

Supporting Information

Solvation sheath reorganization enables fast ion transfer kinetics in lithium-ion battery

Menglu Li¹⁺, Di Lu¹⁺, Jinze Wang^{1,2+}, Shuoqing Zhang¹, Ling Lv¹, Baochen Ma¹,
Haotian Zhu¹, Long Li¹, Sheng Yang³, Zirui Li³, Yuefei Wu³, Jiacheng Qi^{1,4}, Liwu
Fan³, Ruhong Li^{1,2*}, Lixin Chen^{1,4}, Tao Deng⁵, Xiulin Fan^{1*}

¹State Key Laboratory of Silicon and Advanced Semiconductor Materials, School of
Materials Science and Engineering, Zhejiang University, Hangzhou 310027, China.

²ZJU-Hangzhou Global Scientific and Technological Innovation Center, Zhejiang
University, Hangzhou 311215, China.

³Institute of Thermal Science and Power Systems School of Energy Engineering,
Zhejiang University, Hangzhou 310027, China

⁴Key Laboratory of Hydrogen Storage and Transportation Technology of Zhejiang
Province, Hangzhou 310027, Zhejiang, China.

⁵China-UK Low Carbon College, Shanghai Jiao Tong University, Shanghai, China.

⁺These authors contributed equally to this work.

^{*}Corresponding author: Email: ruhong@zju.edu.cn; xlfan@zju.edu.cn.

Supplementary Note 1

By combining the two expressions of ionic conductivity, we observe a negative correlation between the natural logarithm of the ion transport barrier and the number of effective charge carriers.

$$\sigma = \frac{A}{T} C e^{\frac{E_{\text{trans}}}{k_B T}} \quad (1)$$

$$\sigma = \sum n_i \mu_i Z_i e_0 \quad (2)$$

where C is the molar concentration of diffused Li^+ ; T is the absolute temperature; E_{trans} is the transport energy barrier; A and k_B are the pre-exponential factor and Boltzmann constant, respectively; Z_i is the valence order; n_i is the number of charge carriers; μ_i is the mobility; e_0 is elementary charge.

Combining Equation (1) with Equation (2), we derive

$$E_{\text{trans}} \propto \ln \sum n_i \quad (3)$$

According to formula (3), it is evident that the energy barrier of ion transport decreases as the number of effective charge carrier increases. The response of the energy barrier of ion transport to the number of effective conductive clusters varies across different types of electrolytes due to differences in ionic mobilities.

$$\sigma = \frac{Z_i e_0}{6\pi\eta r} \quad (4)$$

where η is the viscosity of electrolyte, and r is the Stokes radius of solvated Li^+ . From Equation (4), the viscosity and the Stokes radius of solvated Li^+ vary in different electrolyte.

Supplementary Note 2

The ion transport behaviors are dependent on the spatial configuration and electrostatic interactions within the ionic cloud¹⁻³. The distortion of an ionic cloud creates two separate counterforces on the movement of the central ion: relaxation force (F_R) and electrophoresis force (F_E), so that the net force (F_{Net}) felt by the moving central ion would be

$$F_{Net} = F_C - (F_R + F_E) \quad (5)$$

where F_C is the force applied by the external Coulombic field.

Correspondingly, the drift velocity should be modified by correcting the two velocity components generated by these two counterforces:

$$v_d = v_0 - (v_R + v_E) \quad (6)$$

where v_d is the drift velocity, v_0 is the drift velocity component generated by the external Coulombic field, v_R is the drift velocity component generated by relaxation force, v_E is the drift velocity component generated by electrophoresis force.

As Li^+ migrates, the negative center of its surrounding electron cloud remains misaligned with the ion, requiring compensatory forces to restore equilibrium, thereby restricting its movement. Put the central ion back and apply an external field, the average distance traveled by ionic cloud during relaxation time (τ_R) can be calculated as

$$d = \tau_R v_0 = \frac{v_0 (K^{-1})^2}{2\mu k_B T} \quad (7)$$

where d is the distance to quantify the asymmetric degree of the ionic cloud, μ is the mobility, k_B is Boltzmann's constant, K^{-1} is the Debye–Hückel thickness, which can be approximated as the distance between anions and ions.

The Coulombic force between Li^+ and anion is expressed as

$$F_R = \frac{z^2 e_0^2}{\varepsilon (K^{-1})^2} \quad (8)$$

where z is the valence order, e_0 is elementary charge, ε is the dielectric constant.

When the ionic cloud is distorted by a degree d , its charge center no longer coincides with the central ion but instead moves further away from it. This distortion introduces an additional counterforce, the relaxation force (F_R), which is proportional to the ratio of the distortion to the Debye–Hückel thickness (d/K^{-1}):

$$F_R = \frac{z^2 e_0^2}{\varepsilon (K^{-1})^2} \cdot \frac{d}{K^{-1}} \quad (9)$$

From F_R , the corresponding drift velocity component (v_R) is derived as

$$v_R = \mu F_R = \frac{z^2 e_0^3 \omega}{6 \varepsilon k_B T K^{-1}} \mu X \quad (10)$$

where ω is related to the ionic strength, and X is the applied external field. As the interionic distance (K^{-1}) increases, the strength of cation-anion interactions weakens, promoting faster ion migration.

Under an externally applied field X , the central ion experiences an electrophoretic force

$$F = z e_0 X \quad (11)$$

The electrophoresis component of the drift velocity should be

$$v_E = \frac{z e_0 X}{6 \pi K^{-1} \eta} \quad (12)$$

Therefore, the diminished presence of anions near Li^+ alleviates electrophoretic resistance, enhancing its overall mobility.

Supplementary Note 3

Supplementary Table 1. The costs of various electrolytes.

Electrolyte	Cost (\$/t)	Reference
1.5 M LiFSI/AN-DCM (1:4, vol)	\$12,374.4	This work
1.5 M LiFSI/DME-BTFE (1:2, vol)	\$14,209.2	4
1.8 M LiFSI/DOL	\$15,650.4	5
1.5 M LiFSI/DMK-VC (7:3, vol) + 5wt% FEC	\$18,919.0	6
1 M LiTFSI/ETFA-FEC (7:3, vol)	\$58,721.2	7
LiDFOB/NMTFA (1:5, mol)	\$72,448.0	8
2 M LiTFSI/EA	\$77,710.5	9
1.28 M LiFSI-FEMC/FEC in D2	\$106,075.4	10
4.2 M LiTFSI/AN	\$120,633.6	11
1 M LiTFSI MDFA/MDFS-A-TTE (4:1:5, vol)	\$201,769.3	12
1 M LiDFOB/FEC-IZ (1:10, vol)	\$356,660.0	13
1.3 M LiFSI/FAN	\$19,695,732.4	14

Supplementary Table 2. The costs of various lithium salts and solvents.

Abbreviation	Name	Cost \$/t
LiDFOB	Lithium difluoro(oxalato)borate	\$13,927.6
LiFSI	Lithium Bis(fluorosulfonyl)imide	\$55,710.3
LiTFSI	Lithium bis(trifluoromethanesulphonyl)imide	\$198,607.2
AN	Acetonitrile	\$1,016.7
BTFE	bis(2,2,2-trifluoroethyl) ether	\$3,899.7
D2	1,1,2,2-tetrafluoro-1-(2,2,2-trifluoroethoxy)ethane	\$28,830.1
DCM	Dichloromethane	\$292.5

DME	dimethoxyethane	\$1,922.0
DMK	Acetone	\$724.2
DOL	1,3-dioxolane	\$2,924.8
EA	Ethyl acetate	\$752.1
ETFA	Ethyl trifluoroacetate	\$6,267.4
FAN	Fluoroacetonitrile	\$24,889,972.1
FEC	Fuoroethylene carbonate	\$48,746.5
FEMC	Methyl (2,2,2-trifluoroethyl) carbonate	\$480,341.2
IZ	Isoxazole	\$448,468.0
MDFA	Methyl Difluoroacetate	\$192,200.6
MDFSFA	Methyl 2,2-difluoro-2-(fluorosulfonyl)acetate	\$288,348.9
NMTFA	N-methyl-2,2,2-trifluoroacetamide	\$85,689.4
TTE	1,1,2,2-Tetrafluoroethyl-2,2,3,3-tetrafluoropropylether	\$192,200.6
VC	Vinylene carbonate	\$7,242.3

Supplementary tables 1 and 2 present the costs of electrolytes for low-temperature and fast-charging conditions, along with the costs of the required lithium salts and moderators. Owing to the low price and ready availability of its constituents, the FA-DCM electrolyte exhibits a lower overall cost, which is conducive to large-scale production and application.

Supplementary Note 4

The interactions between moderators and anions, as well as between moderator and solvents, are described by equations (13) and (14), respectively¹⁵.

$$U_{\text{ion-dipole}} = -\frac{ze\mu_{\text{moderator}}\cos\theta}{4\pi\epsilon_0r_1^2} \quad (13)$$

$$U_{\text{dipole-dipole}} = -\frac{2\mu_{\text{moderator}}^2\mu_{\text{solvent}}^2}{(4\pi\epsilon_0)^23Tr_2^6k_B} \quad (14)$$

where U is the electrostatic potential energy, ϵ_0 is the dielectric constant, ze is the charge of the ion, r_1 is the distance between moderator molecule center and negative charge center, and r_2 is the distance between moderator molecule center and solvent molecule center. The μ is the dipole moment, where θ is the dipole angle relative to the line joining the ion and the center of the dipole, k_B is the Boltzmann constant, and T is the absolute temperature.

We define the degree of solvated structure disintegration (D) as

$$D = \frac{V_{\text{sol-structure}}}{V_{\text{moderator}}} \cdot \frac{U_{\text{ion-dipole}}}{U_{\text{dipole-dipole}}} \quad (15)$$

where $V_{\text{sol-structure}}$ is the volume of the solvation shell, $V_{\text{moderator}}$ is the volume of moderator molecule.

Substituting equations (13) and (14), we obtain

$$D = \frac{6\pi ze\epsilon_0r_2^6k_BT}{r_1^2\mu_2^2} \cdot \frac{1}{\mu_{\text{moderator}}} \cdot \frac{1}{V_{\text{moderator}}} \quad (16)$$

Since the coefficient term can be considered nearly constant (C), we obtain

$$D = C \cdot \frac{1}{\mu_{\text{moderator}}} \cdot \frac{1}{V_{\text{moderator}}} \quad (17)$$

Supplementary Table 3. Summary of all moderators in Fig. 1c.

Moderator	Abbreviation	Volume/Å ³	μ/debye	Structure
Dichloromethane	DCM	85.11	2.36	
Dichloroethane	DCE	108.41	2.91	
Fluorobenzene	FB	120.62	2.08	
1,1,2,2-Tetrafluoroethyl-2,2,3,3-tetrafluoropropylether	TTE	184.63	4.94	
1,1,1,3,3-Pentafluorobutane	PFB	134.85	2.35	
1,1,2,2,3,3,4-Heptafluorocyclopentane	HFC	152.22	3.66	
(Trifluoromethyl)cyclohexane	TFMCH	176.00	3.47	
Benzotrifluoride	TFMB	153.19	3.71	
(Trifluoromethoxy)benzene	TFMOB	164.34	3.26	
Bis(2,2,2-trifluoroethyl) ether	BTFE	152.62	5.16	
1H,1H,5H-Perfluoropentyl-1,1,2,2-tetrafluoroethylether	OTFOP	248.53	4.26	
1,1,2,2-Tetrafluoroethyl 2,2,2-trifluoroethyl ether	TFTFE	156.96	3.58	
Chlorobenzene	CLB	137.26	2.44	

Supplementary Table 4. Relative percentages of each cluster type for different electrolytes in Supplementary Fig. 8.

Electrolyte	AGGs propotion (%)	CIPs propotion (%)	SSIP propotion (%)
FAHCE	61.6	33.3	5.1
FA-DCM	18.4	69.7	11.9
FA-TTE	62.0	33.4	4.6

Supplementary Table 5. Self-diffusion coefficient of different electrolytes at 25 °C obtained by diffusion ordered spectroscopy NMR in Supplementary Fig. 10.

Electrolyte	FA-DCM	FA-TTE
Self-diffusion coefficient (D) ($\text{cm}^2 \text{ s}^{-1}$)	$D_{\text{Li}^+}=3.330\times 10^{-7}$	$D_{\text{Li}^+}=1.133\times 10^{-7}$
	$D_{\text{FSI}^-}=1.030\times 10^{-7}$	$D_{\text{FSI}^-}=4.268\times 10^{-8}$
	$D_{\text{AN}}=3.825\times 10^{-8}$	$D_{\text{AN}}=1.514\times 10^{-8}$
	$D_{\text{DCM}}=1.267\times 10^{-7}$	$D_{\text{TTE}}=9.657\times 10^{-8}$

Supplementary Table 6. Density of different electrolytes.

Electrolyte	Density (g mL ⁻¹)
BE	1.317
BEMP	1.227
FA-DCM	1.426
FA-TTE	1.776
FALCE	0.992
FAHCE	1.353

Supplementary Table 7. Charge-transfer resistance (R_{ct}) and interfacial resistance (R_{SEI}) of Li||graphite cells using different electrolytes at different rates, obtained from equivalent circuit fitting of EIS spectra in Supplementary Fig. 26.

Electrolyte	Rate	R_{ct} (ohm)	R_{SEI} (ohm)	χ^2
BE	2 C	5.290	9.035	1.21
	4 C	8.420	7.273	1.35
	6 C	8.790	7.687	1.42
	8 C	9.500	8.717	1.58
	10 C	12.850	9.180	1.73
FA-TTE	2 C	6.056	1.438	1.92
	4 C	7.660	1.990	1.05
	6 C	8.720	3.116	1.18
	8 C	9.720	4.651	1.33
	10 C	10.980	4.637	1.46
FA-DCM	2 C	0.367	1.757	1.48
	4 C	0.237	0.973	1.52
	6 C	0.366	1.359	1.61
	8 C	0.754	1.670	1.69
	10 C	0.544	1.417	1.73

Supplementary Table 8. Transport parameters of different electrolytes at different temperatures extracted from MD simulations in Supplementary Fig. 15 and 33-38.

Electrolyte	Transport parameters	25 °C	0 °C	-20 °C	-40 °C
FA-DCM	Calculated Li ⁺ diffusion coefficients ($\times 10^{-6}$ cm ² s ⁻¹)	5.11	3.19	2.01	0.66
	Residence times for AN (ps)	152.26	193.81	—	—
	Residence times for FSI ⁻ (ps)	115.66	144.28	—	—
	Average migration distance of FSI ⁻ (Å)	49.00	45.86	—	—
	Root mean square displacement of Li ⁺ over 3000 ps (Å)	32.48	25.99	20.81	11.67
FA-TTE	Calculated Li ⁺ diffusion coefficients ($\times 10^{-6}$ cm ² s ⁻¹)	1.77	0.45	0.14	0.03
	Residence times for AN (ps)	234.44	348.18	—	—
	Residence times for FSI ⁻ (ps)	178.63	249.01	—	—
	Average migration distance of FSI ⁻ (Å)	71.02	226.13	—	—
	Root mean square displacement of Li ⁺ over 3000 ps (Å)	15.92	9.12	5.00	2.16

Supplementary Table 9. Rietveld refinement results of pristine NMC811 positive electrode and NMC811 positive electrodes recovered from Li||NMC811 half-cells after 50 cycles using different electrolytes.

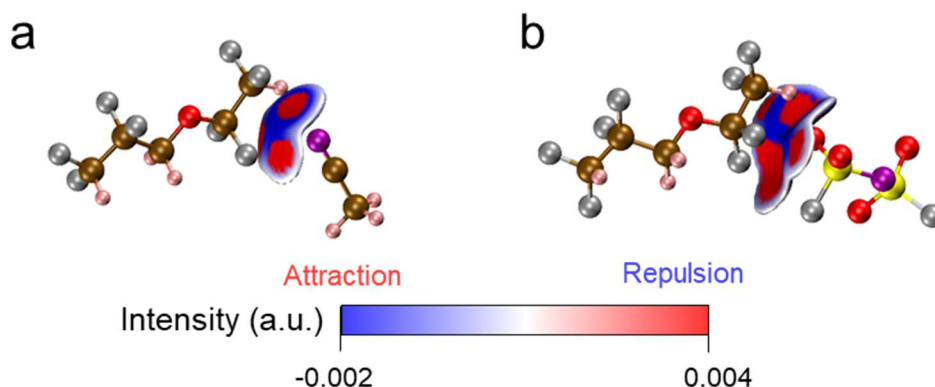
NMC811	<i>a</i> axis (Å)	<i>c</i> axis (Å)	Vol (Å ³)	R _{wp}	R _p
Pristine	2.8703	14.1892	101.241	14.10	9.78
BE	2.8324	14.3956	100.019	2.78	5.22
FA-DCM	2.8733	14.1850	101.418	14.40	9.93

Supplementary Table 10. The proportion of each atom in SEI and the fraction of organic and inorganic components after cycled in FA-DCM electrolyte.

Elements	N	O	C	S	F	Cl
Atom ratio (%)	3.30	12.48	9.25	4.56	25.90	9.04
Percentage of organic components (%)	0	38	100	0	0	55
Percentage of inorganic components (%)	100	62	0	100	100	45

Supplementary Table 11. The atomic percentages of key elements with different electrolytes at different sputtering depths.

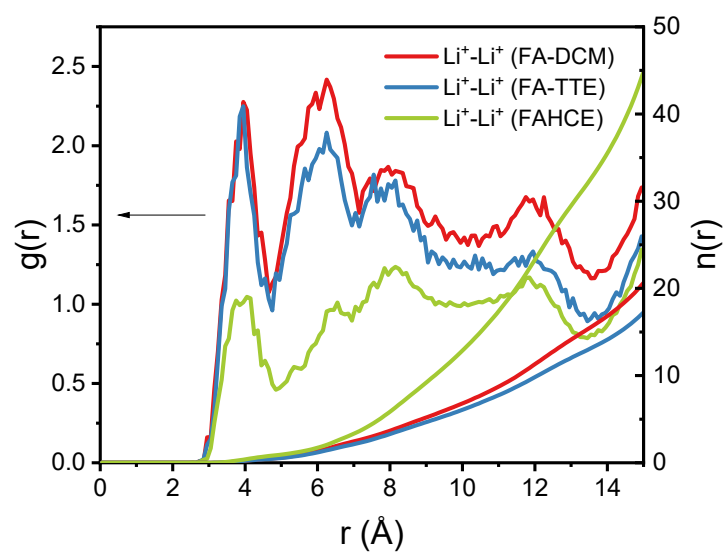
Electrolyte	Sputtering depth	0.0 nm	2.4 nm	6.0 nm
	Element	Atomic %	Atomic %	Atomic %
FA-DCM	F 1s	10.21	25.63	25.90
	N 1s	6.67	2.65	3.30
	S 2p	9.84	4.92	4.56
	Cl 2p	4.20	8.89	9.04
BE	F 1s	15.86	23.17	24.84
	P 2p	2.18	2.80	2.80
	C 1s	34.55	11.83	9.93
	O 1s	27.89	21.62	20.3



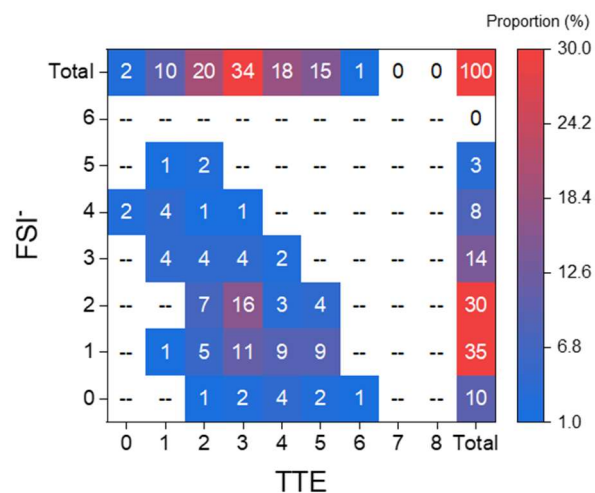
Supplementary Fig. 1 | IGMH analysis of TTE-AN and TTE-FSI⁻ complexes.

Sign(λ_2) ρ colored isosurfaces of $\delta g^{\text{inter}} = 0.005$ a.u. corresponding to IGMH analysis for TTE-AN (a), TTE-FSI⁻ (b) complexes (red, O atom; yellow, S atom; purple, N atom; silver, F atom; tan, C atom; white, H atom). The color bar represents interaction intensity (a.u.) (-0.002-0.004), where red indicates attractive interactions, white denotes van der Waals interactions, and blue corresponds to steric repulsion. The data are provided in Supplementary Data 1. Source data are provided as a Source Data file.

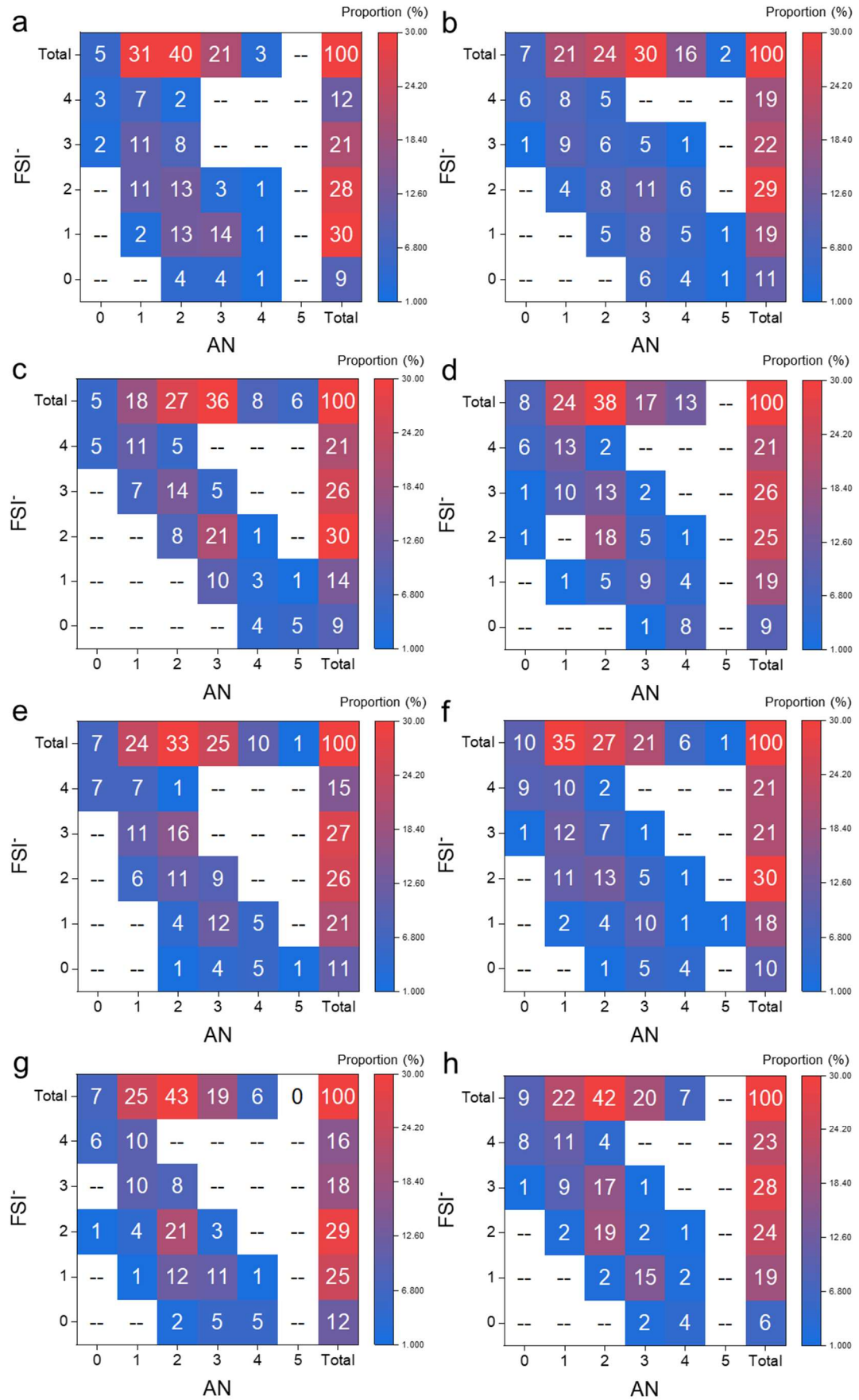
The main interaction was graphically depicted between specific sites of TTE-AN (TTE-H and TTE-F interacting with AN-N) and TTE-FSI⁻ (TTE-H interacting with FSI⁻-O).

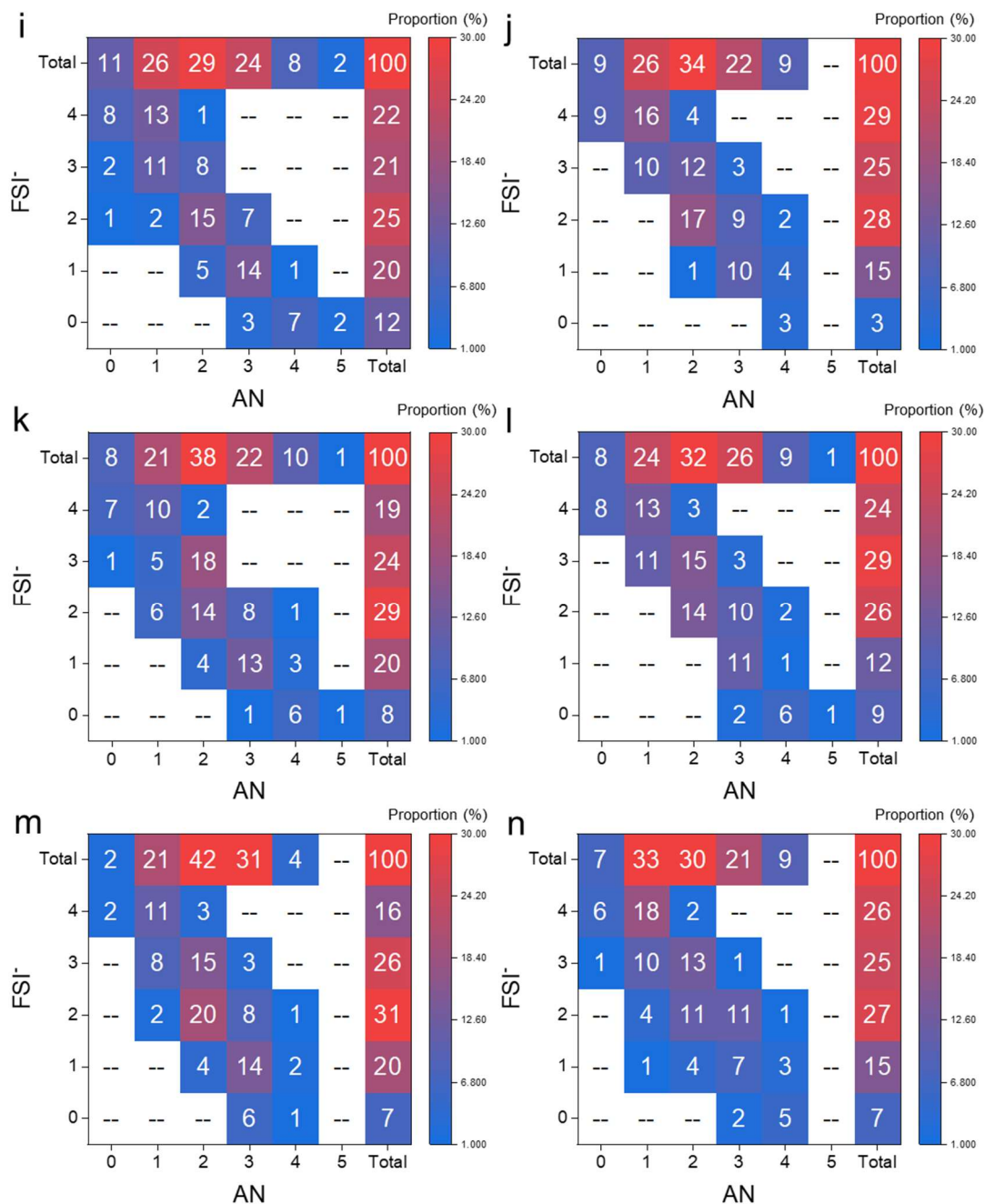


Supplementary Fig. 2 | MD simulations. Radial distribution function $g(r)$ and coordination numbers $n(r)$ in different electrolytes. Source data are provided as a Source Data file.

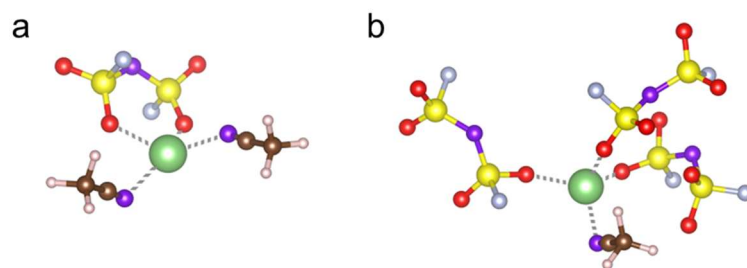


Supplementary Fig. 3 | MD simulations. Heatmaps of Li^+ solvating environment (3 Å to 5 Å around Li^+) in FA-TTE electrolyte, the color bar represents the proportion of the number of this species to the total number of clusters. Source data are provided as a Source Data file.

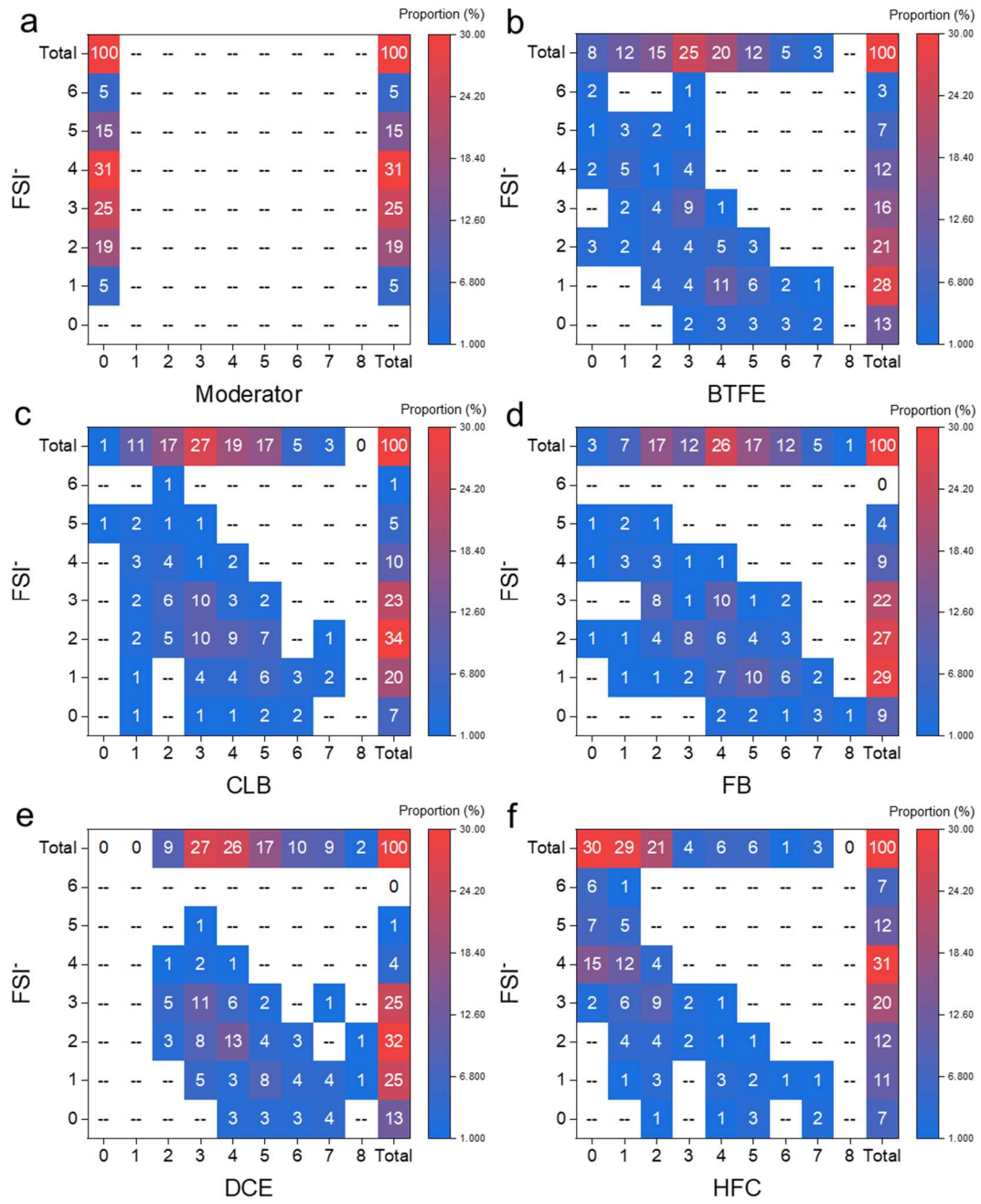


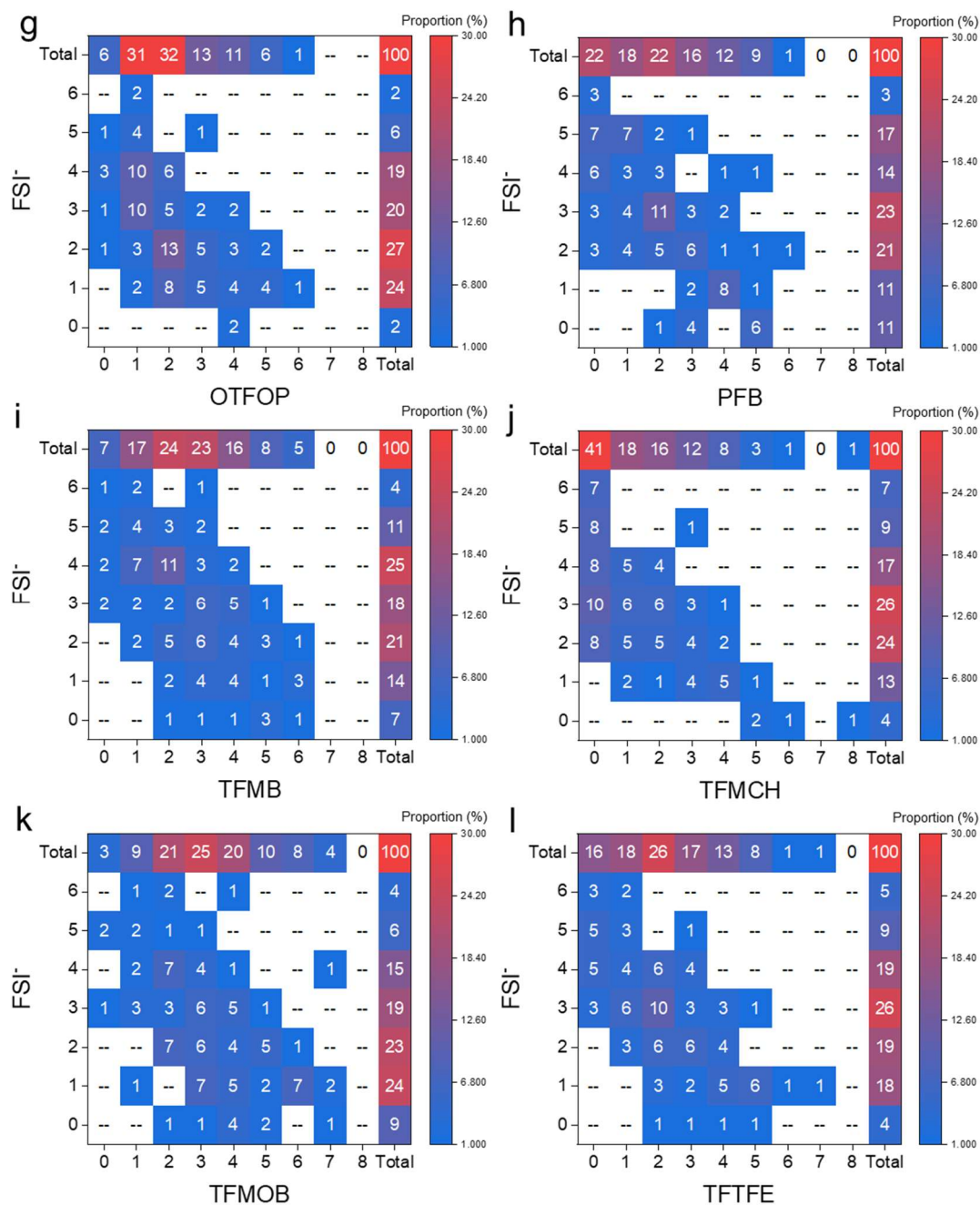


Supplementary Fig. 4 | Heatmaps of Li^+ solvation sheath in different electrolytes, the color bar represents the proportion of the number of this species to the total number of clusters. FA-DCM electrolyte (a), FA-TTE electrolyte (b), FAHCE electrolyte (c), FA-BTFE electrolyte (d), FA-CLB electrolyte (e), FA-FB electrolyte (f), FA-DCE electrolyte (g), FA-HFC electrolyte (h), FA-OTFOP electrolyte (i), FA-PFB electrolyte (j), FA-TFMB electrolyte (k), FA-TFMCH electrolyte (l), FA-TFMOB electrolyte (m) and FA-TFTFE electrolyte (n). Source data are provided as a Source Data file.

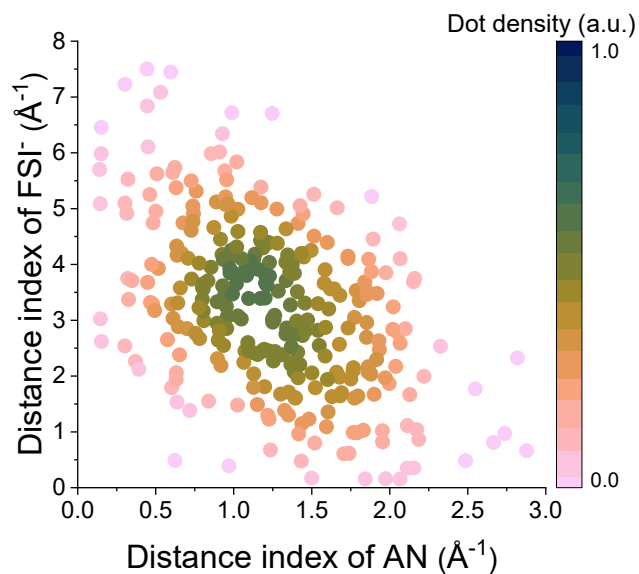


Supplementary Fig. 5 | Typical Li^+ solvation structures in different electrolyte extracted from the MD simulations. FA-DCM electrolyte (a) and FA-TTE electrolyte (b). (olive green, Li atom; red, O atom; yellow, S atom; purple, N atom; silver, F atom; tan, C atom; white, H atom). The data are provided in Supplementary Data 4. Source data are provided as a Source Data file.



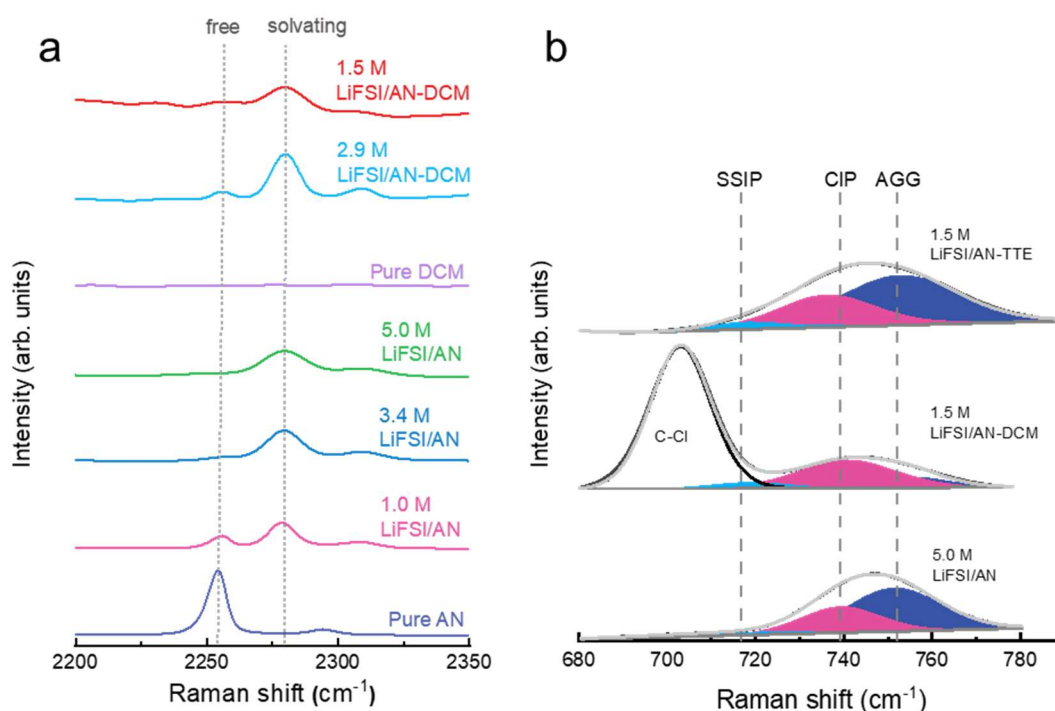


Supplementary Fig. 6 | Heatmaps of Li^+ solvating environment (3 Å to 5 Å) in different electrolytes, the color bar represents the proportion of the number of this species to the total number of clusters. FAHCE electrolyte (a), FA-BTFE electrolyte (b), FA-CLB electrolyte (c), FA-FB electrolyte (d), FA-DCE electrolyte (e), FA-HFC electrolyte (f), FA-OTFOP electrolyte (g), FA-PFB electrolyte (h), FA-TFMB electrolyte (i), FA-TFMCH electrolyte (j), FA-TFMOB electrolyte (k) and FA-TFTFE electrolyte (l). Source data are provided as a Source Data file.



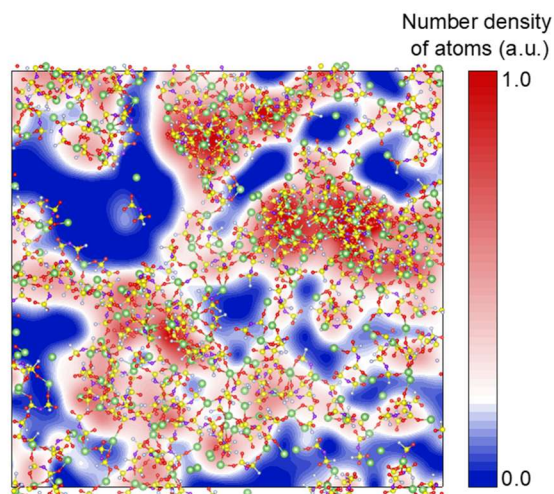
Supplementary Fig. 7 | Distance index of FSI⁻ and AN in FA-TTE electrolyte.

Distance index = $\sum 1/x_n$, where x_n represents the distance between Li⁺ and N (AN), O (FSI⁻), the color bar represents the density of Li⁺. Source data are provided as a Source Data file.



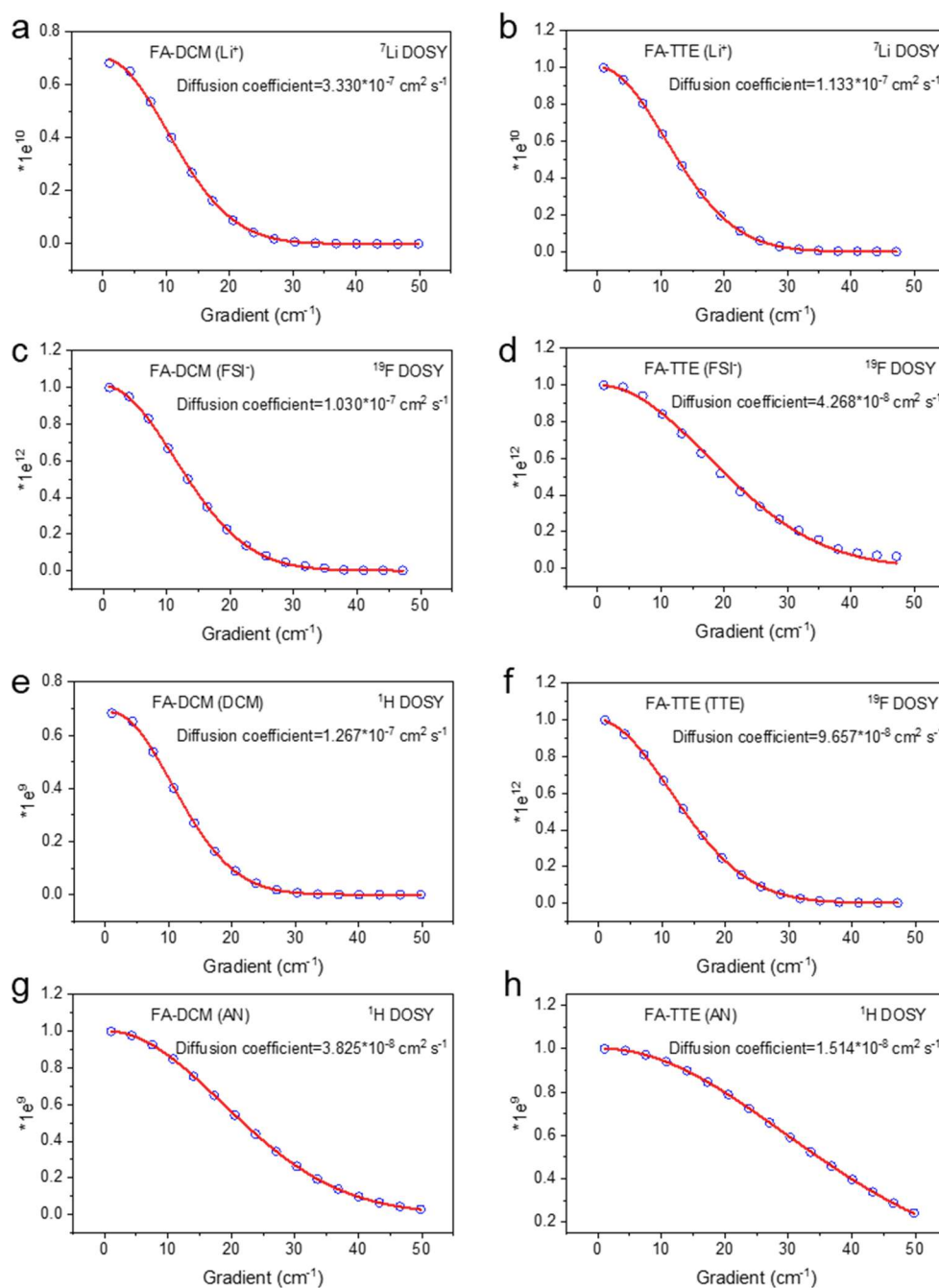
Supplementary Fig. 8 | Raman spectra of various concentrations of LiFSI/AN, FA-DCM and FA-TTE electrolytes in different ranges. 2200-2350 cm^{-1} (a) and 680-780 cm^{-1} (b), solvent-separated ion pair (SSIP, non-coordinated FSI⁻) locates at $\sim 717 \text{ cm}^{-1}$, contact ion pair (CIP, one FSI⁻ bonding with one Li⁺) locates at 740 cm^{-1} , aggregate (AGG, one FSI⁻ bonding with two or more Li⁺) locates at 751 cm^{-1} . Source data are provided as a Source Data file.

In Supplementary Fig. 8a, the peak at $\sim 2252 \text{ cm}^{-1}$, assigned to the C $\equiv$ N stretching vibration of free AN molecules, gradually disappears with the increasing LiFSI concentration. Concurrently, a new peak emerges at $\sim 2280 \text{ cm}^{-1}$, corresponding to the formation of Li⁺-AN coordinated interactions¹⁶⁻¹⁸. In Supplementary Fig. 8b, upon adding DCM to the highly concentrated electrolyte (5.0 M LiFSI/AN), a significant portion of AGGs was converted into CIPs, confirming the regulatory role of DCM in tailoring solvation structures. While with the addition of TTE, the fraction of AGG clusters increases, hindering the facilitation of fast ion conduction.



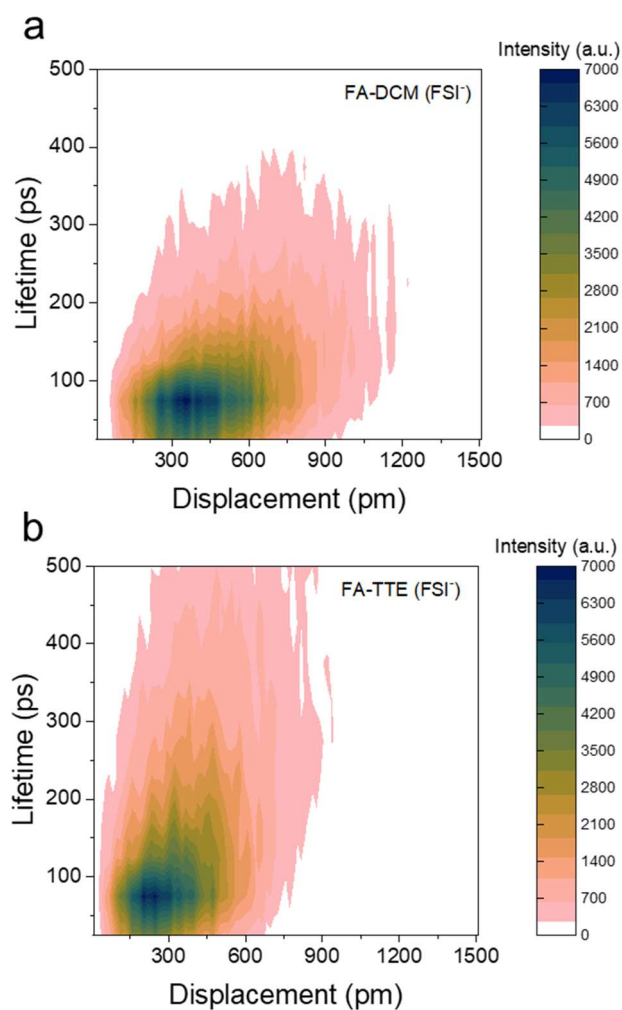
Supplementary Fig. 9 | MD simulations. Snapshots of FA-TTE electrolyte extracted from MD simulations. (olive green, Li atom; red, O atom; yellow, S atom; purple, N atom; silver, F atom; tan, C atom; white, H atom), the color bar represents the number density of atoms. The data are provided in Supplementary Data 2. Source data are provided as a Source Data file.

The FA-TTE electrolyte exhibits microscopic heterogeneity due to the aggregation of large ionic clusters.



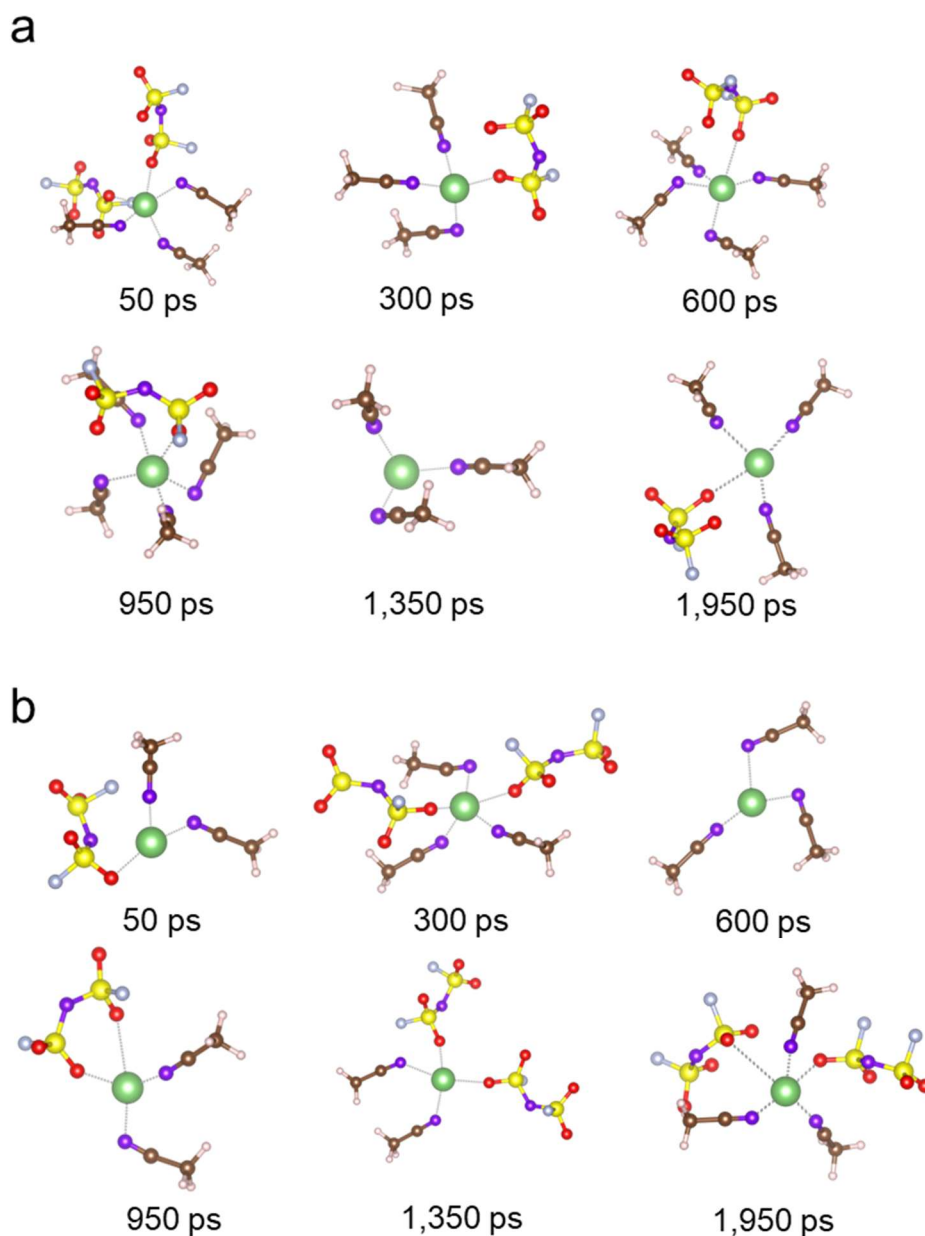
Supplementary Fig. 10 | Self-diffusion coefficient measurement of different electrolytes. ⁷Li DOSY NMR spectrum of FA-DCM (a) and FA-TTE electrolyte (b). ¹⁹F DOSY NMR spectra of FA-DCM (c) and FA-TTE electrolyte (d, f). ¹H DOSY NMR spectrum of FA-DCM (e, g) and FA-TTE electrolyte (h). Source data are provided as a Source Data file.

The self-diffusion coefficients obtained by DOSY NMR of FSI⁻ and solvent molecules in FA-DCM electrolyte ($1.030 \times 10^{-7} \text{ cm}^2 \text{ s}^{-1}$ of FSI⁻, $3.825 \times 10^{-8} \text{ cm}^2 \text{ s}^{-1}$ of AN, $1.267 \times 10^{-7} \text{ cm}^2 \text{ s}^{-1}$ of DCM) are higher than those of FA-TTE electrolyte ($4.268 \times 10^{-8} \text{ cm}^2 \text{ s}^{-1}$ of FSI⁻, $1.514 \times 10^{-8} \text{ cm}^2 \text{ s}^{-1}$ of AN, $9.657 \times 10^{-8} \text{ cm}^2 \text{ s}^{-1}$ of TTE).

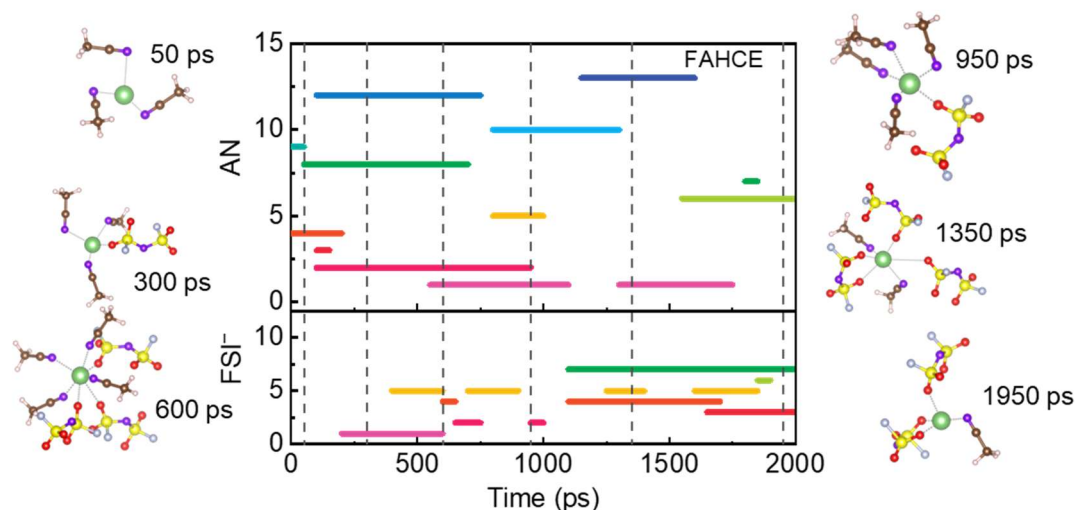


Supplementary Fig. 11 | Lifetime/displacement function of FSI⁻ for different electrolytes. FA-DCM electrolyte (a) and FA-TTE electrolyte (b), where color bar represents the statistical intensity of FSI⁻ anions at a given combination of lifetime and displacement. Source data are provided as a Source Data file.

During the same lifetime of Li⁺-AN/FSI⁻, the clusters migrated a longer distance in FA-DCM electrolyte. Additionally, the clusters in FA-DCM electrolyte have a shorter lifetime, reflecting the enhanced mobility of Li⁺. These results demonstrate significantly enhanced Li⁺ migration kinetics in the FA-DCM electrolyte compared to the FA-TTE system, driven by DCM-induced modulation of Li⁺ transport mechanisms.

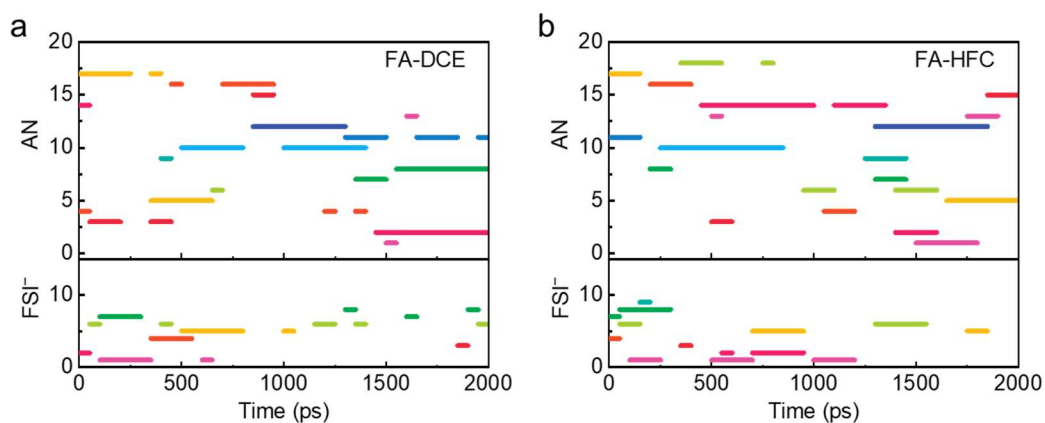


Supplementary Fig. 12 | Evolution of Li^+ solvation structures in FA-DCM and FA-TTE electrolytes. The representative Li^+ solvation structures corresponding to different residence times of FA-DCM electrolyte (a) and FA-TTE electrolyte (b) are shown ($t = 50$ ps, 300 ps, 600 ps, 950 ps, 1,350 ps, 1,950 ps; olive green, Li atom; red, O atom; yellow, S atom; purple, N atom; silver, F atom; tan, C atom; white, H atom). The data are provided in Supplementary Data 4. Source data are provided as a Source Data file.

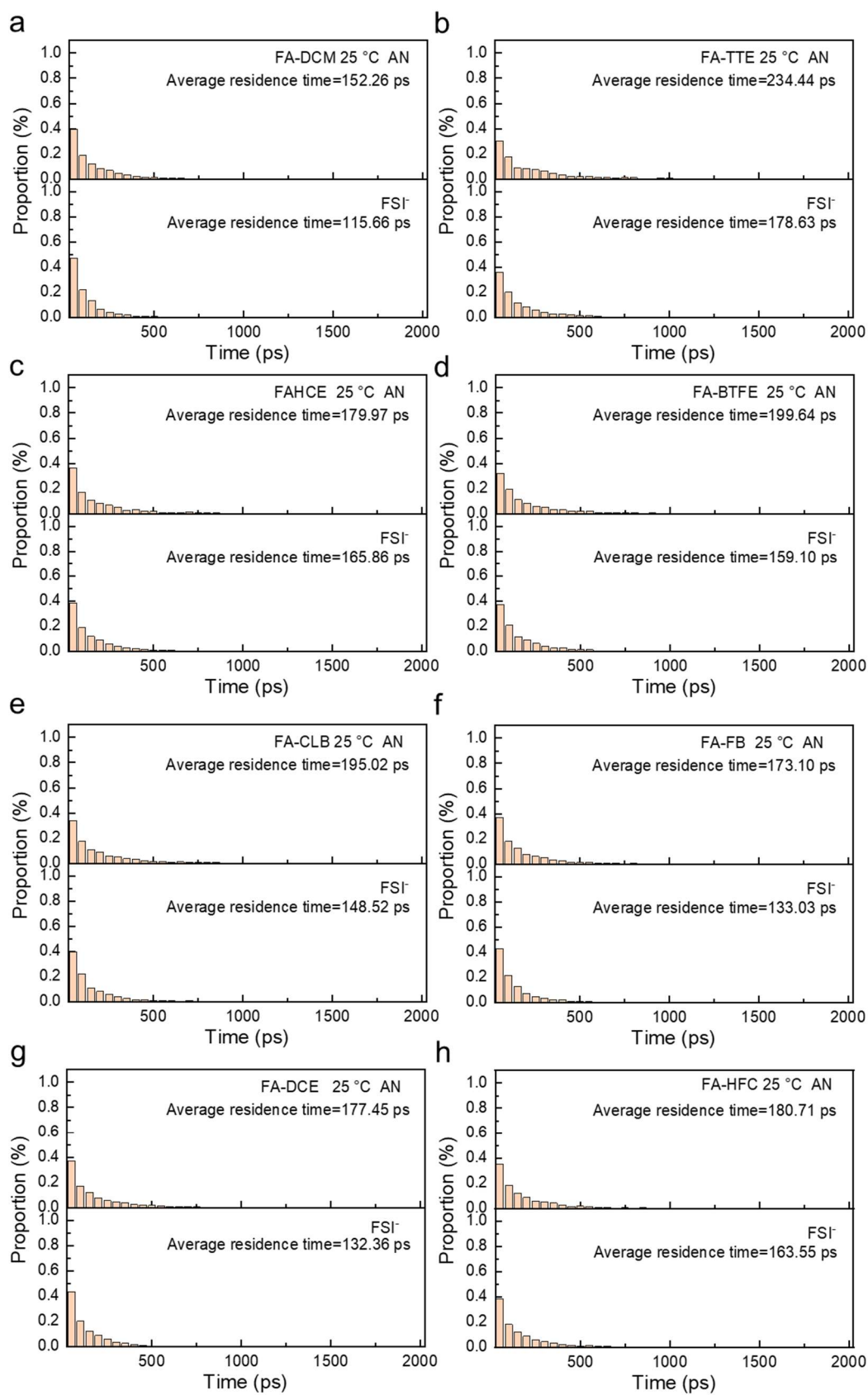


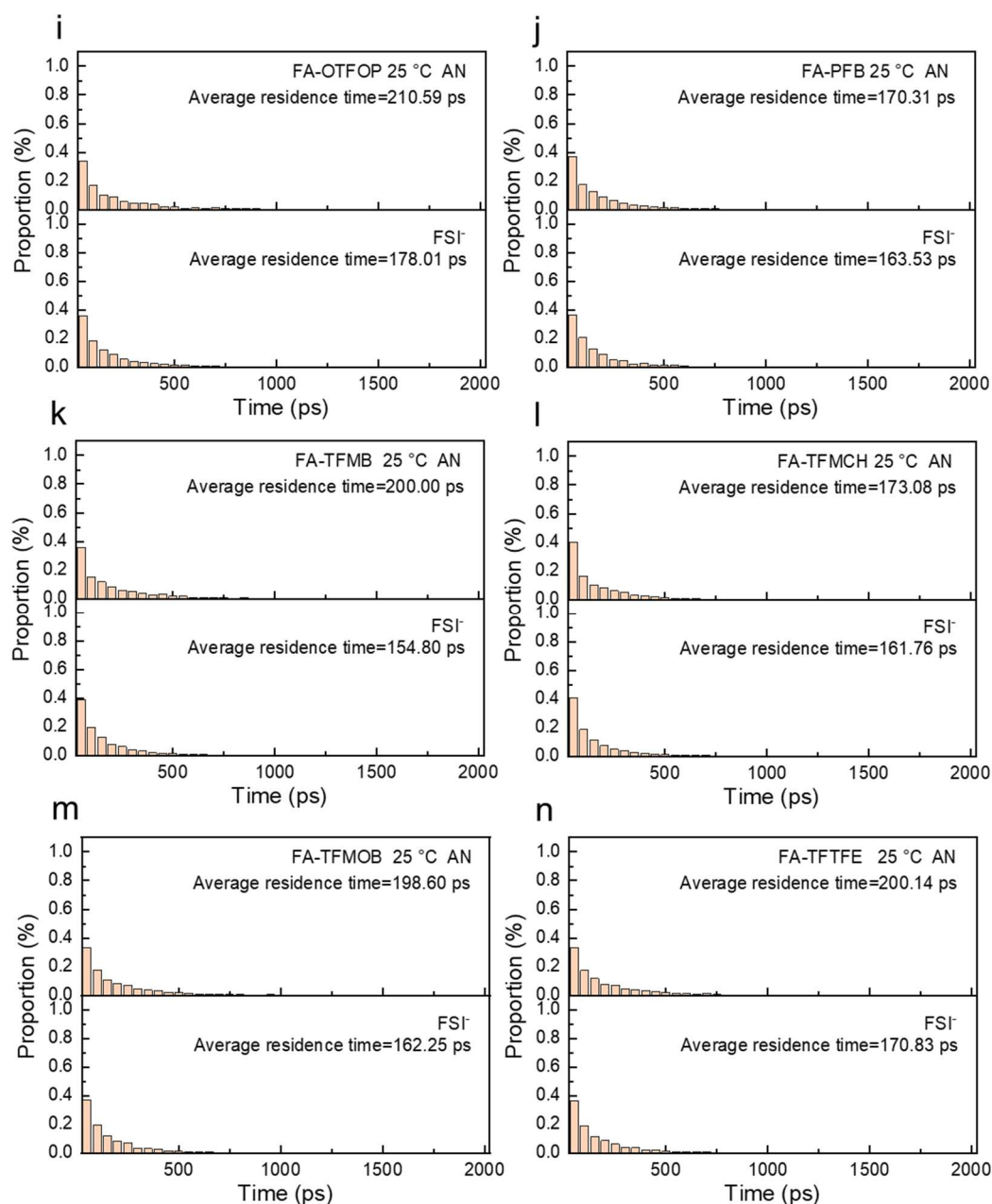
Supplementary Fig. 13 | Evolution of Li^+ solvation environment in FAHCE electrolyte from MD simulations at 298 K. The vertical axis represents the serial number of different solvents or anions coordinated with the investigated Li^+ in the simulation time of 2,000 ps. The representative Li^+ solvation structures corresponding to different residence times indicated by dashed vertical lines are also shown ($t = 50$ ps, 300 ps, 600 ps, 950 ps, 1,350 ps, 1,950 ps; olive green, Li atom; red, O atom; yellow, S atom; purple, N atom; silver, F atom; tan, C atom; white, H atom). The data are provided in Supplementary Data 4. Source data are provided as a Source Data file.

In the FAHCE electrolyte, Li^+ is predominantly surrounded by numerous anions within 2,000 ps. The strong coordination between Li^+ , anions, and solvent molecules increases the desolvation energy barrier, impeding Li^+ hopping dynamics and leading to an extended residence time.

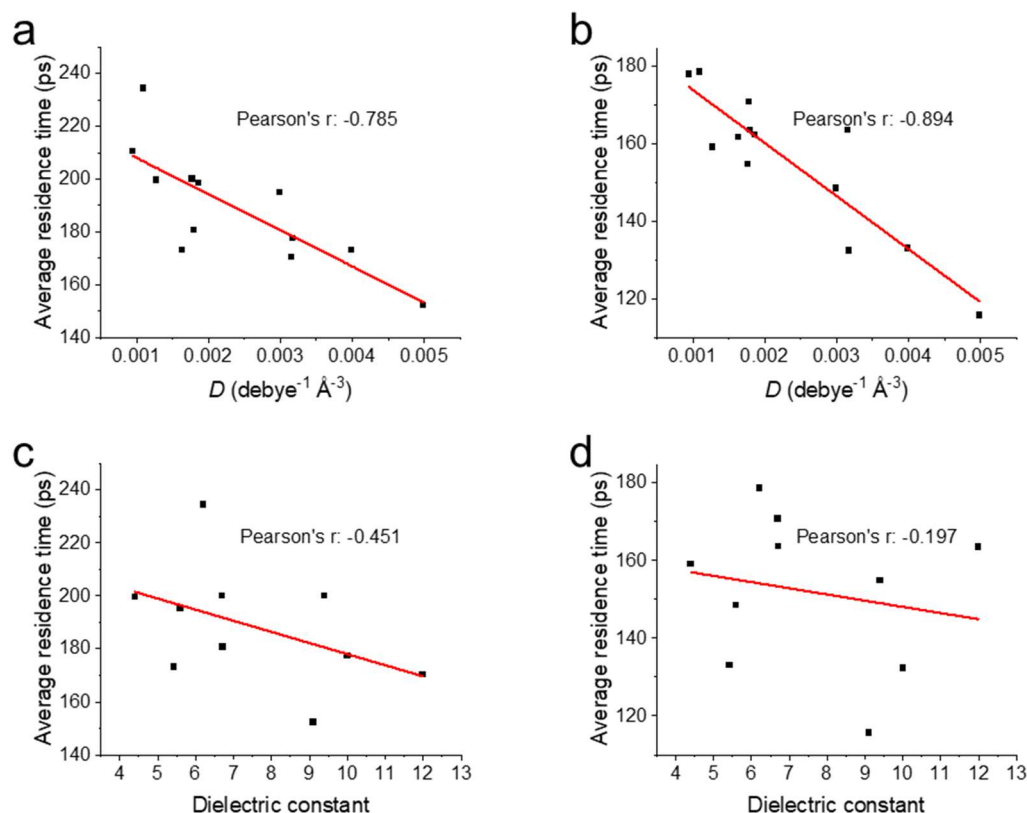


Supplementary Fig. 14 | Evolution of Li^+ solvation environment in FA-DCE (a) and FA-HFC (b) electrolyte from MD simulations at 298 K. The vertical axis represents the serial number of different solvents or anions coordinated with the investigated Li^+ in the simulation time of 2,000 ps. Source data are provided as a Source Data file.





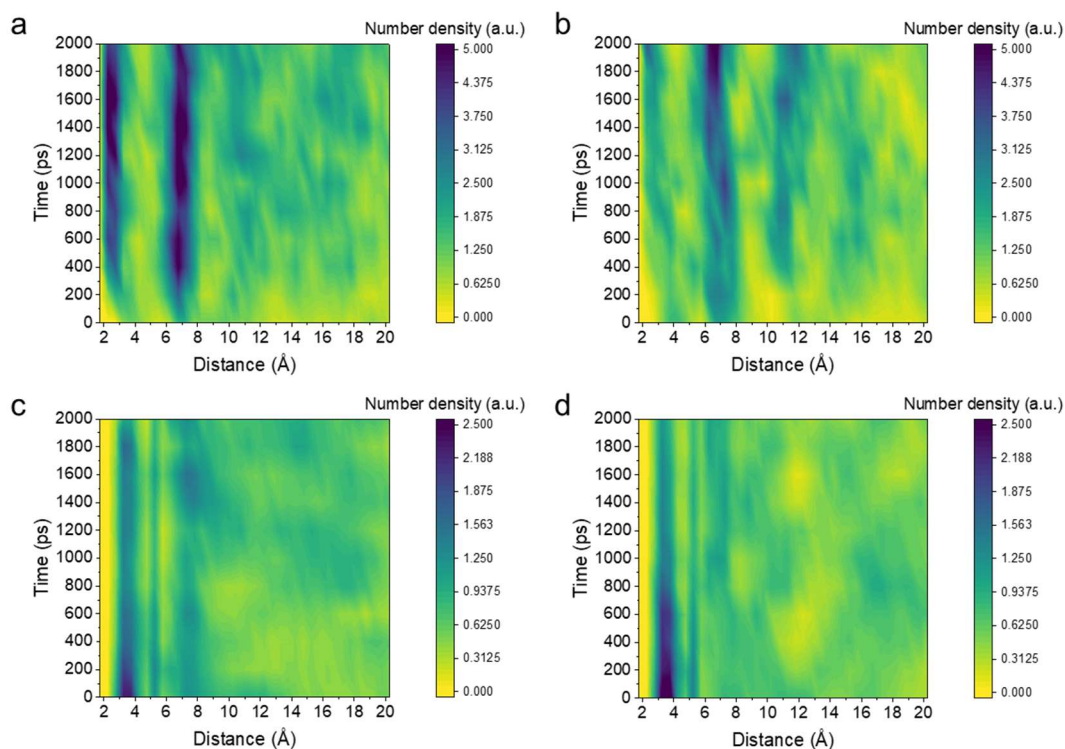
Supplementary Fig. 15 | Residence time distribution of AN and FSI⁻ in different electrolytes at 25 °C. FA-DCM electrolyte (a), FA-TTE electrolyte (b), FAHCE electrolyte (c), FA-BTFE electrolyte (d), FA-CLB electrolyte (e), FA-FB electrolyte (f), FA-DCE electrolyte (g), FA-HFC electrolyte (h), FA-OTFOP electrolyte (i), FA-PFB electrolyte (j), FA-TFMB electrolyte (k), FA-TFMCH electrolyte (l), FA-TFMOB electrolyte (m) and FA-TFTFE electrolyte (n). Source data are provided as a Source Data file.



Supplementary Fig. 16 | Functional relationship between average residence time and the disintegration of solvation structures (D). AN (a) and FSI $^{-}$ (b). Functional relationship between average residence time and dielectric constant. AN (c) and FSI $^{-}$ (d). Source data are provided as a Source Data file.

To quantitatively validate the proposed descriptor $D=C/(\mu \cdot V)$, we plotted the correlation between D values and the average Li $^{+}$ residence times (both with AN and FSI $^{-}$) obtained from MD simulations. As shown, a negatively correlated linear function relationship is observed: larger D values correspond to shorter residence times, in agreement with our theoretical framework. Pearson's correlation analysis yields $r=-0.785$ for AN and $r=-0.894$ for FSI $^{-}$, confirming a strong negative correlation between the descriptor and Li $^{+}$ solvation dynamics. This quantitative analysis supports the predictive capability of the proposed descriptor in capturing key ion transport

characteristics. While the known dielectric constant does not exhibit a strong linear correlation with solvation dynamics, indicating that these parameters alone are insufficient to capture the complex interplay ion-anion-solvent interactions.

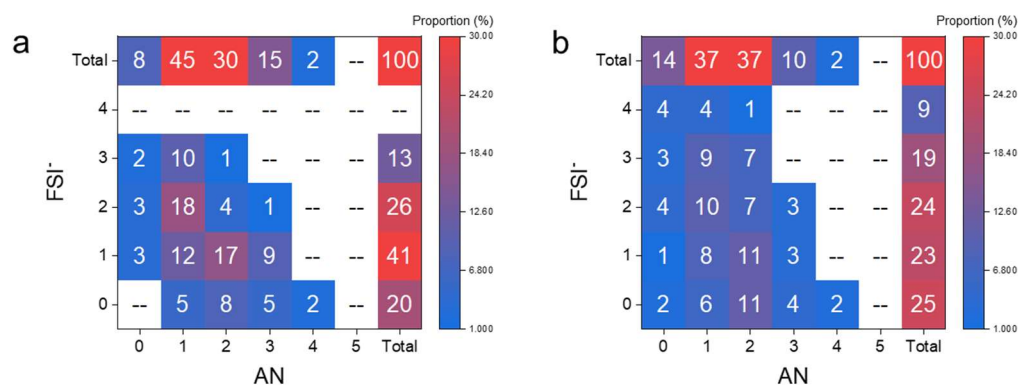


Supplementary Fig. 17 | Li^+ evolution at the negative electrode interface in FA-DCM electrolyte (a) and FA-TTE electrolyte (b). FSI^- evolution at the negative electrode interface in FA-DCM electrolyte (c) and FA-TTE electrolyte (d), $E=0.1 \text{ V } \text{\AA}^{-1}$. The vertical axis in the figure represents the time at which the electric field is applied, following system equilibration, with electrode slabs positioned at both ends of the electrolyte region along the Z-axis. The relative number density shown in the figure represents the number density of Li^+/FSI^- , which is normalized with respect to the average value of the entire electrolyte system. Source data are provided as a Source Data file.

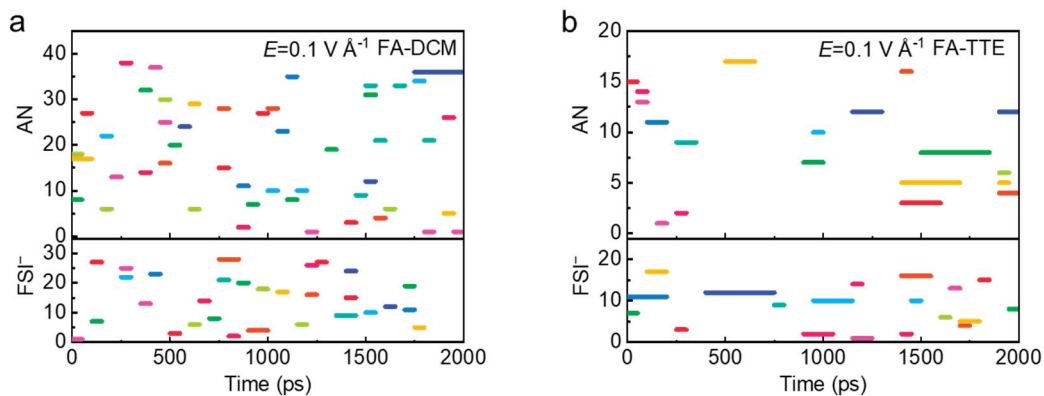
MD simulations were carried out under applied electric fields ($E=0.1 \text{ V } \text{\AA}^{-1}$) to directly probe the interfacial behavior of Li^+ and FSI^- in the FA-DCM electrolyte, in comparison with the FA-TTE electrolyte. The horizontal axis in the Supplementary Fig. 17 represents the time at which the electric field is applied, after the system has reached equilibrium. The relative number density shown in the figure is normalized with respect to the average value of the entire electrolyte system.

Our simulations reveal that in FA-DCM, Li^+ ions indeed migrate rapidly toward

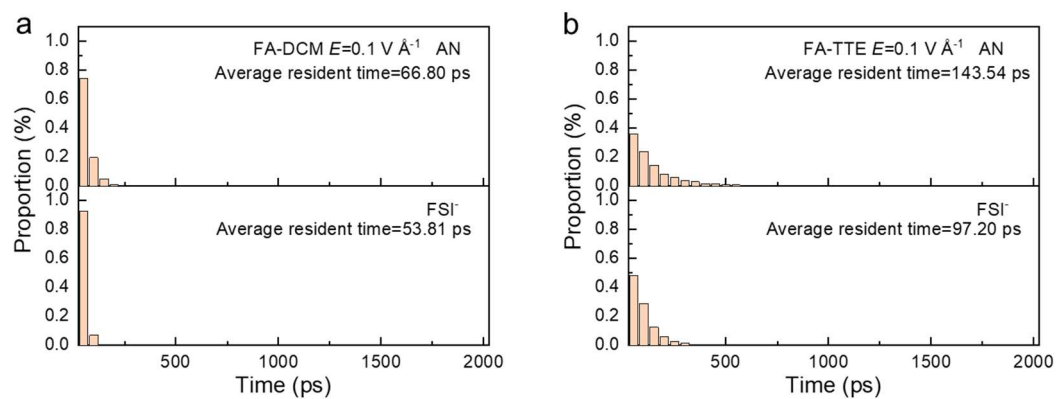
the negative electrode interface, consistent with the enhanced bulk mobility. Meanwhile, although the FSI⁻ concentration at the interface initially decreases due to electrostatic exclusion, it quickly reaches a dynamic equilibrium rather than continuing to diminish. It is also worth noting that the number density of FSI⁻ at the interface is much higher than the average value of the entire electrolyte. This stabilization can be attributed to the rapid accumulation of Li⁺ ions, which effectively screens the interfacial electric field and stabilizes the anion distribution at the interface, thereby suppressing interfacial heterogeneity. As a result, the interfacial environment remains relatively stable instead of exhibiting increasing kinetic heterogeneity.



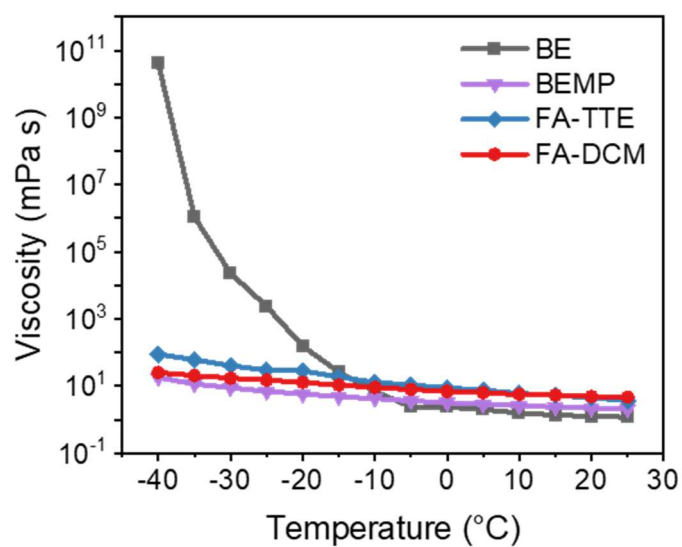
Supplementary Fig. 18 | MD simulations. Heatmaps of Li^+ solvation sheath in FA-DCM (a) and FA-TTE electrolyte (b) at 298 K, $E=0.1 \text{ V } \text{\AA}^{-1}$, the color bar represents the proportion of the number of this species to the total number of clusters. Source data are provided as a Source Data file.



Supplementary Fig. 19 | Evolution of Li⁺ solvation environment in FA-DCM (a) and FA-TTE electrolyte (b) from MD simulations at 298 K, $E=0.1 \text{ V } \text{\AA}^{-1}$. The vertical axis represents the serial number of different solvents or anions coordinated with the investigated Li⁺ in the simulation time of 2,000 ps. Source data are provided as a Source Data file.

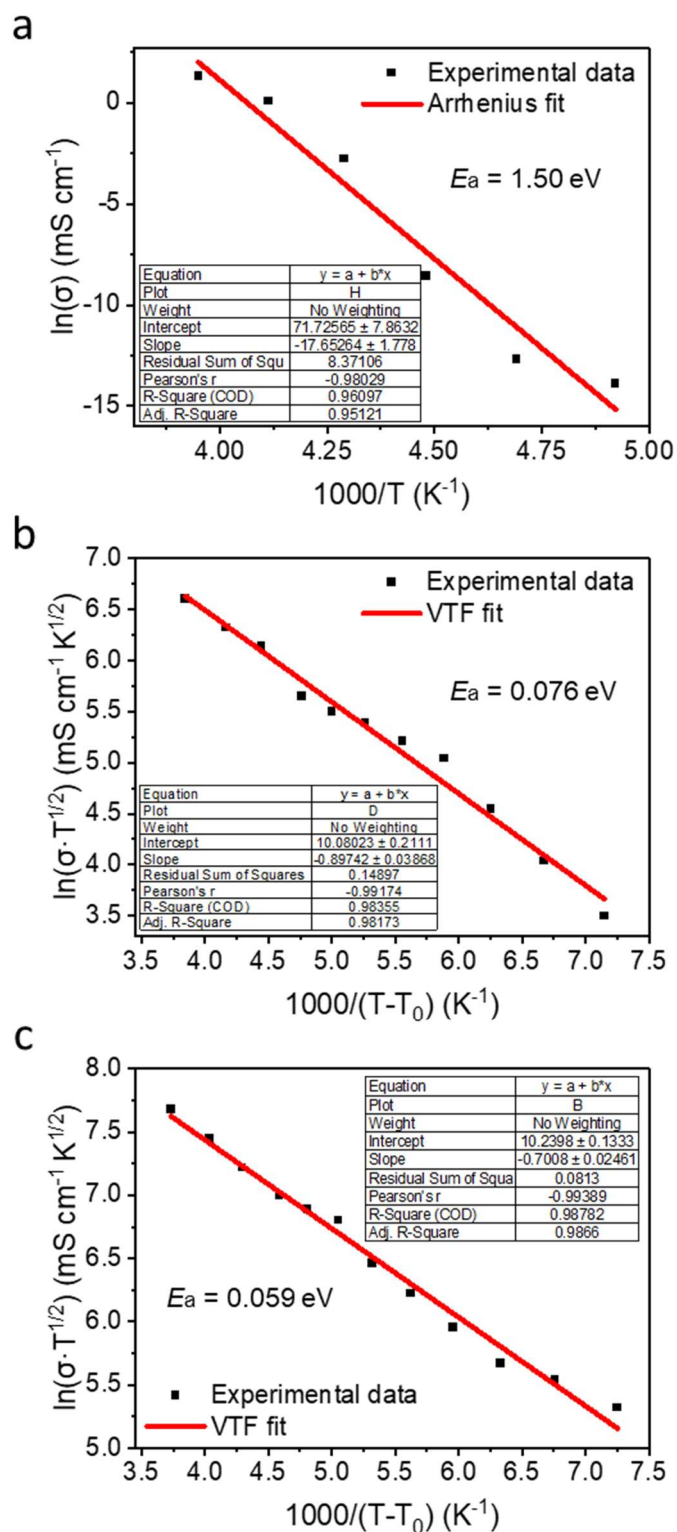


Supplementary Fig. 20 | MD simulations. Residence time distribution of AN and FSI^- in FA-DCM (a) and FA-TTE electrolyte (b) at 298 K, $E=0.1 \text{ V } \text{\AA}^{-1}$. Source data are provided as a Source Data file.



Supplementary Fig. 21 | Viscosity measurements. Viscosities of different electrolytes under different temperatures. Source data are provided as a Source Data file.

The FA-DCM electrolyte exhibits relatively low viscosity, particularly at low temperatures.



Supplementary Fig. 22 | Ionic conductivity-temperature fitting. The fitting results for BE electrolyte (a), FA-TTE electrolyte (b) and FA-DCM electrolyte (c). Source data are provided as a Source Data file.

For BE electrolyte, the data were fitted by the Arrhenius equation, because of the solidification of the electrolyte under -38 °C.

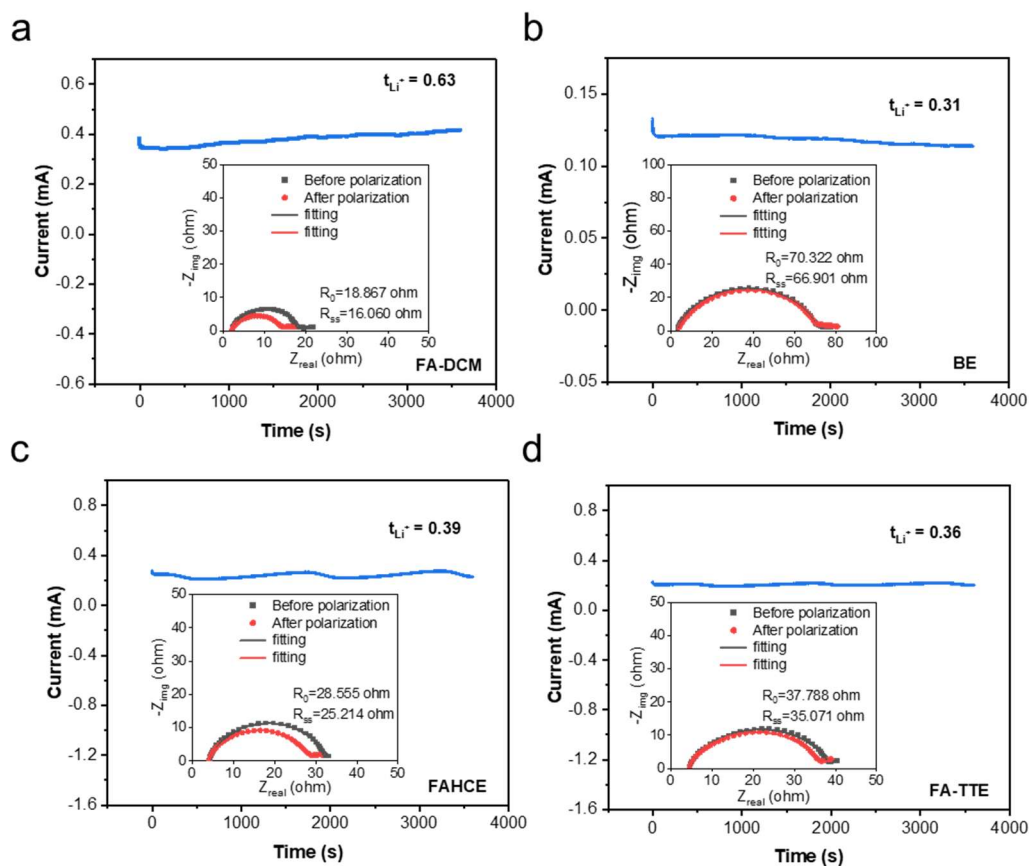
$$\sigma = Ae^{-\frac{E_a}{RT}} \quad (4.1)$$

where E_a is the pseudo-activation energy, A is the pre-exponential factor and R is the gas constant. FA-TTE and FA-DCM electrolyte was fitted by the Vogel-Tamman-Fulcher (VTF) empirical equation.

$$\sigma = \sigma_0 T^{-\frac{1}{2}} e^{\left(\frac{-E_a}{R(T-T_0)}\right)} \quad (4.2)$$

where σ_0 is the pre-exponential factor, T_0 is the ideal glass transition temperature.

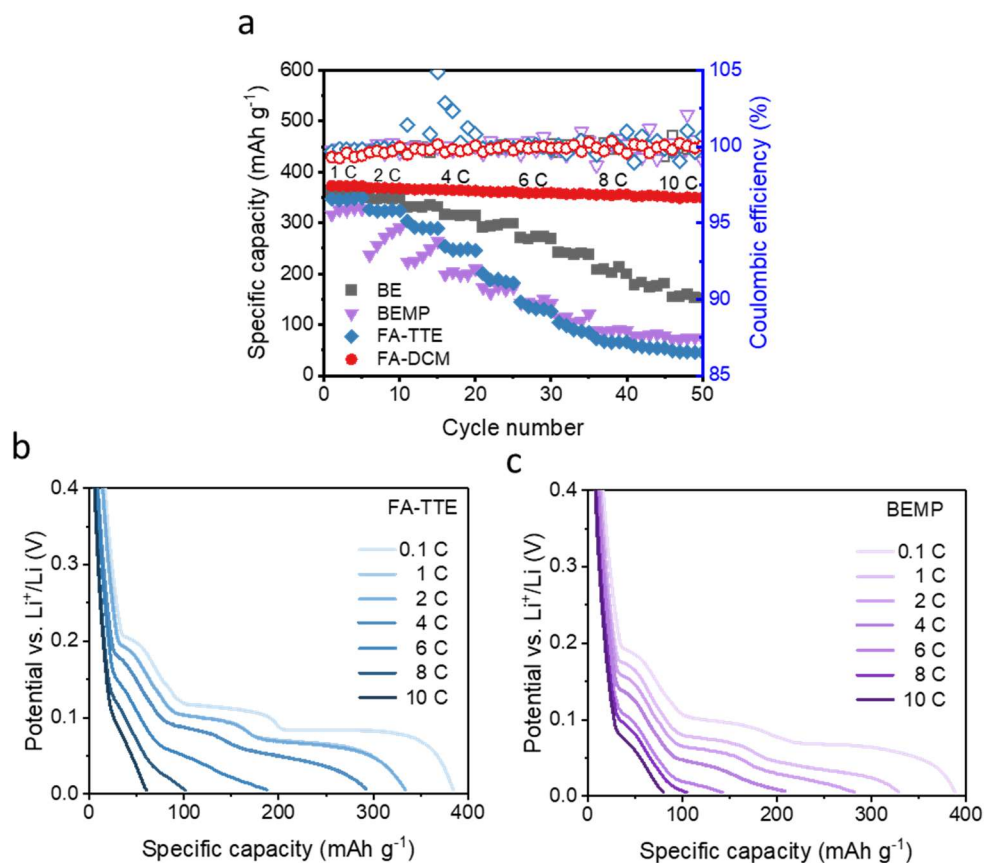
According to the fitted results, the BE electrolyte undergoes a transition into a glassy state as the temperature approaches T_0 , wherein the restricted molecular motion significantly decreases the number of mobile Li^+ and markedly reduces ionic conductivity. This deterioration directly compromises the available capacity and rate capability of batteries. Conversely, the FA-DCM electrolyte with the lowest observed T_0 , implies an optimized solvation structure that minimizes Li^+ coordination with solvents and anions, thereby promoting fast desolvation kinetics at low temperatures.



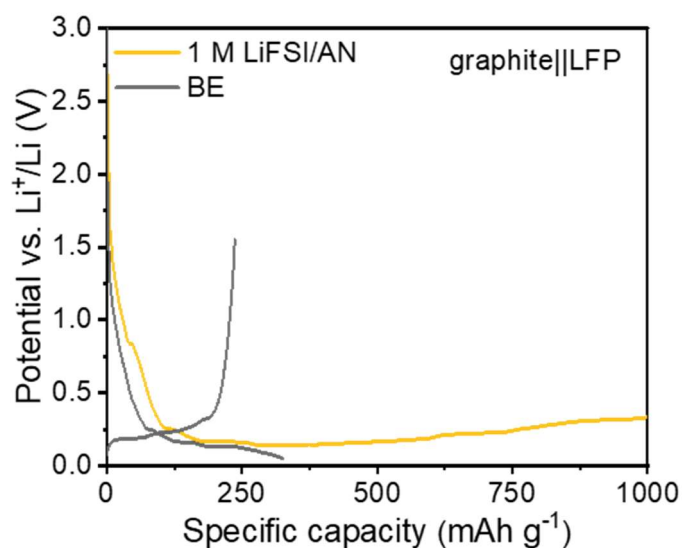
Supplementary Fig. 23 | Li^+ transference numbers of different electrolytes.

Polarization curves of the $Li||Li$ cells with FA-DCM (a), BE (b), FAHCE (c) and FA-TTE (d) electrolytes. Insets are impedance spectra before and after the polarization.

Source data are provided as a Source Data file.



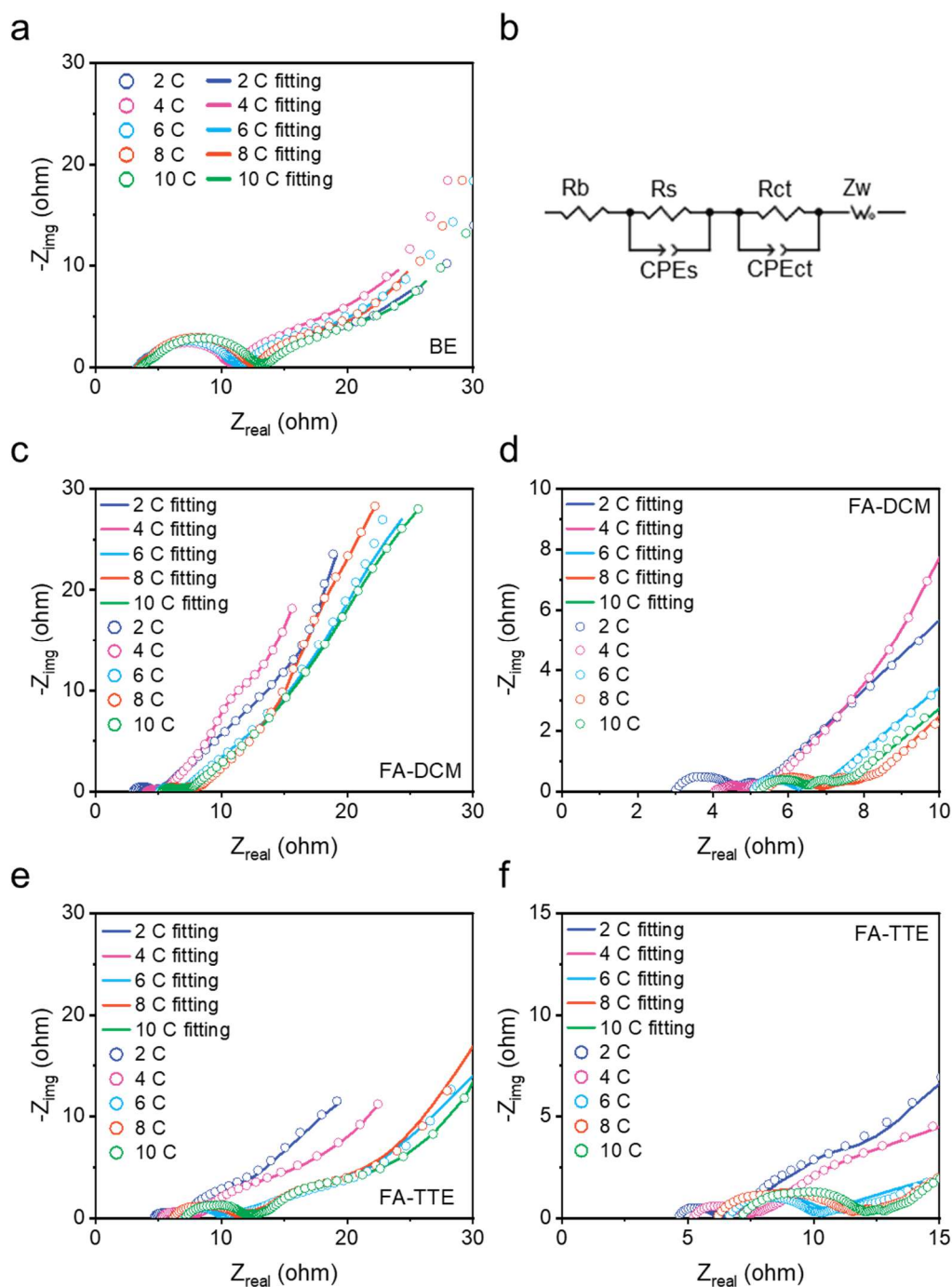
Supplementary Fig. 24 | Electrochemical performance of Li||graphite half cells with different electrolytes. Rate performance of Li||graphite cells with different electrolytes in the range of 0.005-1.5 V at 25 °C (a), solid symbols correspond to capacity values (left y-axis), while open symbols correspond to Coulombic efficiency (right y-axis). The discharge curves of Li||graphite cells with FA-TTE (b) and BEMP (c) electrolytes at different rates. Source data are provided as a Source Data file.



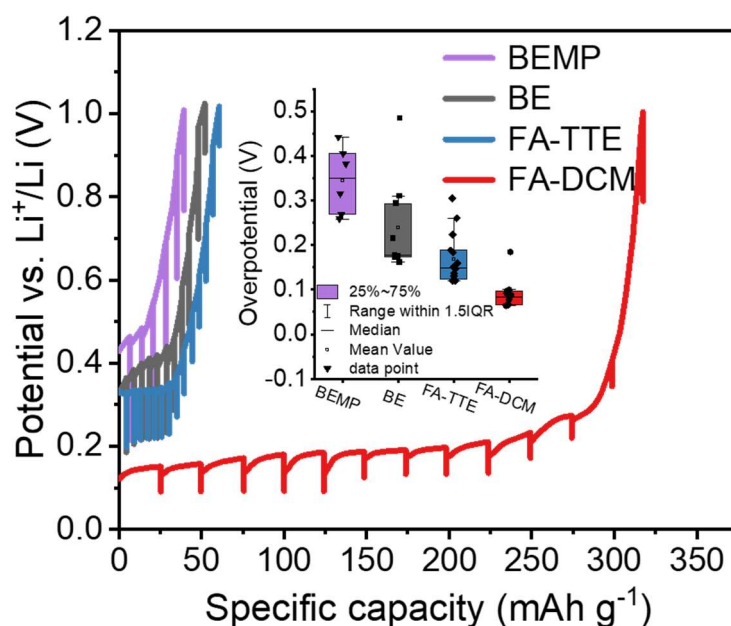
Supplementary Fig. 25 | Electrochemical performance of graphite||LFP full cells.

The charge/discharge curves of graphite||LFP full cells with different electrolytes at 0.1 C, 25 °C. Source data are provided as a Source Data file.

We employed graphite||LiFePO₄ (LFP) full cells, in which the high-loading LFP positive electrode serves primarily as the lithium reservoir. This design circumvents direct contact between AN and metallic lithium, thereby preventing the parasitic side reactions that would otherwise occur¹⁹. As shown in the Supplementary Fig. 25, the graphite||LFP cell assembled with the commercial BE electrolyte delivers three characteristic lithiation plateaus, in sharp contrast to the cell using the low-concentration LiFSI/AN electrolyte, which proves incompatible with the graphite electrode.

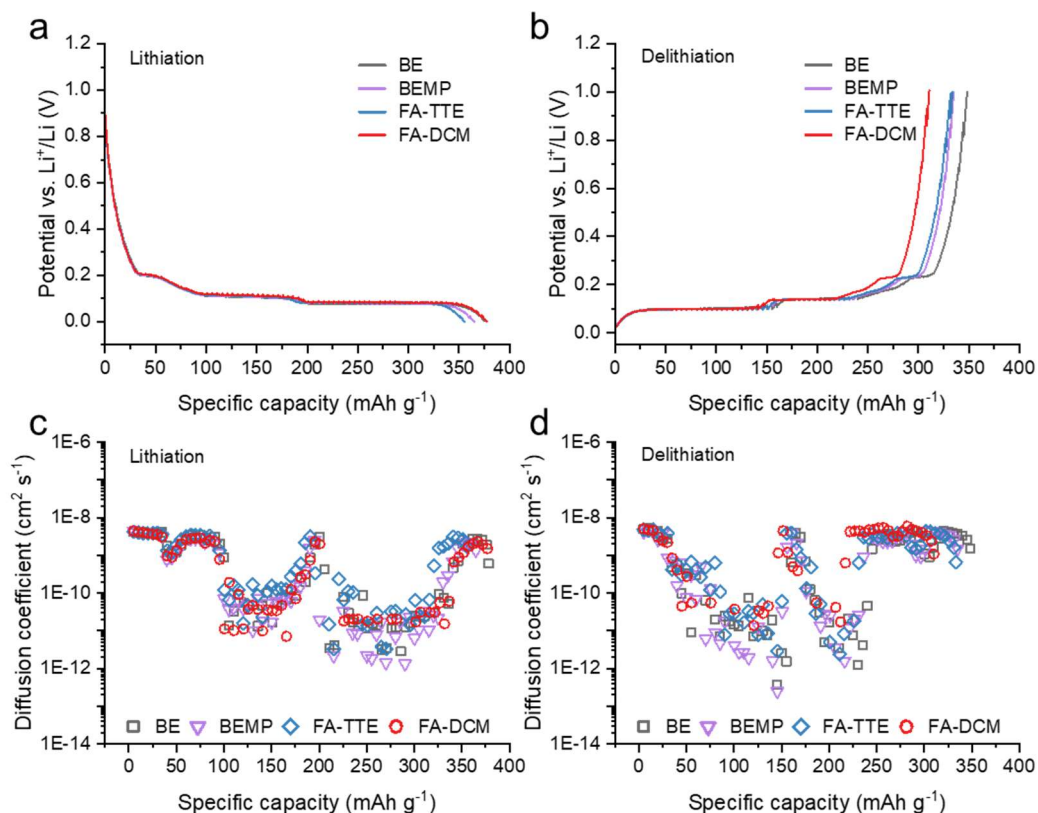


Supplementary Fig. 26 | Impedance evaluations. Electrochemical impedance spectra of Li||graphite cells at different rates for BE electrolyte (a), FA-DCM electrolyte (c-d) and FA-TTE electrolyte (e-f) at 25 °C. In electrochemical impedance spectra, the solid lines represent the fits using an equivalent circuit (b), EIS were obtained at 0% SOC. Source data are provided as a Source Data file.

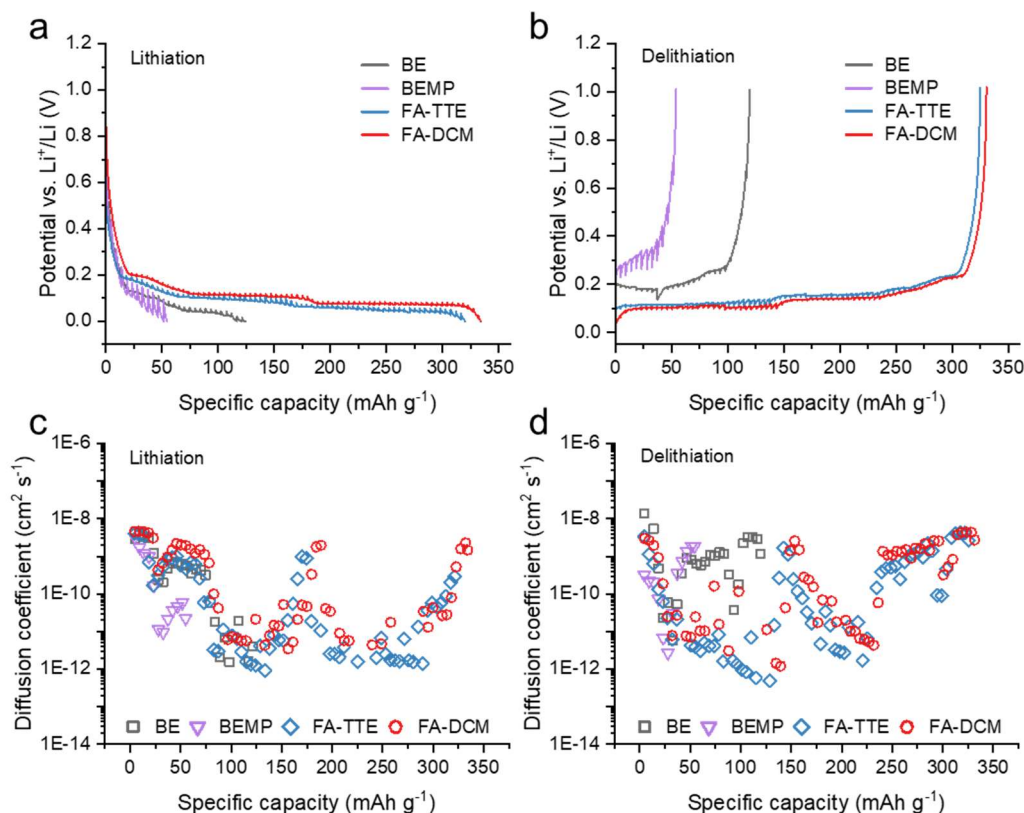


Supplementary Fig. 27 | GITT evaluations. Charge curves of the GITT measurements conducted after the 60th cycle of Li||graphite cells with different electrolytes at 10 C, 25 °C. The corresponding overpotentials obtained from GITT measurements are presented as box-and-whisker plots. The center line represents the median; the box limits indicate the upper and lower quartiles; whiskers extend to 1.5× the interquartile range; data points correspond to the overpotentials extracted from an individual GITT current pulse. $n = 6, 9, 14, 12$ for BEMP, BE, FA-TTE, FA-DCM electrolytes, respectively, where n denotes the number of constant-current pulses applied during the GITT measurements. Source data are provided as a Source Data file.

Notably, during the delithiation phase, the Li||graphite cells with FA-DCM electrolyte facilitates a specific capacity exceeding 317.3 mAh g⁻¹ (FA-TTE, 61.3 mAh g⁻¹; BEMP, 39.3 mAh g⁻¹; BE, 51.9 mAh g⁻¹). The overpotential of the Li||graphite cell with the commercial carbonate electrolyte is 240 mV, while the cell with the FA-DCM electrolyte shows a significantly lower overpotential of 89 mV.

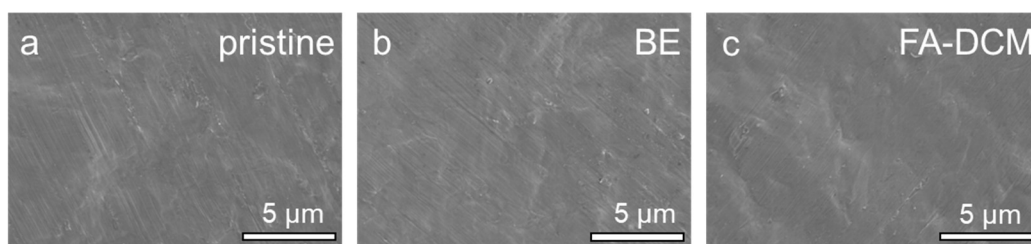


Supplementary Fig. 28 | GITT evaluations of Li||graphite (0.53 mAh cm⁻²). Curves of the GITT measurements conducted after the 60th cycle of Li||graphite (0.53 mAh cm⁻²) cells with different electrolytes at 0.1 C, 25 °C during lithiation (a) and delithiation (b). The calculated chemical diffusion coefficients of Li⁺ during lithiation (c) and delithiation (d). Source data are provided as a Source Data file.

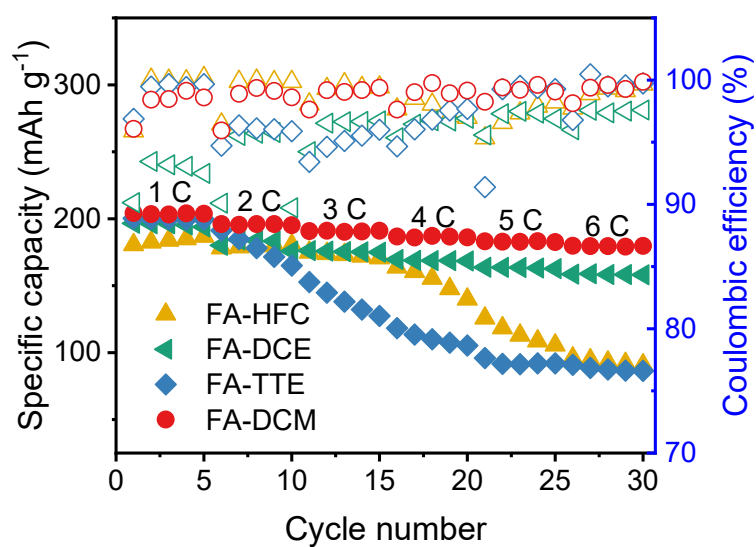


Supplementary Fig. 29 | GITT evaluations of Li||graphite (3.40 mAh cm⁻²).

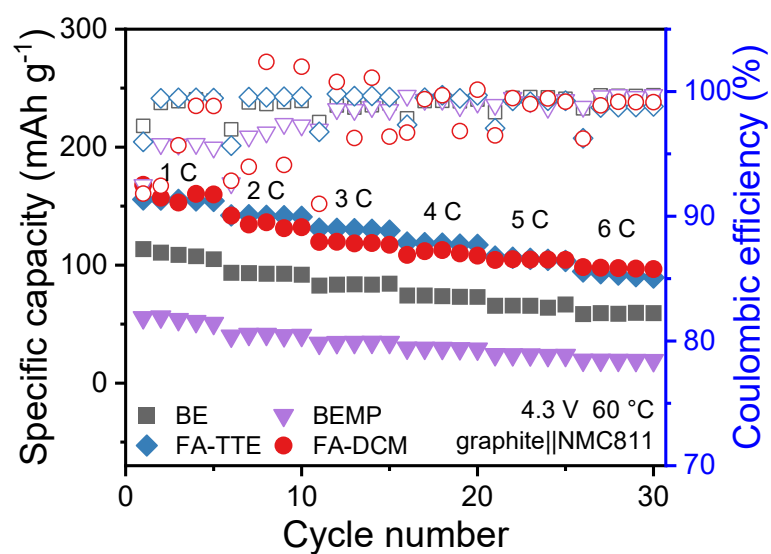
Curves of the GITT measurements conducted after the 60th cycle of Li||graphite (3.40 mAh cm⁻²) cells with different electrolytes at 0.1 C, 25 °C during lithiation (a) and delithiation (b). The calculated chemical diffusion coefficients of Li⁺ during lithiation (c) and delithiation (d). Source data are provided as a Source Data file.



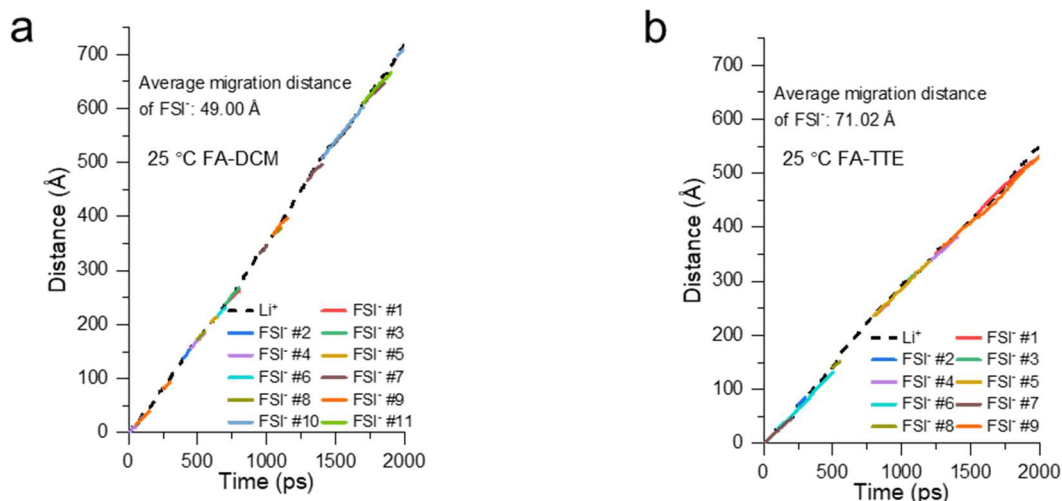
Supplementary Fig. 30 | The corrosivity of different electrolytes to Al foils. SEM images of pristine Al foils (a) and Al foils recovered from Li||Al cells held at 5.0 V, 25 °C for 24 h in BE (b) and FA-DCM (c) electrolytes. No corrosions were detected in neither BE or FA-DCM electrolytes. Scale bars, 5 μm. Source data are provided as a Source Data file.



Supplementary Fig. 31 | Rate performance of graphite||NMC811 cells with different electrolytes in the range of 2.8-4.5 V at 25 °C. Solid symbols correspond to capacity values (left y-axis), while open symbols correspond to Coulombic efficiency (right y-axis). Source data are provided as a Source Data file.

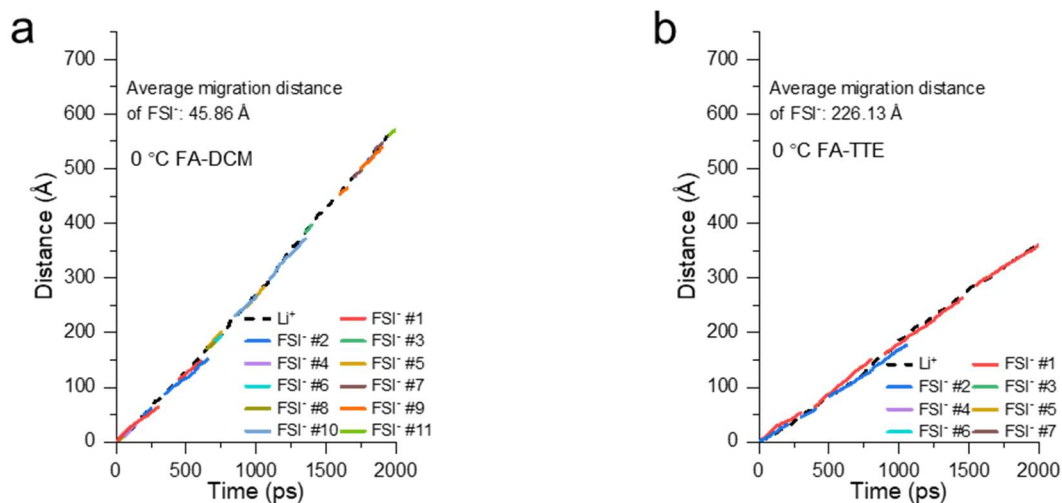


Supplementary Fig. 32 | Rate performance of graphite||NMC811 cells with different electrolytes in the range of 2.8-4.3 V at 60 °C. Solid symbols correspond to capacity values (left y-axis), while open symbols correspond to Coulombic efficiency (right y-axis). Source data are provided as a Source Data file.



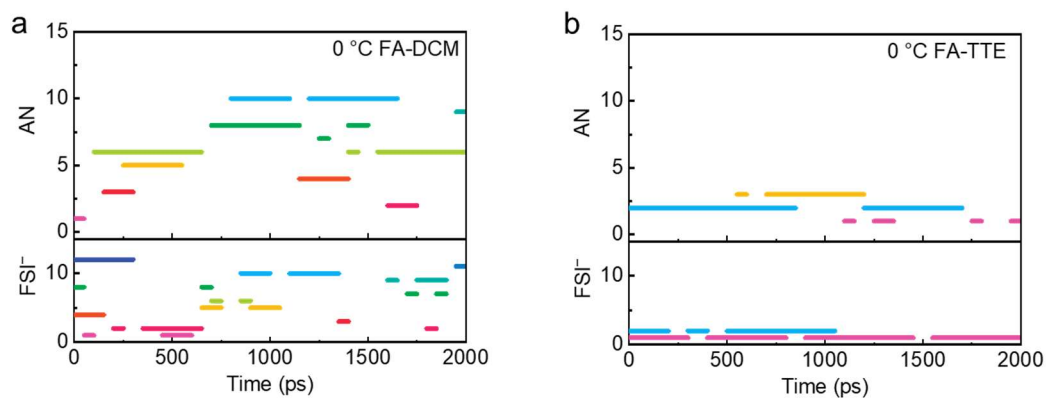
Supplementary Fig. 33 | MD simulations. Li⁺-anion correlated motion in FA-DCM (a) and FA-TTE electrolyte (b) at 25 °C. Source data are provided as a Source Data file.

To specifically address the role of Li⁺-anion correlated motions, we carried out MD simulations to quantify the average interaction distance between Li⁺ and each coordinating anion. In the FA-DCM electrolyte, the mean Li⁺-anion interaction distance was calculated to be 49.0 Å, which is notably shorter than that observed in the FA-TTE electrolyte (71.0 Å). This closer spacing reflects more frequent but transient Li⁺-anion encounters, which facilitate efficient hopping rather than long-lived ion-pair drag.

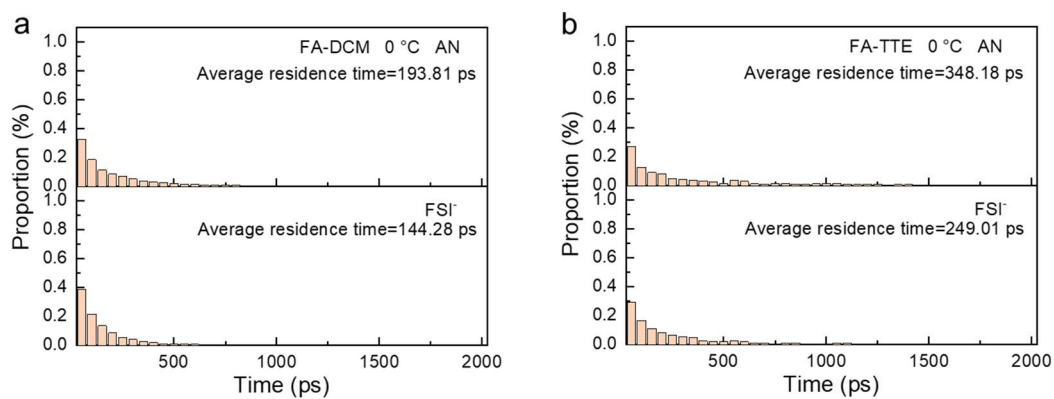


Supplementary Fig. 34 | MD simulations. Li⁺-anion correlated motion in FA-DCM (a) and FA-TTE electrolyte (b) at 0 °C. Source data are provided as a Source Data file.

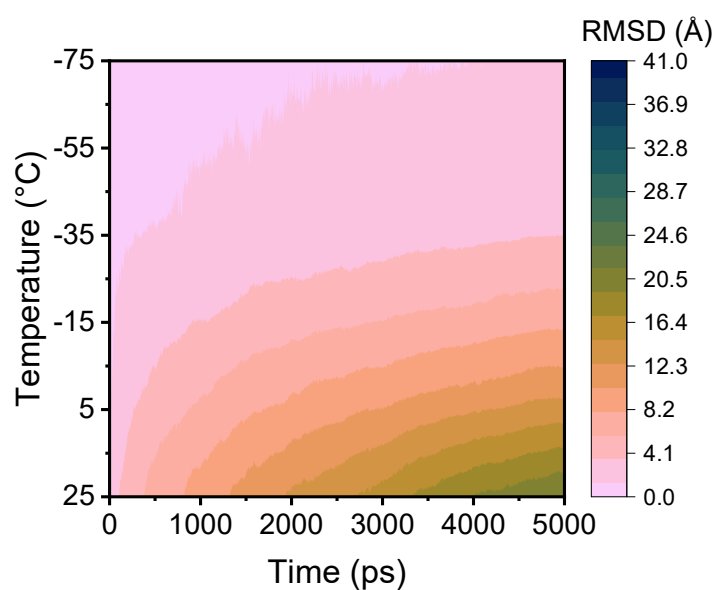
Importantly, this trend persists at lower temperature (0 °C), indicating that FA-DCM systems (45.86 Å) preserve favorable solvation dynamics even under kinetically demanding conditions, while the interaction between Li⁺-anions in the FA-TTE electrolyte become more heavily (226.13 Å), impeding the transfer of Li⁺.



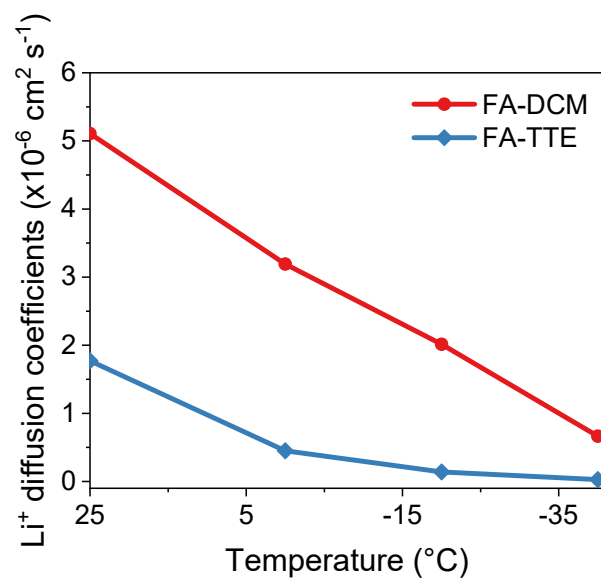
Supplementary Fig. 35 | Evolution of Li^+ solvation environment in FA-DCM (a) and FA-TTE electrolyte (b) from MD simulations at 273K. The vertical axis represents the serial number of different solvents or anions coordinated with the investigated Li^+ in the simulation time of 2,000 ps. Source data are provided as a Source Data file.



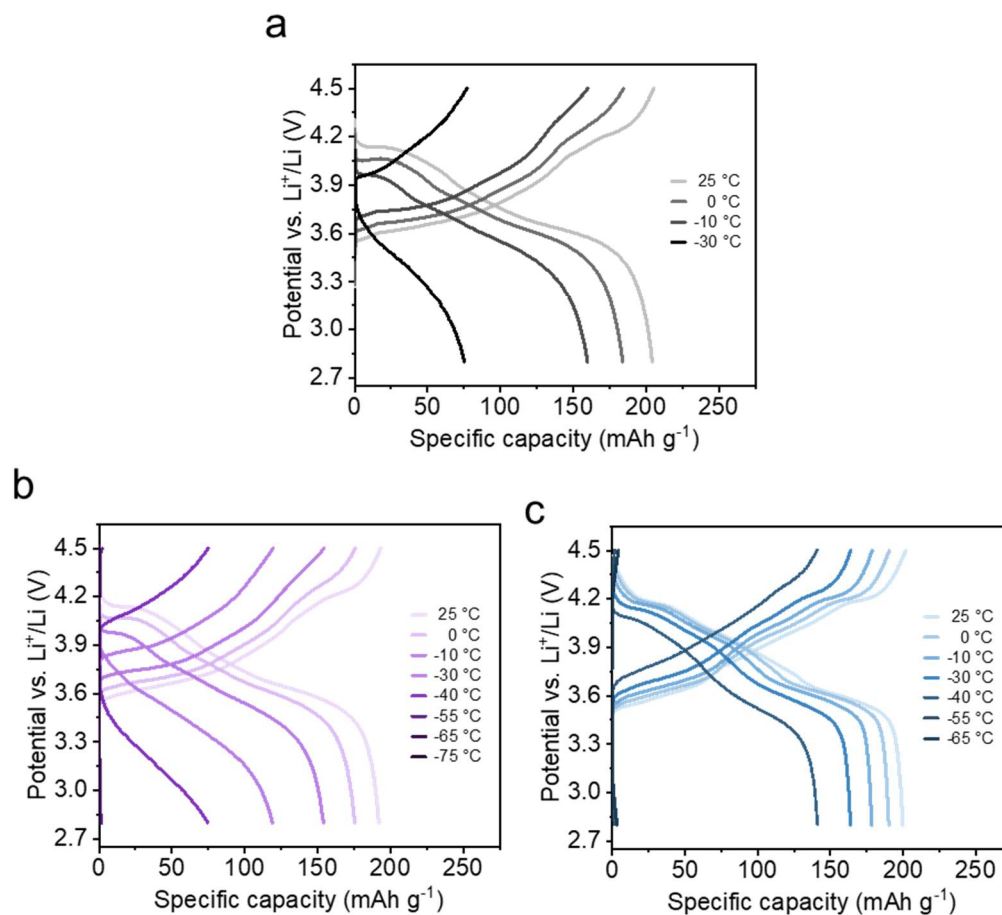
Supplementary Fig. 36 | MD simulations. Residence time distribution of AN and FSI⁻ in FA-DCM (a) and FA-TTE electrolyte (b) at 273K. Source data are provided as a Source Data file.



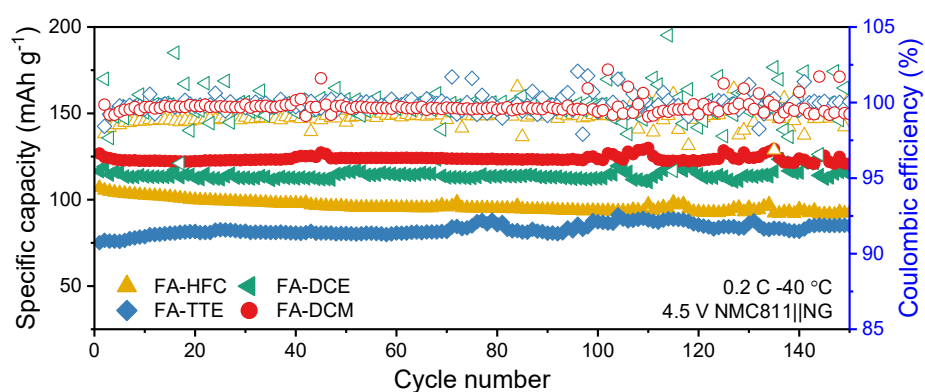
Supplementary Fig. 37 | MD simulations. Temperature- and time- dependence of Li^+ root mean square displacement (RMSD) in FA-TTE electrolyte, color bar represents the magnitude of the Li^+ RMSD (in $\text{\AA}$), with darker colors indicating larger displacements. Source data are provided as a Source Data file.



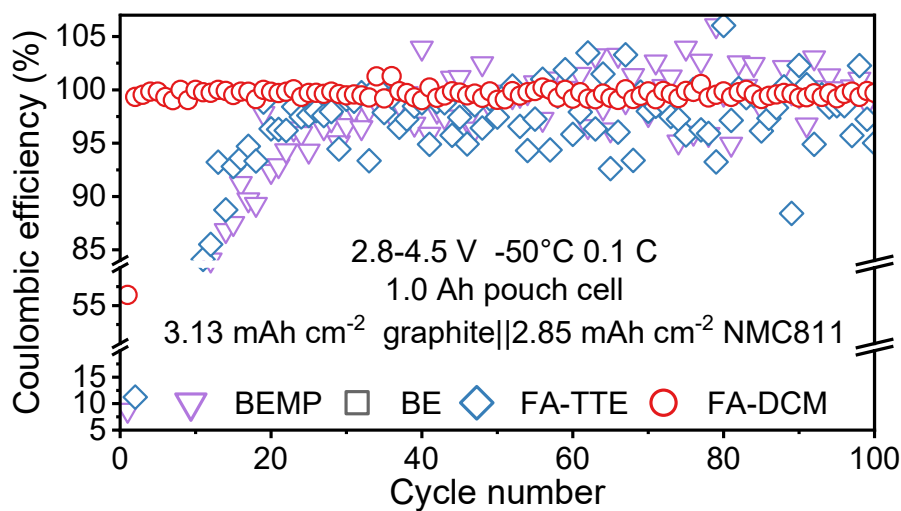
Supplementary Fig. 38| MD simulations. Li⁺ diffusion coefficients varied with temperatures in different electrolytes. Source data are provided as a Source Data file.



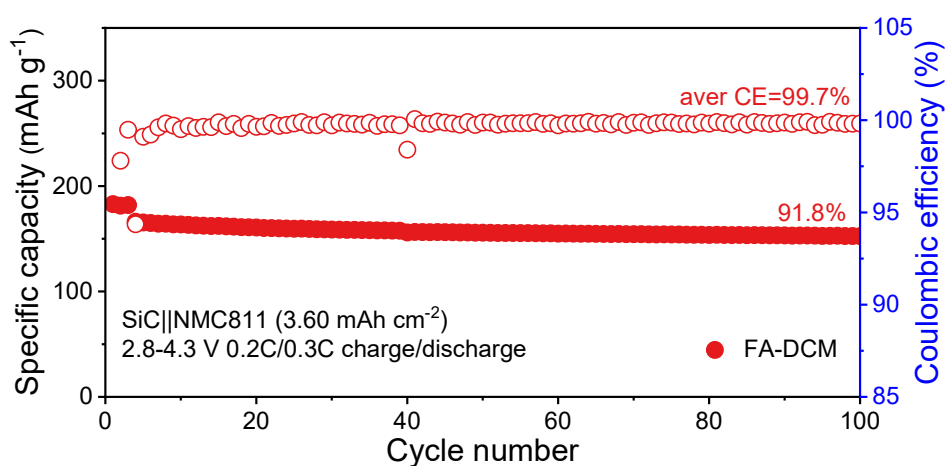
Supplementary Fig. 39 | The charge/discharge curves of graphite||NMC811 full cells with different electrolytes at 0.1 C under varied temperatures. BE electrolyte (a), BEMP electrolyte (b), and FA-TTE electrolyte (c). Source data are provided as a Source Data file.



Supplementary Fig. 40 | Cycling performance with different electrolytes in the range 2.8-4.5 V at 0.2 C under -40 °C. Solid symbols correspond to capacity values (left y-axis), while open symbols correspond to Coulombic efficiency (right y-axis). Source data are provided as a Source Data file.

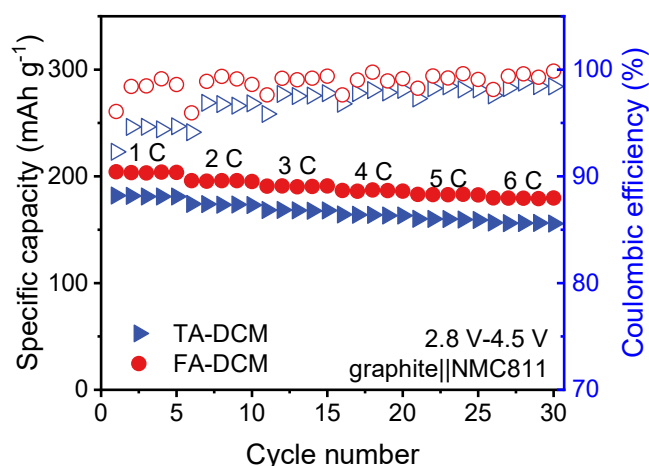


Supplementary Fig. 41 | Cycling performance of graphite||NMC811 pouch cells with different electrolytes in the range of 2.8-4.5 V at -50 °C. To improve data readability, the coulombic efficiency is plotted with a broken y-axis: the main axis range (85-105%) highlights the steady-state cycling behavior, while the lower segment displays the initial cycles with coulombic efficiency below 90%. Source data are provided as a Source Data file.



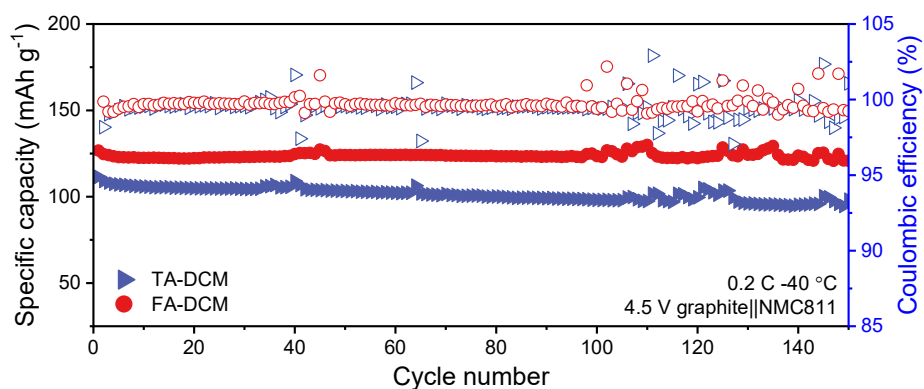
Supplementary Fig. 42 | Cycling performance of SiC||NMC811 (3.60 mAh cm⁻²) cell with FA-DCM electrolytes in the range of 2.8-4.3 V at 25 °C. Solid symbols correspond to capacity values (left y-axis), while open symbols correspond to Coulombic efficiency (right y-axis). Source data are provided as a Source Data file.

The applicability of our DCM-mediated solvation strategy can be extended beyond graphite to high-capacity Si negative electrodes. As shown in Supplementary Fig. 42, after 100 cycles, the cells retained 91.8% of their initial capacity with an average Coulombic efficiency of 99.7%.



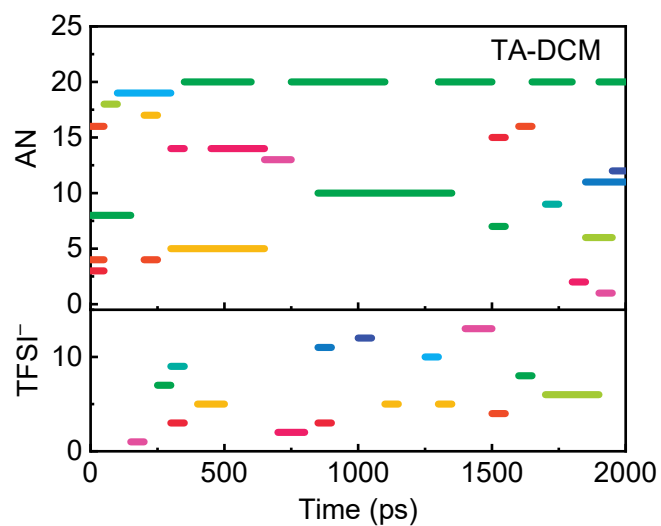
Supplementary Fig. 43 | Rate performance of graphite||NMC811 cells with different electrolytes in the range of 2.8-4.5 V at 25 °C. Solid symbols correspond to capacity values (left y-axis), while open symbols correspond to Coulombic efficiency (right y-axis). Source data are provided as a Source Data file.

To disentangle the respective effects of the LiFSI salt and the DCM moderator, we additionally prepared an electrolyte with lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) replacing LiFSI. Graphite||NMC811 full-cell tests with this LiTFSI-based electrolyte (“TA-DCM electrolyte” for short) demonstrate that the incorporation of DCM still enables stable operation under high-rate 6 C conditions.

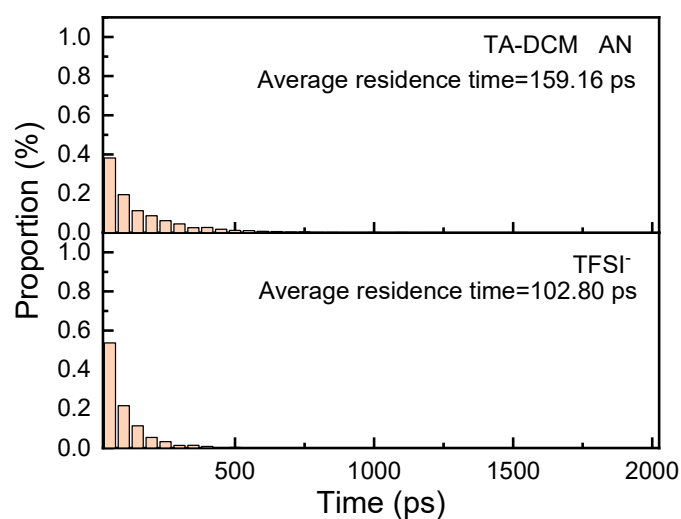


Supplementary Fig. 44 | Cycling performance with different electrolytes in the range 2.8-4.5 V at 0.2 C under -40 °C. Solid symbols correspond to capacity values (left y-axis), while open symbols correspond to Coulombic efficiency (right y-axis). Source data are provided as a Source Data file.

Graphite||NMC811 full-cell tests with TA-DCM electrolyte demonstrate that the incorporation of DCM still enhances low-temperature (-40 °C) cycling.

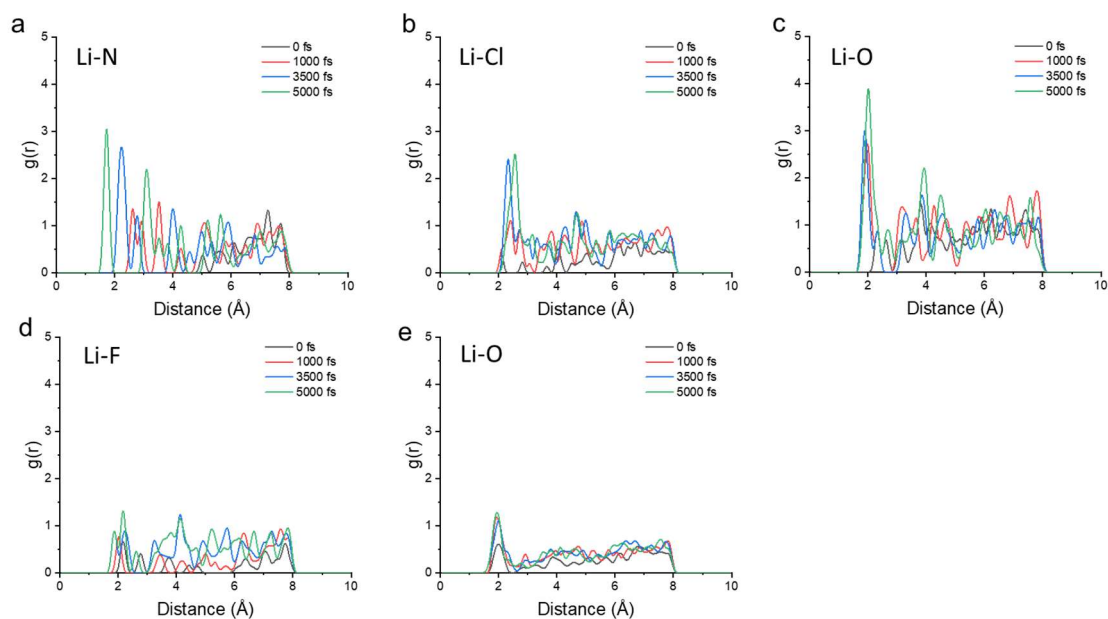


Supplementary Fig. 45 | Evolution of Li⁺ solvation environment in TA-DCM electrolyte from MD simulations at 298 K. The vertical axis represents the serial number of different solvents or anions coordinated with the investigated Li⁺ in the simulation time of 2,000 ps. Source data are provided as a Source Data file.

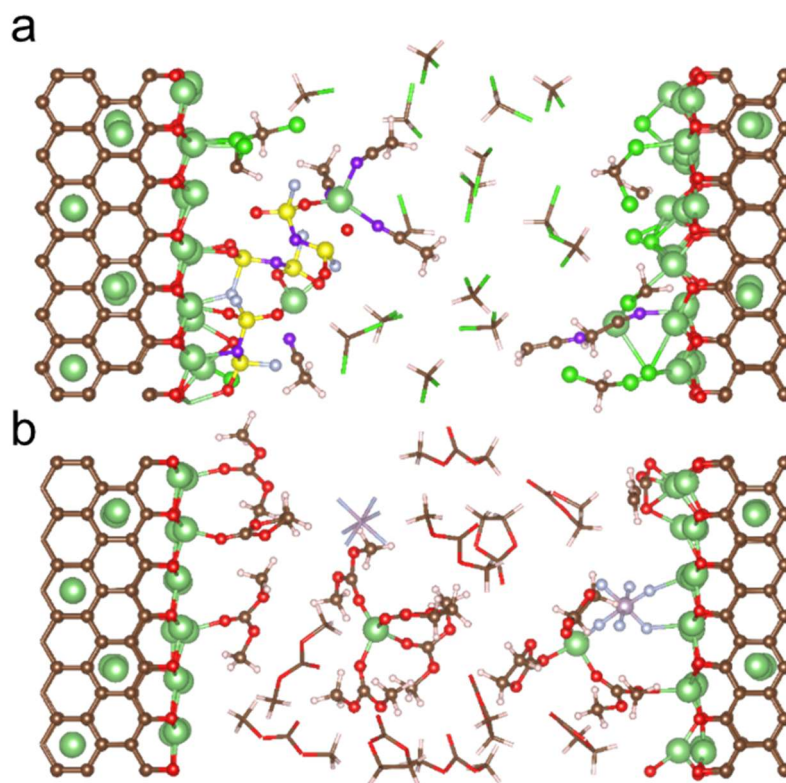


Supplementary Fig. 46 | MD simulations. Residence time distribution of AN and FSI⁻ in TA-DCM electrolyte at 298K. Source data are provided as a Source Data file.

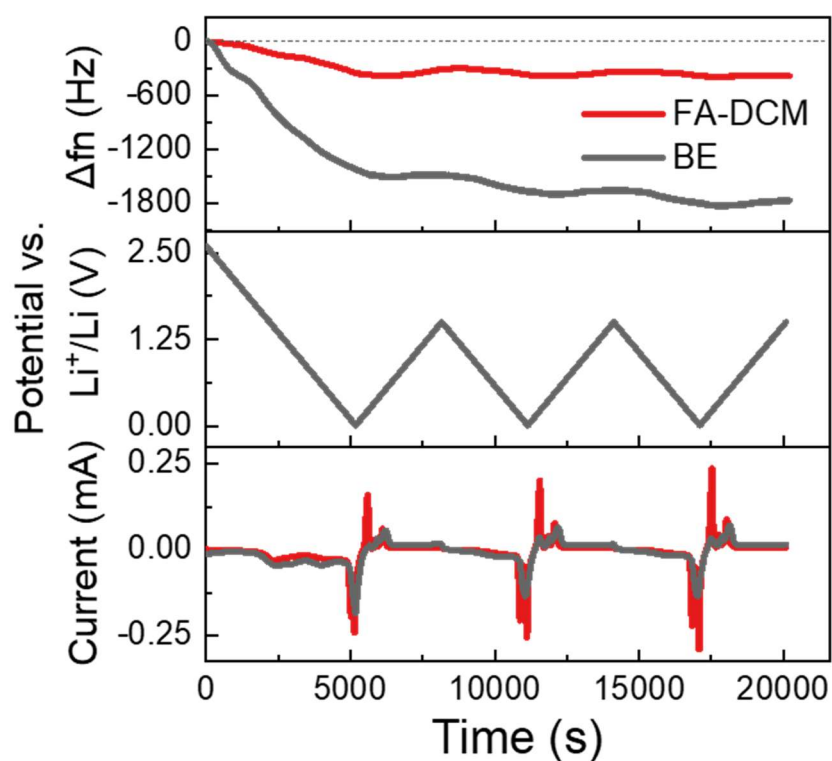
MD simulations reveal a shortened Li⁺ residence time consistent with the disruption of large solvation clusters, in line with our proposed mechanism. These results confirm that the beneficial role of DCM as a moderator is not exclusively dependent on the choice of LiFSI salt, but represents a generalizable strategy for tailoring solvation structure and improving ion transport under demanding conditions (Supplementary Fig. 45 and 46).



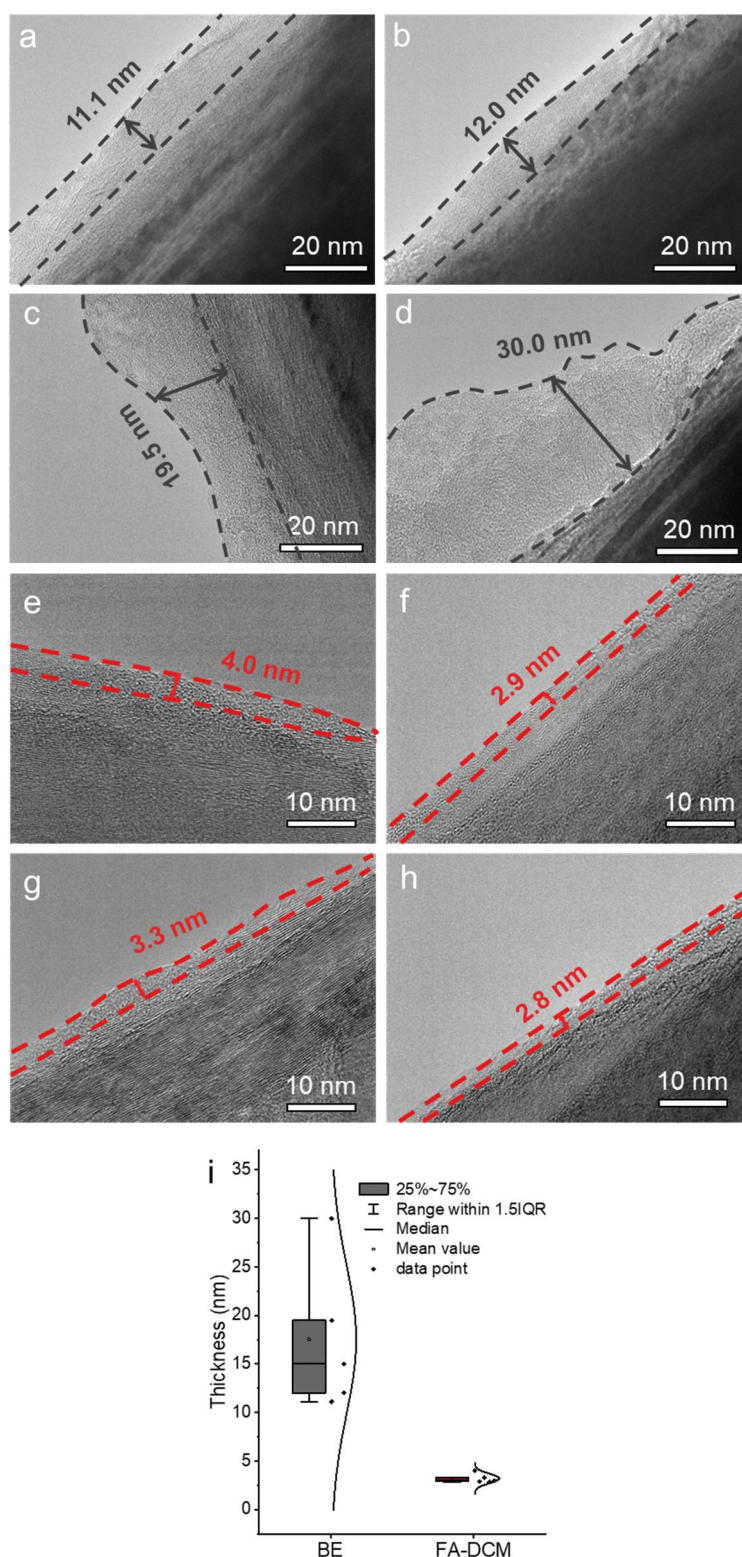
Supplementary Fig. 47 | AIMD simulations. RDF curves of FA-DCM electrolyte Li-N (AN) species (a), Li-Cl (DCM) species (b), Li-O (FSI⁻) species (c) and BE electrolyte Li-F (PF₆⁻) species (d), Li-O (EC, DMC) species (e). Source data are provided as a Source Data file.



Supplementary Fig. 48 | The initial decomposition reaction of different electrolytes on the negative electrode interphase calculated by AIMD. FA-DCM electrolyte (a) and BE electrolyte (b), lime green, Cl atom; red, O atom; yellow, S atom; purple, N atom; silver, F atom; tan, C atom; white, H atom. The data are provided in Supplementary Data 3. Source data are provided as a Source Data file.



Supplementary Fig. 49 | *in-situ* EQCM-D evaluations. EQCM-D profiles of frequency baseline shift (Δf_n) versus time (top), frequency is taken at the 3rd overtone ($n = 3$). The corresponding and potential versus time (medium) current versus time (bottom). Cells are scanned at a potential window from open circuit voltage to 0.01 V and then back to 1.50 V (vs. Li^+/Li) at a scan rate of 5 mV s^{-1} , at 25°C for 3 cycles. Source data are provided as a Source Data file.

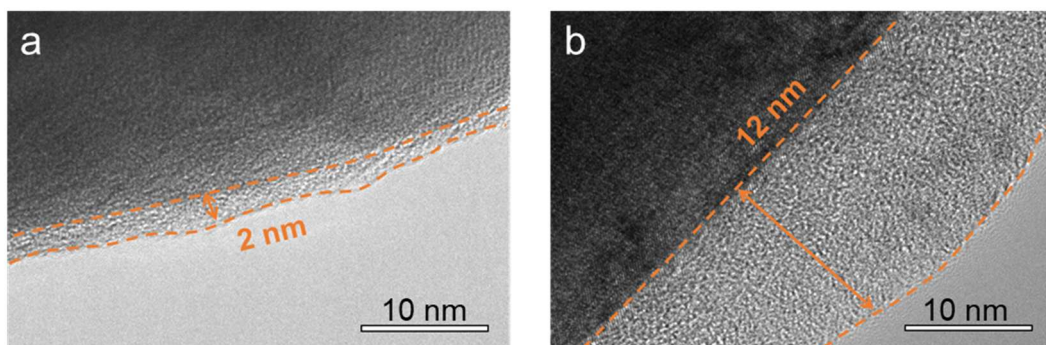


Supplementary Fig. 50 | TEM characterizations. TEM images of multiple graphite particles recovered from graphite||NMC811 cells using BE electrolyte (a-d) and FA-DCM electrolyte (e-h) after 100 cycles at 0.5 C, 25 °C. Data are presented as box-and-

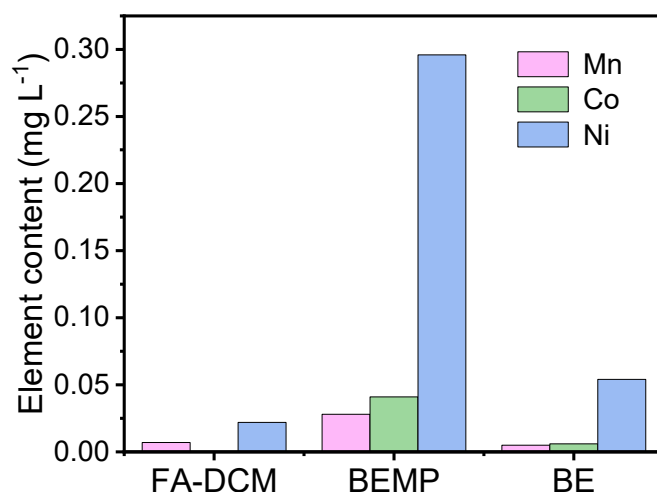
whisker plots overlaid with normal distribution curves to illustrate data distribution (i). Source data are provided as a Source Data file.

The center line of each box indicates the median; the box limits represent the upper and lower quartiles; whiskers extend to $1.5\times$ the interquartile range; points denote individual measurements. The overlaid curves represent fitted normal distributions based on the corresponding datasets. The number of independent samples is $n = 5$ for each electrolyte.

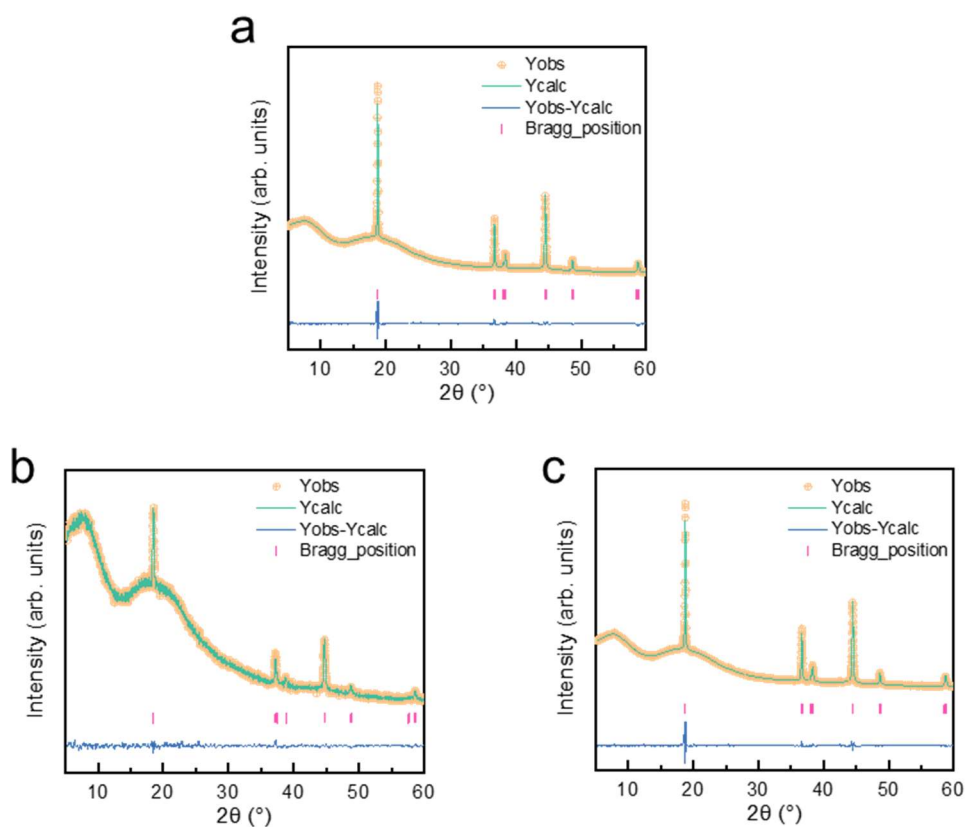
Statistical analysis of TEM images reveals that the BE electrolyte forms a thick, non-uniform SEI (17.52 ± 7.71 nm) on graphite, significantly thicker than the uniform SEI (3.20 ± 0.48 nm) formed by the FA-DCM electrolyte.



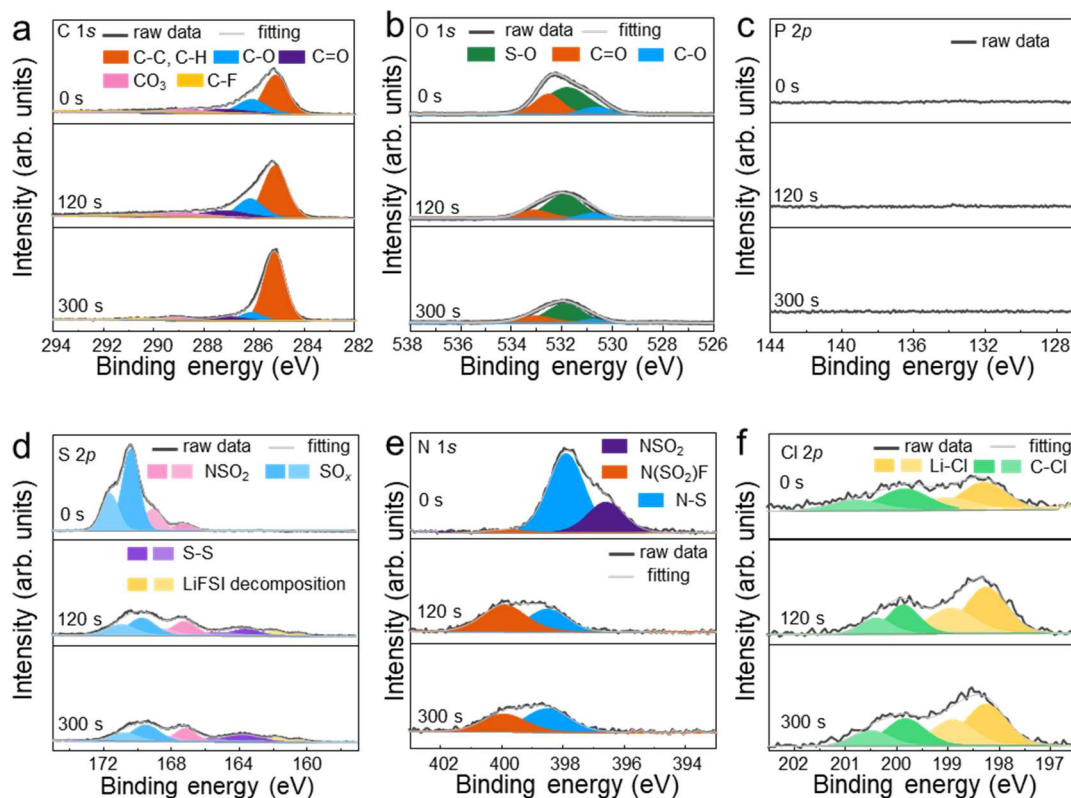
Supplementary Fig. 51 | TEM characterizations. TEM images of NMC811 Positive electrodes recovered from graphite||NMC811 cells using FA-DCM electrolyte (a) and BE electrolyte (b) after 100 cycles at 0.5 C, 25 °C. Scale bars, 10 nm.



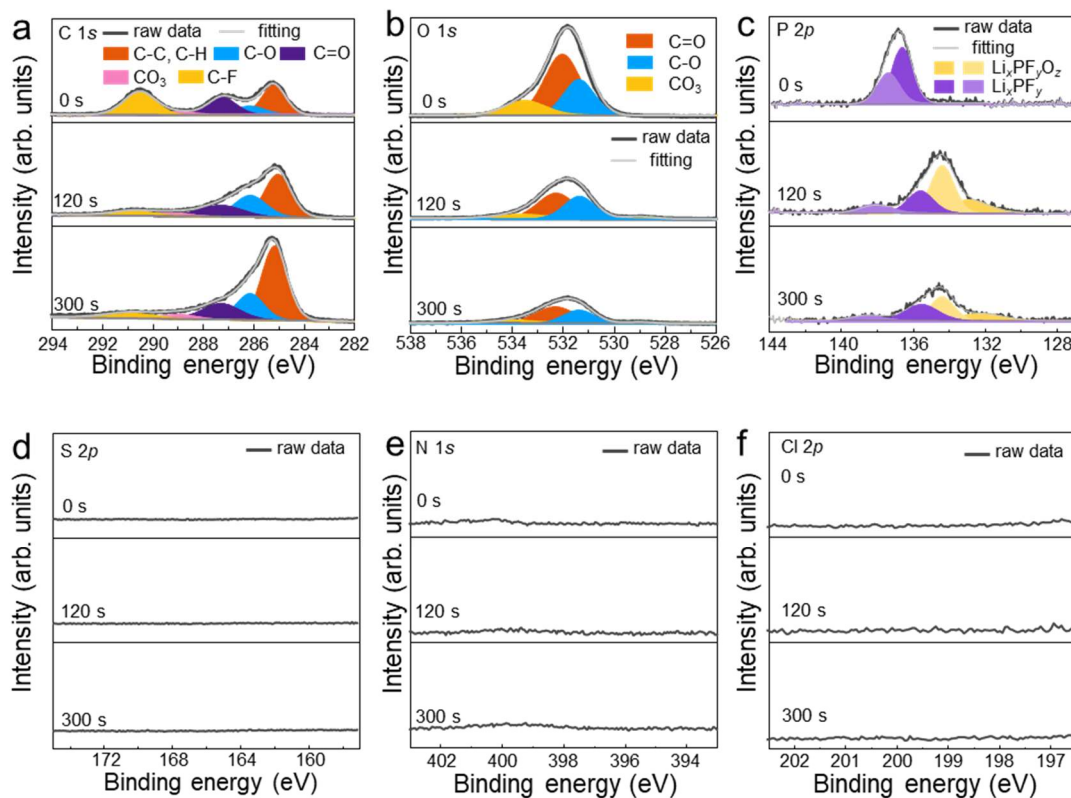
Supplementary Fig. 52 | ICP-OES evaluations. Transition metal (Mn, Co and Ni) dissolution of fully-charged-state NMC811 positive electrodes recovered from graphite||NMC811 cells using different electrolyte after 100.5 cycles at 0.5 C, 25 °C, which were measured using inductively coupled plasma optical emission spectrometer. Source data are provided as a Source Data file.



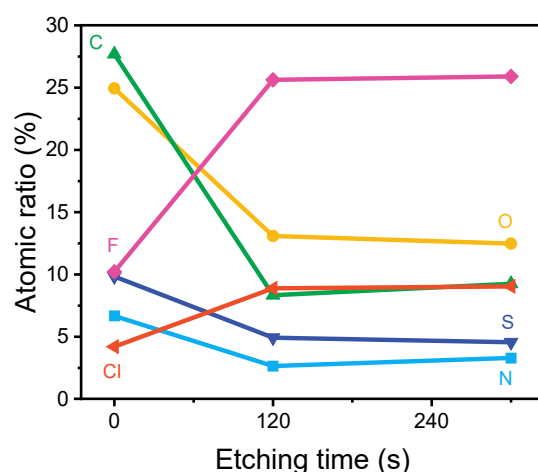
Supplementary Fig. 53 | XRD refinement patterns. Pristine NMC811 (a) and NMC811 positive electrode recovered from graphite||NMC811 cells using BE (b) and FA-DCM electrolyte (c) after 100 cycles at 0.5 C, 25 °C. Source data are provided as a Source Data file.



Supplementary Fig. 54 | XPS analysis of SEI in FA-DCM electrolyte. XPS spectra of C 1s (a), O 1s (b), P 2p (c), S 2p (d), N 1s (e) and Cl 2p (f) for graphite negative electrodes recovered from graphite||NMC811 cells using FA-DCM electrolyte after 100 cycles at 0.5 C, 25 °C. Source data are provided as a Source Data file.

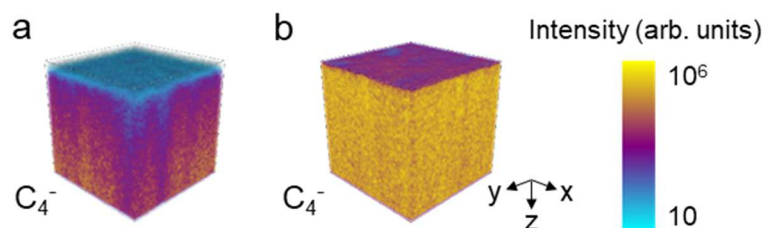


Supplementary Fig. 55 | XPS analysis of SEI in BE electrolyte. XPS spectra of C 1s (a), O 1s (b), P 2p (c), S 2p (d), N 1s (e) and Cl 2p (f) for cycled graphite negative electrode recovered from graphite||NMC811 cells using BE electrolyte after 100 cycles at 0.5 C, 25 °C. Source data are provided as a Source Data file.



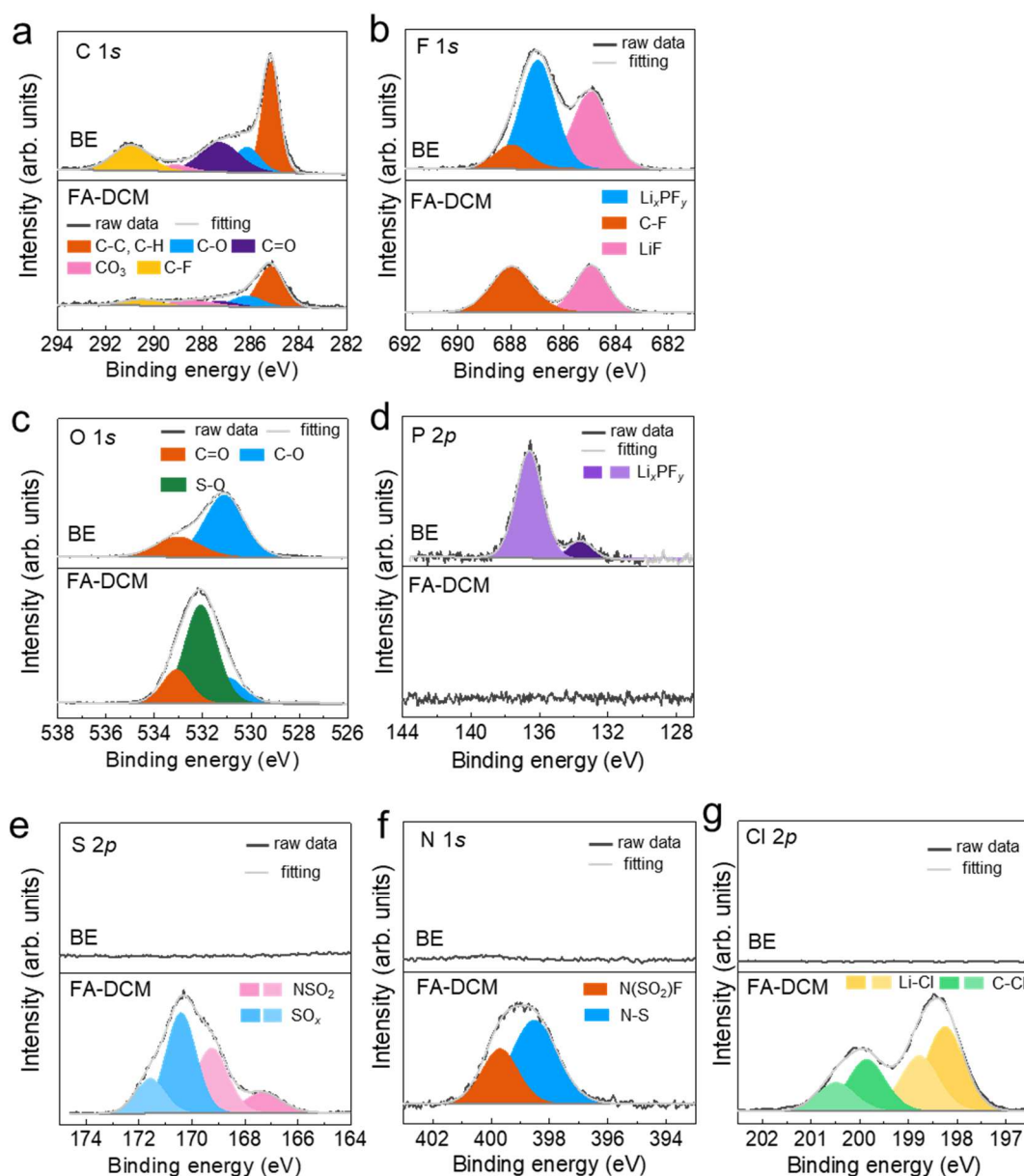
Supplementary Fig. 56 | Distribution analysis of atomic concentration. The atomic concentration percentage of the SEI composition after different durations of Ar^+ sputtering on graphite negative electrode recovered from graphite||NMC811 cells using FA-DCM electrolyte after 100 cycles at 0.5 C, 25 °C. Source data are provided as a Source Data file.

To provide a more quantitative understanding of the SEI composition, we analyzed the XPS depth profiles at a sputtering time of 300 s, where the atomic ratios reach a relatively stable state. Based on the atomic concentrations at this depth and the corresponding peak assignments to inorganic (like LiF, LiCl) and organic (like ROCO_2Li , polymeric carbonates) species, we estimated the relative contributions of the inorganic and organic fractions. The detailed atomic composition and the calculated organic/inorganic ratio are summarized in Supplementary Table 10. The results indicate an inorganic-to-organic ratio of ~ 2.4 , confirming that the SEI formed in the FA-DCM electrolyte is dominated by inorganic species (LiF and LiCl), which is consistent with its superior stability and ionic transport properties.

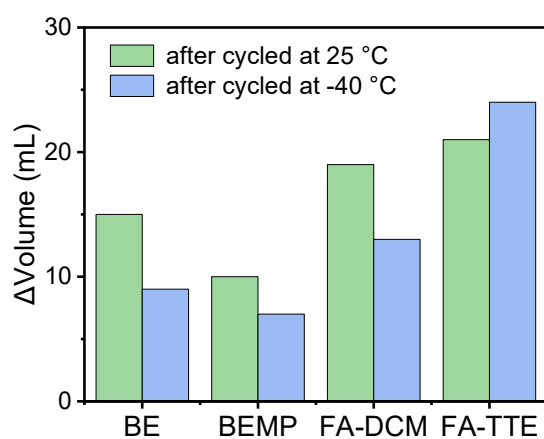


Supplementary Fig. 57 | TOF-SIMS. 3D-rendering images of C_4^- species on the graphite negative electrode surface recovered from graphite||NMC811 cells using FA-DCM electrolyte (a) and BE electrolyte (b) after 100 cycles at 0.5 C, 25 °C, the color bar represents the range of signal intensity corresponding to the pixel colors in the image. The analysis area was $100 \times 100 \mu\text{m}^2$ and 820 s etching time. Source data are provided as a Source Data file.

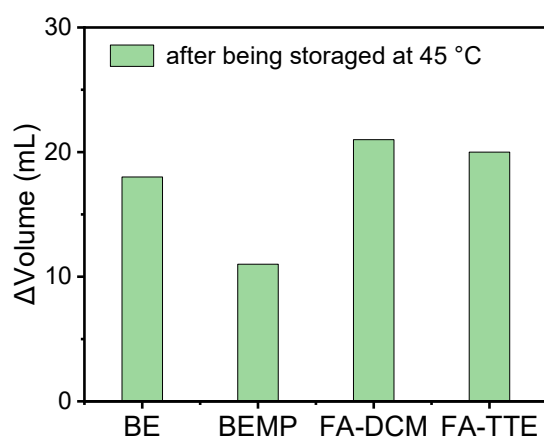
On the graphite surface cycled in the FA-DCM electrolyte, a dense SEI layer is formed, and with increasing depth, partial derivatives are also detected between the graphite layers; in contrast, graphite cycled in the BE electrolyte predominantly exhibits a strong C signal.



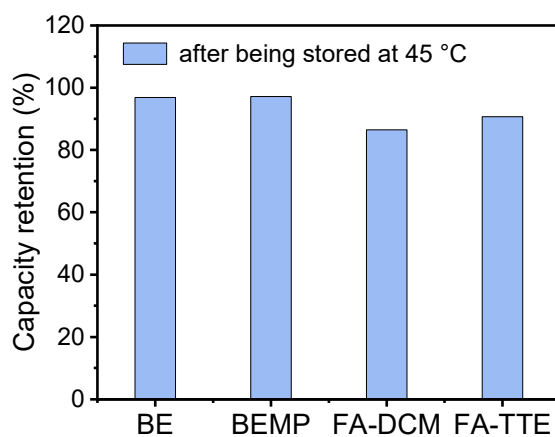
Supplementary Fig. 58 | XPS analysis of CEI. XPS spectra of C 1s (a), F 1s (b), O 1s (c), P 2p (d), S 2p (e), N 1s (f) and Cl 2p (g) for cycled NMC811 positive electrode recovered from graphite||NMC811 cells using BE electrolyte (top) and FA-DCM electrolyte (bottom) after 100 cycles at 0.5 C, 25 °C after 50 cycles at 0.5 C, 25 °C. Source data are provided as a Source Data file.



Supplementary Fig. 59 | Gas generation test. The change in volume of gas bag in the graphite||NMC811 pouch cells before and after 50 cycles at 0.1 C under different temperatures using different electrolytes. Source data are provided as a Source Data file.



Supplementary Fig. 60 | Gas generation test. The change in volume of gas bag in the graphite||NMC811 pouch cells before and after being stored at 45 °C for 7 days in different electrolytes. Prior to placement in the constant-temperature oven, the pouch cells were preconditioned by cycling at 0.1 C and 25 °C for three cycles. Source data are provided as a Source Data file.



Supplementary Fig. 61 | Capacity retention of the graphite||NMC811 pouch cells after being stored at 45 °C for 7 days in different electrolytes. Prior to placement in the constant-temperature oven, the pouch cells were preconditioned by cycling at 0.1 C and 25 °C for three cycles. Electrochemical testing was then performed at 0.1 C and 25 °C, and the corresponding discharge capacity was defined as C_1 . After removal from the constant-temperature oven, the cells were allowed to equilibrate back to 25 °C. Subsequently, the cells were cycled again at 0.1 C and 25 °C for three cycles, and the discharge capacity was recorded as C_2 . The capacity retention was calculated as the ratio of C_2 to C_1 , multiplied by 100%. Source data are provided as a Source Data file.

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