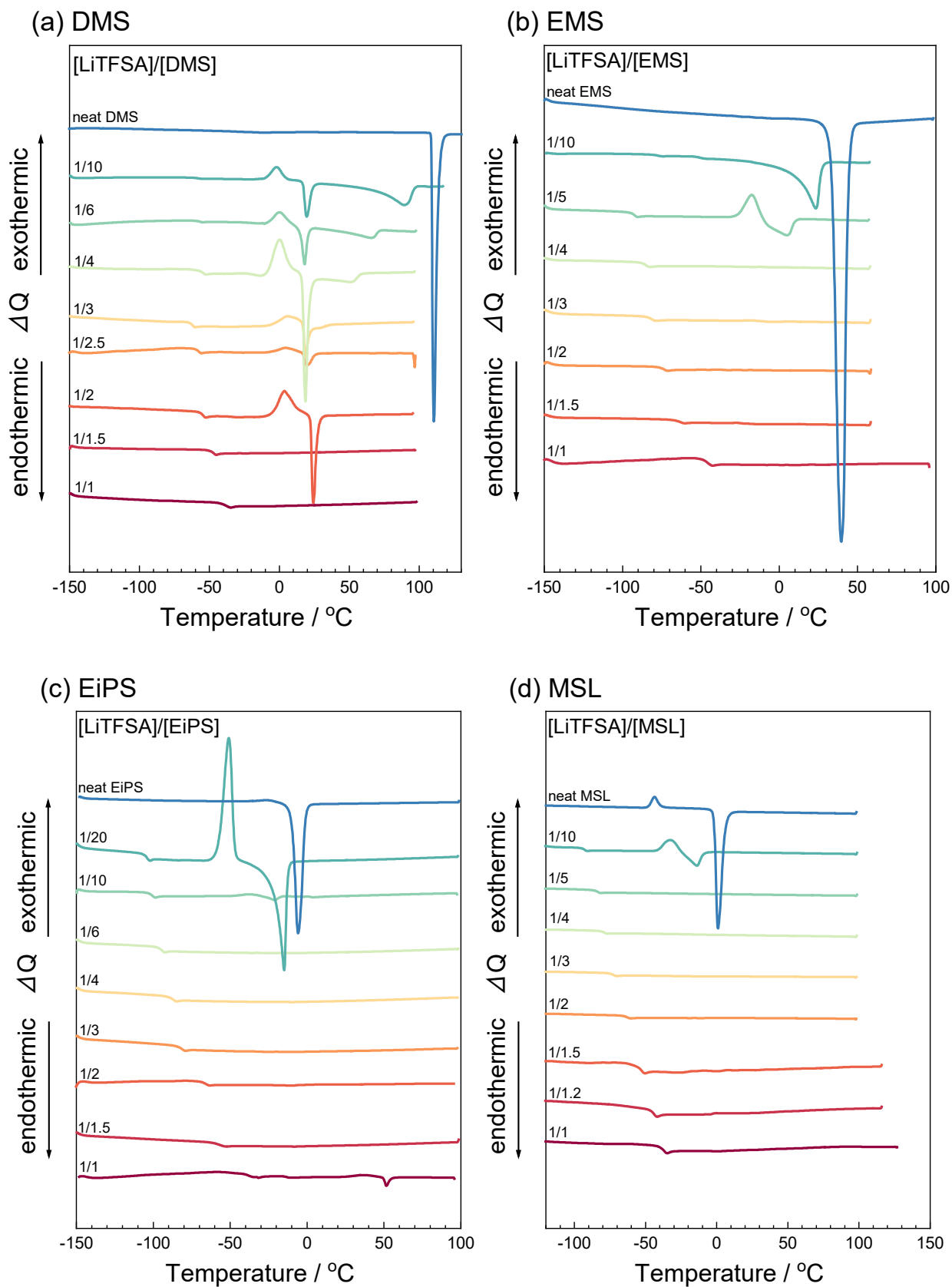


Figure S1. DSC curves of (a) LiTFSA/DMS, (b) LiTFSA/EMS, (c) LiTFSA/EiPS, and (d) LiTFSA/MSL mixtures.

Table S1. Crystallographic data for [LiTFSA]/[EiPS]=1/1 and [LiTFSA]/[MSL]=1/1.

	[LiTFSA]/[EiPS]=1/1	[LiTFSA]/[MSL]=1/1
Chemical formula	C ₁₄ H ₂₄ F ₁₂ Li ₂ N ₂ O ₁₂ S ₆	C ₁₄ H ₂₀ F ₁₂ Li ₂ N ₂ O ₁₂ S ₆
Formula weight	846.59	842.56
Crystal system	monoclinic	orthorhombic
Space group	P 1 21/c 1	P n a 21
<i>a</i> / Å	18.9850(9)	17.8545(10)
<i>b</i> / Å	8.7718(4)	12.6864(7)
<i>c</i> / Å	21.8241(12)	14.6399(8)
α / °	90	90
β / °	111.777(6)	90
γ / °	90	90
<i>V</i> / Å ³	3375.1(3)	3316.1(3)
<i>Z</i>	4	4
<i>D</i> _{calc} / g cm ⁻³	1.666	1.688
μ / mm ⁻¹	0.524	0.533
Temp. / K	223	223
Reflections collected	65601	29957
Independent reflection, <i>R</i> _{int}	9251, 0.0358	8471, 0.0215
<i>R</i> ₁ [<i>I</i> > 2σ(<i>I</i>)]	0.0467	0.0455
w <i>R</i> ₂ (all data)	0.1534	0.1310
Goodness of fit	0.932	1.030
Largest residual density / eÅ ⁻³	0.659, -0.443	0.568, -0.319

The crystallographic information files (cifs) for [LiTFSA]/[EiPS]=1/1 and [LiTFSA]/[MSL]=1/1 were deposited in the Cambridge Structural Database (CSD) as CCDC 2224170 and 2224171, respectively.

Table S2. Viscosity (η), density (ρ), LiTFSA concentration (c), ionic conductivity (σ), and diffusivity (D) of the LiTFSA–MSL electrolytes at 30 °C.

[MSL]/[LiTFSA]	η mPa s	ρ g cm ⁻³	c mol dm ⁻³	σ mS cm ⁻¹	D_{Li}	D_{sol}	D_{TFSA}
					10 ⁻⁷ cm ² s ⁻¹		
3	176	1.42	2.06	0.75	0.82	0.87	0.74
4	91	1.38	1.67	1.18	1.58	1.84	1.60
5	60	1.35	1.41	1.52	-	-	-
8	31	1.29	0.95	1.96	-	-	-
10	25	1.28	0.78	2.06	4.09	5.56	4.97
20	16	1.23	0.42	1.67	-	-	-

Table S3. Viscosity (η), density (ρ), LiTFSA concentration (c), ionic conductivity (σ), and diffusivity (D) of the LiTFSA–DMS electrolytes at 30 °C.

[DMS]/[LiTFSA]	η mPa s	ρ g cm ⁻³	c mol dm ⁻³	σ mS cm ⁻¹	D_{Li}	D_{sol}	D_{TFSA}
					10 ⁻⁷ cm ² s ⁻¹		
2	861	1.60	3.36	0.34	0.26	0.27	0.19
3	206	1.53	2.68	0.98	0.83	1.00	0.67

Table S4. Viscosity (η), density (ρ), LiTFSA concentration (c), ionic conductivity (σ), and diffusivity (D) of the LiTFSA–EMS electrolytes at 30 °C.

[EMS]/[LiTFSA]	η mPa s	ρ g cm ⁻³	c mol dm ⁻³	σ mS cm ⁻¹	D_{Li}	D_{sol}	D_{TFSA}
					10 ⁻⁷ cm ² s ⁻¹		
1.5	2205	1.57	3.50	0.13	-	-	-
2	592	1.52	3.01	0.34	0.24	0.30	0.21
3	159	1.44	2.36	0.91	0.71	0.98	0.73
4	76	1.40	1.94	1.52	1.31	2.06	1.57
8	22	1.30	1.13	2.67	3.72	6.89	5.35
20	11	1.23	0.50	2.47	-	-	-
50	8	1.19	0.21	1.41	-	-	-

Table S5. Viscosity (η), density (ρ), LiTFSA concentration (c), ionic conductivity (σ), and diffusivity (D) of the LiTFSA–EiPS electrolytes at 30 °C.

[EiPS]/[LiTFSA]	η mPa s	ρ g cm ⁻³	c mol dm ⁻³	σ mS cm ⁻¹	D_{Li}	D_{sol}	D_{TFSA}
					10 ⁻⁷ cm ² s ⁻¹		
2	1409	1.41	2.52	0.10	0.08	0.11	0.10
3	281	1.33	1.92	0.31	0.37	0.56	0.51
4	107	1.29	1.55	0.64	-	-	-
8	22	1.20	0.87	1.76	2.93	6.15	5.26
20	9	1.13	0.38	1.97	-	-	-
50	6	1.10	0.15	1.21	-	-	-

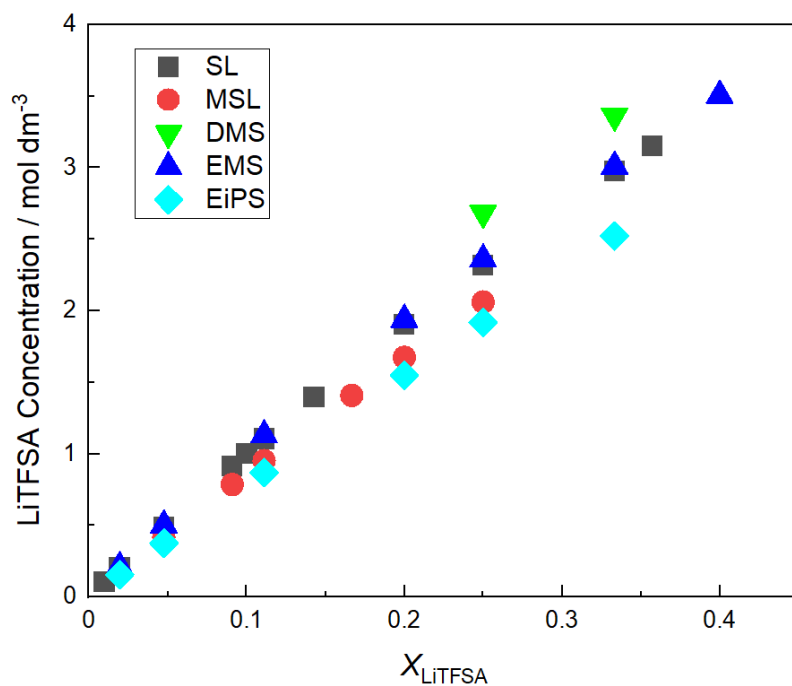


Figure S2. LiTFSA concentration (mol dm⁻³) as a function of the LiTFSA mole fraction (X_{LiTFSA}) in LiTFSA/sulfone solutions at 30 °C.

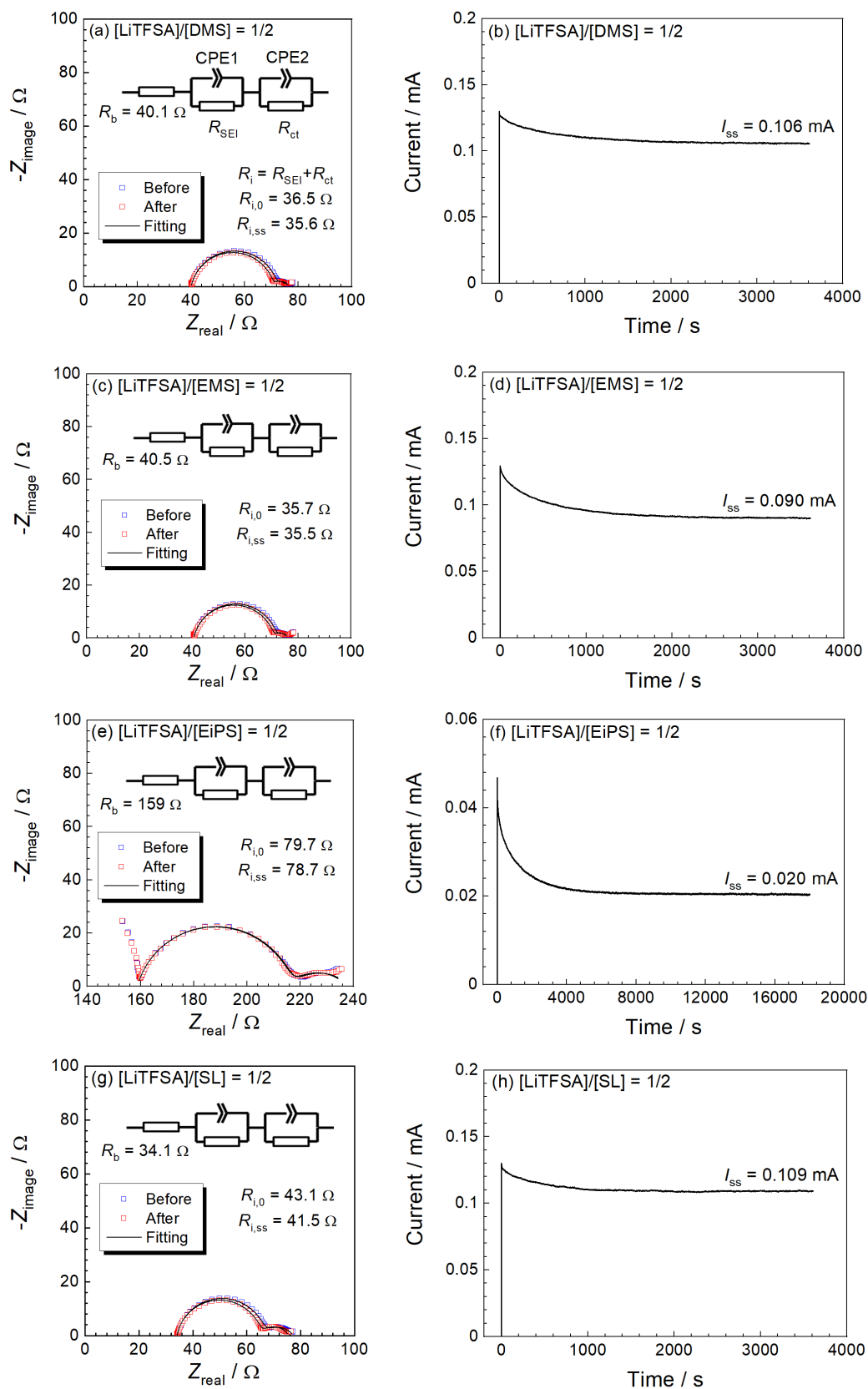


Figure S3. (a, c, e, g) Nyquist plots and (b, d, f, h) chronoamperograms of symmetric Li/Li cells with electrolytes: (a, b) [LiTFSA]/[DMS]=1/2, (c, d) [LiTFSA]/[EMS]=1/2, (e, f) [LiTFSA]/[EiPS]=1/2, and (g, h) [LiTFSA]/[SL]=1/2. Chronoamperometry was performed at a constant voltage of 10 mV at 30 °C. Nyquist plots were obtained before and after chronoamperometry.

Table S6. Resistances in Li/Li symmetric cells evaluated by AC impedance and steady-state current observed by chronoamperometry of Li/Li symmetric cells (**Fig. S3**) for the determination of $t_{\text{Li}}^{\text{abc}}$ in [LiTFSA]/[sulfone] = 1/2 electrolytes.

sulfone	R_b (Ω)	$R_{i,0}$ (Ω)	$R_{i,ss}$ (Ω)	I_{ohm} (mA)	I_{ss} (mA)	ΔV (mV)
SL	34.1	43.1	41.5	0.127	0.109	9.83
DMS	40.1	36.5	35.6	0.130	0.106	9.97
EMS	40.5	35.7	35.5	0.132	0.090	10.05
EiPS	159	79.7	78.7	0.043	0.020	10.21