

Supporting Information for

**Design of sulfonimide anions for rechargeable lithium batteries**

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Table S1. Summarization of historical development of sulfonimide anions utilized as rechargeable lithium batteries.

Entry	Year	Abbreviation	Sulfonimide anion	Ref.
1	1962	HFSI	$[(\text{FSO}_2)_2\text{N}]\text{H}$	1
		AgFSI	$[(\text{FSO}_2)_2\text{N}]\text{Ag}$	
2	1965	KFSI	$[(\text{FSO}_2)_2\text{N}]\text{K}$	2
		RbFSI	$[(\text{FSO}_2)_2\text{N}]\text{Rb}$	
		CsFSI	$[(\text{FSO}_2)_2\text{N}]\text{Cs}$	
3	1972	HTFSI	$[(\text{CF}_3\text{SO}_2)_2\text{N}]\text{H}$	3
4	1983	NaTFSI	$[(\text{CF}_3\text{SO}_2)_2\text{N}]\text{Na}$	4
5	1989	HTNFSI	$[(\text{CF}_3\text{SO}_2)(n\text{-C}_4\text{F}_9\text{SO}_2)\text{N}]\text{H}$	5
		AgTNFSI	$[(\text{CF}_3\text{SO}_2)(n\text{-C}_4\text{F}_9\text{SO}_2)\text{N}]\text{Ag}$	
6	1990	KTNFSI	$[(\text{CF}_3\text{SO}_2)(n\text{-C}_4\text{F}_9\text{SO}_2)\text{N}]\text{K}$	6
		CsTNFSI	$[(\text{CF}_3\text{SO}_2)(n\text{-C}_4\text{F}_9\text{SO}_2)\text{N}]\text{Cs}$	
7	1992	Substituent	$=\text{NSO}_2\text{CF}_3$ $[(\text{CF}_3\text{CF}_2\text{SO}_2)_2\text{N}]\text{H}$ $[(\text{CF}_3\text{CF}_2\text{SO}_2)(\text{CF}_3\text{SO}_2)\text{N}]\text{H}$ $[(\text{CF}_3\text{CF}_2\text{CF}_2\text{SO}_2)_2\text{N}]\text{H}$	7
8	1993		$[(\text{CF}_3\text{SO}_2)(\text{CF}_3\text{CF}_2\text{CF}_2\text{SO}_2)\text{N}]\text{H}$ $[(\text{CF}_3\text{SO}_2)(\text{CFCI}=\text{CF}_2\text{CF}_2\text{SO}_2)\text{N}]\text{H}$ $[(\text{CF}_3\text{SO}_2)(\text{CF}_2=\text{CFC}_2\text{F}_4\text{SO}_2)\text{N}]\text{H}$ $[(\text{CF}_3\text{CCl}_2\text{SO}_2)_2\text{N}]\text{H}$	8
9	1995	LiFSI	$[(\text{FSO}_2)_2\text{N}]\text{Li}$	9
		LiTFSI	$[(\text{CF}_3\text{SO}_2)_2\text{N}]\text{Li}$	
10	1997	LiBETI	$[(\text{CF}_3\text{CF}_2\text{SO}_2)_2\text{N}]\text{Li}$ $[(\text{CF}_3\text{CH}_2\text{OSO}_2)_2\text{N}]\text{H}$	10
11	1997		$[(\text{CF}_3\text{CF}_2\text{CH}_2\text{OSO}_2)_2\text{N}]\text{H}$ $[(\text{HCF}_2\text{CF}_2\text{CH}_2\text{OSO}_2)_2\text{N}]\text{H}$ $[(\text{CF}_3)_2\text{CHSO}_2)_2\text{N}]\text{H}$ $[(\text{CF}_3\text{SO}_2)(n\text{-C}_4\text{F}_9\text{SO}_2)\text{N}]\text{Li}$ $[(\text{CF}_3\text{SO}_2)(\text{C}_6\text{F}_5\text{SO}_2)\text{N}]\text{Li}$ $[(\text{CF}_3\text{SO}_2)(n\text{-C}_8\text{F}_{17}\text{SO}_2)\text{N}]\text{Li}$	11
12	1997		$[(\text{CF}_3\text{CHOSO}_2)_2\text{N}]\text{Li}$ $[(\text{CF}_3\text{CF}_2\text{CHOSO}_2)_2\text{N}]\text{Li}$ $[(\text{HCF}_2\text{CF}_2\text{CHOSO}_2)_2\text{N}]\text{Li}$ $[(\text{CF}_3)_2\text{CHOSO}_2)_2\text{N}]\text{Li}$	12
13	2002	$(\text{CF}_3\text{SO}_2)(\text{CF}_3\text{SO})\text{NM}$	$[(\text{CF}_3\text{SO}_2)(\text{CF}_3\text{SO})\text{N}]\text{K}$ $[(\text{CF}_3\text{SO}_2)(\text{CF}_3\text{SO})\text{N}]\text{Cs}$ $[\text{C}_6\text{H}_5\text{SO}(\text{NSO}_2\text{CF}_3)_2\text{N}]\text{K}$	13
14	2005		$[(\text{C}_6\text{H}_5\text{SO}(\text{NSO}_2\text{CF}_3))(\text{CF}_3\text{SO}(\text{NSO}_2\text{CF}_3))\text{N}]\text{K}$ $[\text{CF}_3\text{SO}(\text{NSO}_2\text{CF}_3)_2\text{N}]\text{K}$ $[(\text{CF}_3\text{SO}_2)(\text{CF}_3\text{SO}(\text{NSO}_2\text{CF}_3))\text{N}]\text{K}$	14
		LiFPFSI	$[(\text{FSO}_2)(\text{C}_2\text{F}_5\text{SO}_2)\text{N}]\text{Li}$	
		NaFPFSI	$[(\text{FSO}_2)(\text{C}_2\text{F}_5\text{SO}_2)\text{N}]\text{Na}$	
15	2010	KFPFSI	$[(\text{FSO}_2)(\text{C}_2\text{F}_5\text{SO}_2)\text{N}]\text{K}$	15
		RbFPFSI	$[(\text{FSO}_2)(\text{C}_2\text{F}_5\text{SO}_2)\text{N}]\text{Rb}$	
		CsFPFSI	$[(\text{FSO}_2)(\text{C}_2\text{F}_5\text{SO}_2)\text{N}]\text{Cs}$	
16	2011	LiFNFSI	$[(\text{FSO}_2)(n\text{-C}_4\text{F}_9\text{SO}_2)\text{N}]\text{Li}$ $[(\text{CF}_3\text{SO}_2)(\text{CH}_2=\text{CHC}_6\text{H}_4\text{SO}_2)\text{N}]\text{K}$	16
17	2011	KSTFSI	$-(\text{CH}_2\text{CHX})_n-$ , $\text{X} = [(\text{C}_6\text{H}_4\text{SO}_2\text{N}^{(-)}(\text{Li})\text{SO}_2\text{CF}_3)]$ ,	17,
		LiPSTFSI	$\text{LiPSTFSI}$	18

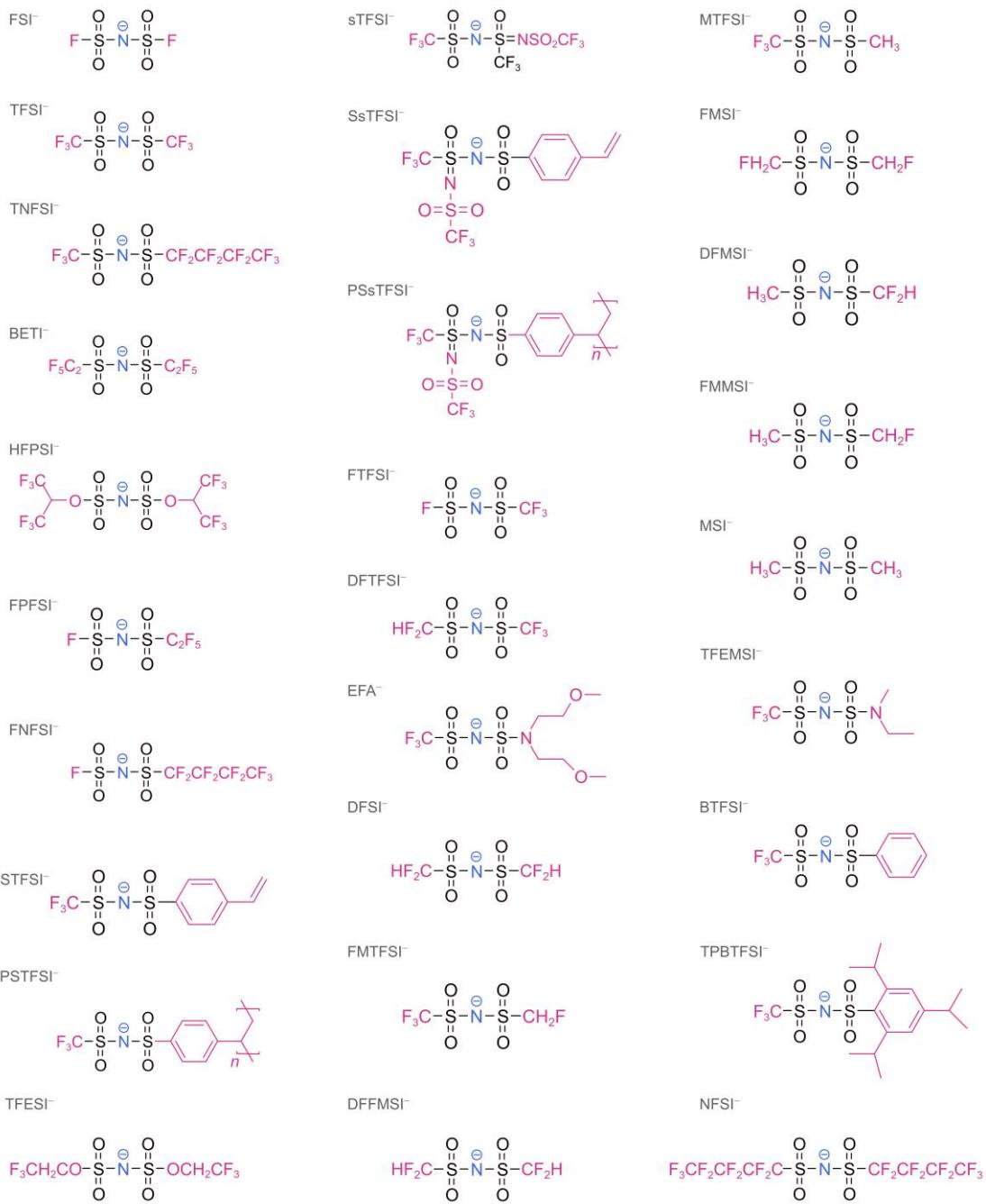
Table S1. Continued.

Entry	Year	Abbreviation	Sulfonimide anion	Ref.
18	2014	LiTFESI	$\{[(CF_3CH_2OSO_2)_2N]Li\}$	
		NaTFESI	$\{[(CF_3CH_2OSO_2)_2N]Na\}$	
		KTFESI	$\{[(CF_3CH_2OSO_2)_2N]K\}$	19
		RbTFESI	$\{[(CF_3CH_2OSO_2)_2N]Rb\}$	
19	2015	CsTFESI	$\{[(CF_3CH_2OSO_2)_2N]Cs\}$	
		LisTFSI	$\{[CF_3SO(=NSO_2CF_3)_2]Li\}$	20
20	2016	LiTNFSI	$\{[(CF_3SO_2)(n-C_4F_9SO_2)_2N]Li\}$	21
21	2016	KSSdTFSI	$\{[(CF_3SO(NSO_2CF_3))(CH_2=CHC_6H_4SO_2)_2N]K\}$	
		LiSSdTFSI	$\{[(CF_3SO(NSO_2CF_3))(CH_2=CHC_6H_4SO_2)_2N]Li\}$	
		LiPSsTFSI	$\{-(CH_2CHX)_n-, X = C_6H_4SO_2N^{(-)}(Li^+)SO_2CF_3\}, LiPSsTFSI$	22
22	2018	LiFTFSI	$\{[(FSO_2)(CF_3SO_2)_2N]Li\}$	23
23	2018	LiFPFSI	$\{[(FSO_2)(C_2F_5SO_2)_2N]Li\}$	24
24	2019	LiDFTFSI	$\{[(CF_3SO_2)(CF_2HSO_2)_2N]Li\}$	25
25	2019	LiEFA	$\{[(CF_3SO_2)((CH_3OC_2H_4)_2NSO_2)_2N]Li\}$	26
		LiFMTFSI	$\{[(CF_3SO_2)(CFH_2SO_2)_2N]Li\}$	
		LiDFFMSI	$\{[(CHF_2SO_2)(CFH_2SO_2)_2N]Li\}$	
		LiMTFSI	$\{[(CF_3SO_2)(CH_3SO_2)_2N]Li\}$	
26	2019	LiFMSI	$\{[(CH_2FSO_2)_2N]Li\}$	27
		LiDFMSI	$\{[(CH_3SO_2)(CF_2HSO_2)_2N]Li\}$	
		LiFMMSI	$\{[(CH_3SO_2)(CFH_2SO_2)_2N]Li\}$	
		LiMSI	$\{[(CH_3SO_2)_2N]Li\}$	
27	2020	LiDFSI	$\{[(CHF_2SO_2)_2N]Li\}$	28
28	2022	LiTFEMSI	$\{[(CF_3SO_2)((CH_3)(C_2H_5)NSO_2)_2N]Li\}$	29
29	2022	LiBTFSI	$\{[(CF_3SO_2)(C_6H_5SO_2)_2N]Li\}$	30
30	2023	LiTPBTFSI	$\{[(CF_3SO_2)(C_6H_2(CH(CH_3)_2)_3SO_2)_2N]Li\}$	
		LiNFSI	$\{[(n-C_4F_9SO_2)_2N]Li\}$	31

Abbreviations are given below: bis(fluorosulfonyl)imide  $\{[(FSO_2)_2N]H, HFSI\}$ , silver bis(fluorosulfonyl)imide  $\{[(FSO_2)_2N]Ag, AgFSI\}$ , potassium bis(fluorosulfonyl)imide  $\{[(FSO_2)_2N]K, KFSI\}$ , rubidium bis(fluorosulfonyl)imide  $\{[(FSO_2)_2N]Rb, RbFSI\}$ , cesium bis(fluorosulfonyl)imide  $\{[(FSO_2)_2N]Cs, CsFSI\}$ , bis(trifluoromethanesulfonyl)imide  $\{[(CF_3SO_2)_2N]H, HTFSI\}$ , sodium bis(trifluoromethanesulfonyl)imide  $\{[(CF_3SO_2)_2N]Na, NaTFSI\}$ , (trifluoromethanesulfonyl)(*n*-nonafluorobutanesulfonyl)imide  $\{[(CF_3SO_2)(n-C_4F_9SO_2)_2N]H, HTNFSI\}$ , silver (trifluoromethanesulfonyl)(*n*-nonafluorobutanesulfonyl)imide  $\{[(CF_3SO_2)(n-C_4F_9SO_2)_2N]Ag, AgTNFSI\}$ , potassium (trifluoromethanesulfonyl)(*n*-nonafluorobutanesulfonyl)imide  $\{[(CF_3SO_2)(n-C_4F_9SO_2)_2N]K, KTNFSI\}$ , cesium (trifluoromethanesulfonyl)(*n*-nonafluorobutanesulfonyl)imide  $\{[(CF_3SO_2)(n-C_4F_9SO_2)_2N]Cs, CsTNFSI\}$ , lithium bis(fluorosulfonyl)imide  $\{[(FSO_2)_2N]Li, LiFSI\}$ , lithium bis(trifluoromethanesulfonyl)imide  $\{[(CF_3SO_2)_2N]Li, LiTFSI\}$ , lithium bis(pentafluoroethanesulfonyl)imide  $\{[(CF_3CF_2SO_2)_2N]Li, LiBETI\}$ , lithium (fluorosulfonyl)(pentafluoroethanesulfonyl)imide  $\{[(FSO_2)(C_2F_5SO_2)_2N]Li, LiFPFSI\}$ , sodium (fluorosulfonyl)(pentafluoroethanesulfonyl)imide  $\{[(FSO_2)(C_2F_5SO_2)_2N]Na, NaFPFSI\}$ , potassium (fluorosulfonyl)(pentafluoroethanesulfonyl)imide  $\{[(FSO_2)(C_2F_5SO_2)_2N]K, KFPFSI\}$ , rubidium (fluorosulfonyl)(pentafluoroethanesulfonyl)imide  $\{[(FSO_2)(C_2F_5SO_2)_2N]Rb, RbFPFSI\}$ , cesium (fluorosulfonyl)(pentafluoroethanesulfonyl)imide  $\{[(FSO_2)(C_2F_5SO_2)_2N]Cs, CsFPFSI\}$ , lithium (fluorosulfonyl)(*n*-nonafluorobutanesulfonyl)imide  $\{[(FSO_2)(n-C_4F_9SO_2)_2N]Li, LiFNFSI\}$ , potassium (4-styrenesulfonyl)(trifluoromethylsulfonyl)imide  $\{[(CF_3SO_2)(CH_2=CHC_6H_4SO_2)_2N]K, KSTFSI\}$ , lithium poly[(4-styrenesulfonyl)(trifluoromethylsulfonyl)imide]  $\{-(CH_2CHX)_n-, X = C_6H_4SO_2N^{(-)}(Li^+)SO_2CF_3; LiPSTFSI\}$ , lithium bis(2,2,2-trifluoroethoxy-sulfonyl)imide  $\{[(CF_3CH_2OSO_2)_2N]Li, LiTFESI\}$ , sodium bis(2,2,2-trifluoroethoxy-sulfonyl)imide  $\{[(CF_3CH_2OSO_2)_2N]Na, NaTFESI\}$ .

xysulfonyl)imide {[[(CF<sub>3</sub>CH<sub>2</sub>OSO<sub>2</sub>)<sub>2</sub>N]Na, NaTFESI], potassium bis(2,2,2-trifluoroethoxysulfonyl)imide {[[(CF<sub>3</sub>CH<sub>2</sub>OSO<sub>2</sub>)<sub>2</sub>N]K, KTFESI}, rubidium bis(2,2,2-trifluoroetho-xysulfonyl)imide {[[(CF<sub>3</sub>CH<sub>2</sub>OSO<sub>2</sub>)<sub>2</sub>N]Rb, RbTFESI}, cesium bis(2,2,2-trifluoroethoxysulfonyl)imide {[[(CF<sub>3</sub>CH<sub>2</sub>OSO<sub>2</sub>)<sub>2</sub>N]Cs, CsTFESI}, lithium (trifluoromethane(S-trifluoromethane sulfonylimino)sulfonyl)(trifluoromethanesulfonyl)imide {[[(CF<sub>3</sub>SO(=NSO<sub>2</sub>CF<sub>3</sub>)<sub>2</sub>]Li, LiTSFSI}, lithium (trifluoromethanesulfonyl)(n-nonafluorobutanesulfonyl)imide {[[(CF<sub>3</sub>SO<sub>2</sub>)(n-C<sub>4</sub>F<sub>9</sub>SO<sub>2</sub>)N]Li, LiTNFSI}, potassium [(4-styrenesulfonyl)(trifluoromethyl(S-trifluoromethylsulfonylimino)sulfonyl)imide]

{[[(CF<sub>3</sub>SO(NSO<sub>2</sub>CF<sub>3</sub>))(CH<sub>2</sub>=CHC<sub>6</sub>H<sub>4</sub>SO<sub>2</sub>)N]K, KSsTFSI], lithium poly[(4-styrenesulfonyl)(trifluoromethyl(S-trifluoromethylsulfonylimino)sulfonyl)imide] {-(CH<sub>2</sub>CHX)<sub>n</sub>-, X = [C<sub>6</sub>H<sub>4</sub>SO<sub>2</sub>N<sup>(-)</sup>(Li<sup>+</sup>)SO(NSO<sub>2</sub>CF<sub>3</sub>)CF<sub>3</sub>], LiPSsTFSI}, lithium (fluorosulfonyl)(trifluoromethanesulfonyl)imide {[[(FSO<sub>2</sub>)(CF<sub>3</sub>SO<sub>2</sub>)N]Li, LiFTFSI}, lithium (fluorosulfonyl)(pentafluoroethanesulfonyl)imide {[[(FSO<sub>2</sub>)(C<sub>2</sub>F<sub>5</sub>SO<sub>2</sub>)N]Li, LiFPFSI}, lithium (difluoromethanesulfonyl)(trifluoromethanesulfonyl)imide {[[(CF<sub>2</sub>HSO<sub>2</sub>)(CF<sub>3</sub>SO<sub>2</sub>)N]Li, LiDFTFSI}, lithium ether-functionalized anion {[[(CF<sub>3</sub>SO<sub>2</sub>)((CH<sub>3</sub>OC<sub>2</sub>H<sub>4</sub>)<sub>2</sub>NSO<sub>2</sub>)N]Li, LiEFA}, lithium (trifluoromethanesulfonyl)(n-heptafluoropropanesulfonyl)imide {[[(CF<sub>3</sub>SO<sub>2</sub>)(n-C<sub>3</sub>F<sub>7</sub>SO<sub>2</sub>)N]Li, LiTPFSI}, lithium bis(difluoromethanesulfonyl)imide {[[(HCF<sub>2</sub>SO<sub>2</sub>)<sub>2</sub>N]Li, LiDFSI}, lithium (fluoromethanesulfonyl)(trifluoromethanesulfonyl)imide {[[(CFH<sub>2</sub>SO<sub>2</sub>)(CF<sub>3</sub>SO<sub>2</sub>)N]Li, LiFMTFSI}, lithium (methanesulfonyl)(trifluoromethanesulfonyl)imide {[[(CH<sub>3</sub>SO<sub>2</sub>)(CF<sub>3</sub>SO<sub>2</sub>)N]Li, LiMTFSI}, lithium bis(fluoromethanesulfonyl)imide {[[(CFH<sub>2</sub>SO<sub>2</sub>)<sub>2</sub>N]Li, LiFMSI}, lithium (difluoromethanesulfonyl)(methanesulfonyl)imide {[[(CF<sub>2</sub>HSO<sub>2</sub>)(CH<sub>3</sub>SO<sub>2</sub>)N]Li, LiDFMSI}, lithium (fluoromethanesulfonyl)(methanesulfonyl)imide {[[(CFH<sub>2</sub>SO<sub>2</sub>)(CH<sub>3</sub>SO<sub>2</sub>)N]Li, LiFMMSI}, lithium bis(methanesulfonyl)imide {[[(CH<sub>3</sub>SO<sub>2</sub>)<sub>2</sub>N]Li, LiMSI}, lithium (trifluoromethanesulfonyl)(N-ethyl-N-methylsulfamoyl)imide {[[(CF<sub>3</sub>SO<sub>2</sub>)((CH<sub>3</sub>)(C<sub>2</sub>H<sub>5</sub>)NSO<sub>2</sub>)N]Li, LiTFEMSI}, lithium (bis(1,1,1,3,3,3-hexafluoro-2propoxy)sulfonyl)imide, {[[(CF<sub>3</sub>)<sub>2</sub>CHOSO<sub>2</sub>)<sub>2</sub>N]Li, LiHFPSI], lithium (benzenesulfonyl)(trifluoromethanesulfonyl)imide {[[(CF<sub>3</sub>SO<sub>2</sub>)(C<sub>6</sub>H<sub>5</sub>SO<sub>2</sub>)N]Li, LiBTFSI}, lithium (2,4,6-triisopropylbenzenesulfonyl)(trifluoromethanesulfonyl)imide {[[(CF<sub>3</sub>SO<sub>2</sub>)(C<sub>6</sub>H<sub>2</sub>(CH(CH<sub>3</sub>)<sub>2</sub>)<sub>3</sub>SO<sub>2</sub>)N]Li, LiTPBTFPSI}, and lithium bis(n-nonafluorobutanesulfonyl)imide {[[(n-C<sub>4</sub>F<sub>9</sub>SO<sub>2</sub>)<sub>2</sub>N]Li, LiNFSI}.



**Fig. S1** Chemical structures of the sulfonimide anions utilized as electrolyte materials.

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