

Supporting Information for

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

Xingxing Wang, Wenfang Feng, Zhibin Zhou, and Heng Zhang*

Key Laboratory of Material Chemistry for Energy Conversion and Storage (Ministry of Education)

School of Chemistry and Chemical Engineering, Huazhong University of Science and Technology

1037 Luoyu Road, Wuhan 430074, China

Corresponding Authors

*H. Zhang: E-mail: hengzhang2020@hust.edu.cn.

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	$=\text{NSO}_2\text{CF}_3$	7
			$[(\text{CF}_3\text{CF}_2\text{SO}_2)_2\text{N}]\text{H}$	
			$[(\text{CF}_3\text{CF}_2\text{SO}_2)(\text{CF}_3\text{SO}_2)\text{N}]\text{H}$	
			$[(\text{CF}_3\text{CF}_2\text{CF}_2\text{SO}_2)_2\text{N}]\text{H}$	
8	1993		$[(\text{CF}_3\text{SO}_2)(\text{CF}_3\text{CF}_2\text{CF}_2\text{SO}_2)\text{N}]\text{H}$	8
			$[(\text{CF}_3\text{SO}_2)(\text{CFCl}=\text{CF}_2\text{CF}_2\text{SO}_2)\text{N}]\text{H}$	
			$[(\text{CF}_3\text{SO}_2)(\text{CF}_2=\text{CFC}_2\text{F}_4\text{SO}_2)\text{N}]\text{H}$	
			$[(\text{CF}_3\text{CCl}_2\text{SO}_2)_2\text{N}]\text{H}$	
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	$[(\text{CF}_3\text{CF}_2\text{SO}_2)_2\text{N}]\text{Li}$	10
			$[(\text{CF}_3\text{CH}_2\text{OSO}_2)_2\text{N}]\text{H}$	
11	1997		$[(\text{CF}_3\text{CF}_2\text{CH}_2\text{OSO}_2)_2\text{N}]\text{H}$	11
			$[(\text{HCF}_2\text{CF}_2\text{CH}_2\text{OSO}_2)_2\text{N}]\text{H}$	
			$[(\text{CF}_3)_2\text{CHSO}_2)_2\text{N}]\text{H}$	
			$[(\text{CF}_3\text{SO}_2)(n\text{-C}_4\text{F}_9\text{SO}_2)\text{N}]\text{Li}$	
			$[(\text{CF}_3\text{SO}_2)(\text{C}_6\text{F}_5\text{SO}_2)\text{N}]\text{Li}$	
			$[(\text{CF}_3\text{SO}_2)(n\text{-C}_8\text{F}_{17}\text{SO}_2)\text{N}]\text{Li}$	
12	1997		$[(\text{CF}_3\text{CHOSO}_2)_2\text{N}]\text{Li}$	12
			$[(\text{CF}_3\text{CF}_2\text{CHOSO}_2)_2\text{N}]\text{Li}$	
			$[(\text{HCF}_2\text{CF}_2\text{CHOSO}_2)_2\text{N}]\text{Li}$	
			$[(\text{CF}_3)_2\text{CHOSO}_2)_2\text{N}]\text{Li}$	
13	2002	$(\text{CF}_3\text{SO}_2)(\text{CF}_3\text{SO})\text{NM}$	$[(\text{CF}_3\text{SO}_2)(\text{CF}_3\text{SO})\text{N}]\text{K}$	13
			$[(\text{CF}_3\text{SO}_2)(\text{CF}_3\text{SO})\text{N}]\text{Cs}$	
			$[\text{C}_6\text{H}_5\text{SO}(\text{NSO}_2\text{CF}_3)_2\text{N}]\text{K}$	
14	2005		$[(\text{C}_6\text{H}_5\text{SO}(\text{NSO}_2\text{CF}_3))(\text{CF}_3\text{SO}(\text{NSO}_2\text{CF}_3))\text{N}]\text{K}$	14
			$[\text{CF}_3\text{SO}(\text{NSO}_2\text{CF}_3)_2\text{N}]\text{K}$	
			$[(\text{CF}_3\text{SO}_2)(\text{CF}_3\text{SO}(\text{NSO}_2\text{CF}_3))\text{N}]\text{K}$	
		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	$[(\text{FSO}_2)(n\text{-C}_4\text{F}_9\text{SO}_2)\text{N}]\text{Li}$	16
			$[(\text{CF}_3\text{SO}_2)(\text{CH}_2=\text{CHC}_6\text{H}_4\text{SO}_2)\text{N}]\text{K}$	
17	2011	KSTFSI	$-(\text{CH}_2\text{CHX})_n-$, X = $[(\text{C}_6\text{H}_4\text{SO}_2\text{N}^{(-)}(\text{Li})\text{SO}_2\text{CF}_3)]$,	17,
		LiPSTFSI	LiPSTFSI	18

Table S1. Continued.

Entry	Year	Abbreviation	Sulfonimide anion	Ref.
18	2014	LiTFESI	$[(CF_3CH_2OSO_2)_2N]Li$	19
		NaTFESI	$[(CF_3CH_2OSO_2)_2N]Na$	
		KTFESI	$[(CF_3CH_2OSO_2)_2N]K$	
		RbTFESI	$[(CF_3CH_2OSO_2)_2N]Rb$	
		CsTFESI	$[(CF_3CH_2OSO_2)_2N]Cs$	
19	2015	LiSTFSI	$[CF_3SO(=NSO_2CF_3)_2]Li$	20
20	2016	LiTNFSI	$[(CF_3SO_2)(n-C_4F_9SO_2)N]Li$	21
21	2016	KSSTFSI	$[(CF_3SO(NSO_2CF_3))(CH_2=CHC_6H_4SO_2)N]K$	22
		LiSSTFSI	$[(CF_3SO(NSO_2CF_3))(CH_2=CHC_6H_4SO_2)N]Li$	
		LiPSSSTFSI	$-(CH_2CHX)_n-$, $X = C_6H_4SO_2N^{(-)}(Li)SO(NSO_2CF_3)CF_3$, LiPSSSTFSI	
22	2018	LiFTFSI	$[(FSO_2)(CF_3SO_2)N]Li$	23
23	2018	LiFPFSI	$[(FSO_2)(C_2F_5SO_2)N]Li$	24
24	2019	LiDFTFSI	$[(CF_3SO_2)(CF_2HSO_2)N]Li$	25
25	2019	LiEFA	$[(CF_3SO_2)((CH_3OC_2H_4)_2NSO_2)N]Li$	26
26	2019	LiFMTFSI	$[(CF_3SO_2)(CFH_2SO_2)N]Li$	27
		LiDFFMSI	$[(CHF_2SO_2)(CFH_2SO_2)N]Li$	
		LiMTFSI	$[(CF_3SO_2)(CH_3SO_2)N]Li$	
		LiFMSI	$[(CH_2FSO_2)_2N]Li$	
		LiDFMSI	$[(CH_3SO_2)(CF_2HSO_2)N]Li$	
		LiFMMSI	$[(CH_3SO_2)(CFH_2SO_2)N]Li$	
27	2020	LiMSI	$[(CH_3SO_2)_2N]Li$	28
		LiDFSI	$[(CHF_2SO_2)_2N]Li$	
		LiDFMSI	$[(CF_3SO_2)((CH_3)(C_2H_5)NSO_2)N]Li$	
28	2022	LiTFEMSI	$[(CF_3SO_2)((CH_3)(C_2H_5)NSO_2)N]Li$	29
29	2022	LiBTFSI	$[(CF_3SO_2)(C_6H_5SO_2)N]Li$	30
		LiTPBTFSI	$[(CF_3SO_2)(C_6H_2(CH(CH_3)_2)_3SO_2)N]Li$	
30	2023	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 $\{[(CF_3SO_2)_2N]Na, NaTFESI\}$, (trifluoromethanesulfonyl)(*n*-nonafluorobutanesulfonyl)imide $\{[(CF_3SO_2)(n-C_4F_9SO_2)N]H, HTNFSI\}$, silver (trifluoromethanesulfonyl)(*n*-nonafluorobutanesulfonyl)imide $\{[(CF_3SO_2)(n-C_4F_9SO_2)N]Ag, AgTNFSI\}$, potassium (trifluoromethanesulfonyl)(*n*-nonafluorobutanesulfonyl)imide $\{[(CF_3SO_2)(n-C_4F_9SO_2)N]K, KTNFSI\}$, cesium (trifluoromethanesulfonyl)(*n*-nonafluorobutanesulfonyl)imide $\{[(CF_3SO_2)(n-C_4F_9SO_2)N]Cs, CsTNFSI\}$, 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 $\{[(FSO_2)(C_2F_5SO_2)N]Li, LiFPFSI\}$, sodium (fluorosulfonyl)(pentafluoroethanesulfonyl)imide $\{[(FSO_2)(C_2F_5SO_2)N]Na, NaFPFSI\}$, potassium (fluorosulfonyl)(pentafluoroethanesulfonyl)imide $\{[(FSO_2)(C_2F_5SO_2)N]K, KFPFSI\}$, rubidium (fluorosulfonyl)(pentafluoroethanesulfonyl)imide $\{[(FSO_2)(C_2F_5SO_2)N]Rb, RbFPFSI\}$, cesium (fluorosulfonyl)(pentafluoroethanesulfonyl)imide $\{[(FSO_2)(C_2F_5SO_2)N]Cs, CsFPFSI\}$, lithium (fluorosulfonyl)(*n*-nonafluorobutanesulfonyl)imide $\{[(FSO_2)(n-C_4F_9SO_2)N]Li, LiFNFSI\}$, potassium (4-styrenesulfonyl)(trifluoromethylsulfonyl)imide $\{[(CF_3SO_2)(CH_2=CHC_6H_4SO_2)N]K, KSTFSI\}$, 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-

xysulfonyl)imide $\{[(CF_3CH_2OSO_2)_2N]Na, NaTFESI\}$, potassium bis(2,2,2-trifluoroethoxysulfonyl)imide $\{[(CF_3CH_2OSO_2)_2N]K, KTFESI\}$, rubidium bis(2,2,2-trifluoroethoxysulfonyl)imide $\{[(CF_3CH_2OSO_2)_2N]Rb, RbTFESI\}$, cesium bis(2,2,2-trifluoroethoxysulfonyl)imide $\{[(CF_3CH_2OSO_2)_2N]Cs, CsTFESI\}$, lithium (trifluoromethane(*S*-trifluoromethane sulfonylimino)sulfonyl)(trifluoromethanesulfonyl)imide $\{[CF_3SO(=NSO_2CF_3)_2]Li, LiSTFSI\}$, lithium (trifluoromethanesulfonyl)(*n*-nonafluorobutanesulfonyl)imide $\{[(CF_3SO_2)(n-C_4F_9SO_2)N]Li, LiTNFSI\}$, potassium [(4-styrenesulfonyl)(trifluoromethyl(*S*-trifluoromethylsulfonylimino)sulfonyl)imide] $\{[(CF_3SO(NSO_2CF_3))(CH_2=CHC_6H_4SO_2)]NK, KSTFSI\}$, lithium poly[(4-styrenesulfonyl)(trifluoromethyl(*S*-trifluoromethylsulfonylimino)sulfonyl)imide] $[-(CH_2CHX)_n-$, $X = [C_6H_4SO_2N^{(-)}(Li^+)SO(NSO_2CF_3)CF_3]$; $LiPSsTFSI$], lithium (fluorosulfonyl)(trifluoromethanesulfonyl)imide $\{[(FSO_2)(CF_3SO_2)N]Li, LiFTFSI\}$, lithium (fluorosulfonyl)(pentafluoroethanesulfonyl)imide $\{[(FSO_2)(C_2F_5SO_2)N]Li, LiFPFSI\}$, lithium (difluoromethanesulfonyl)(trifluoromethanesulfonyl)imide $\{[(CF_2HSO_2)(CF_3SO_2)N]Li, LiDFTFSI\}$, lithium ether-functionalized anion $\{[(CF_3SO_2)((CH_3OC_2H_4)_2NSO_2)N]Li, LiEFA\}$, lithium (trifluoromethanesulfonyl)(*n*-heptafluoropropanesulfonyl)imide $\{[(CF_3SO_2)(n-C_3F_7SO_2)N]Li, LiTPFSI\}$, lithium bis(difluoromethanesulfonyl)imide $\{[(HCF_2SO_2)_2N]Li, LiDFSi\}$, lithium (fluoromethanesulfonyl)(trifluoromethanesulfonyl)imide $\{[(CFH_2SO_2)(CF_3SO_2)N]Li, LiFMTFSI\}$, lithium (difluoromethanesulfonyl)(fluoromethanesulfonyl)imide $\{[(CF_2HSO_2)(CFH_2SO_2)N]Li, LiDFFMSI\}$, lithium (methanesulfonyl)(trifluoromethanesulfonyl)imide $\{[(CH_3SO_2)(CF_3SO_2)N]Li, LiMTFSI\}$, lithium bis(fluoromethanesulfonyl)imide $\{[(CFH_2SO_2)_2N]Li, LiFMSI\}$, lithium (difluoromethanesulfonyl)(methanesulfonyl)imide $\{[(CF_2HSO_2)(CH_3SO_2)N]Li, LiDFMSI\}$, lithium (fluoromethanesulfonyl)(methanesulfonyl)imide $\{[(CFH_2SO_2)(CH_3SO_2)N]Li, LiFMMSI\}$, lithium bis(methanesulfonyl)imide $\{[(CH_3SO_2)_2N]Li, LiMSI\}$, lithium (trifluoromethanesulfonyl)(*N*-ethyl-*N*-methylsulfamoyl)imide $\{[(CF_3SO_2)((CH_3)(C_2H_5)NSO_2)N]Li, LiTFEMSI\}$, lithium (bis(1,1,1,3,3,3-hexafluoro-2-propoxyl)sulfonyl)imide, $[(CF_3)_2CHOSO_2)_2N]Li, LiHFPSI\}$, lithium (benzenesulfonyl)(trifluoromethanesulfonyl)imide $\{[(CF_3SO_2)(C_6H_5SO_2)N]Li, LiBTFSI\}$, lithium (2,4,6-triisopropylbenzenesulfonyl)(trifluoromethanesulfonyl)imide $\{[(CF_3SO_2)(C_6H_2(CH(CH_3)_2)_3SO_2)N]Li, LiTPBTFSI\}$, and lithium bis(*n*-nonafluorobutanesulfonyl)imide $\{[(n-C_4F_9SO_2)N]Li, LiNFSI\}$.

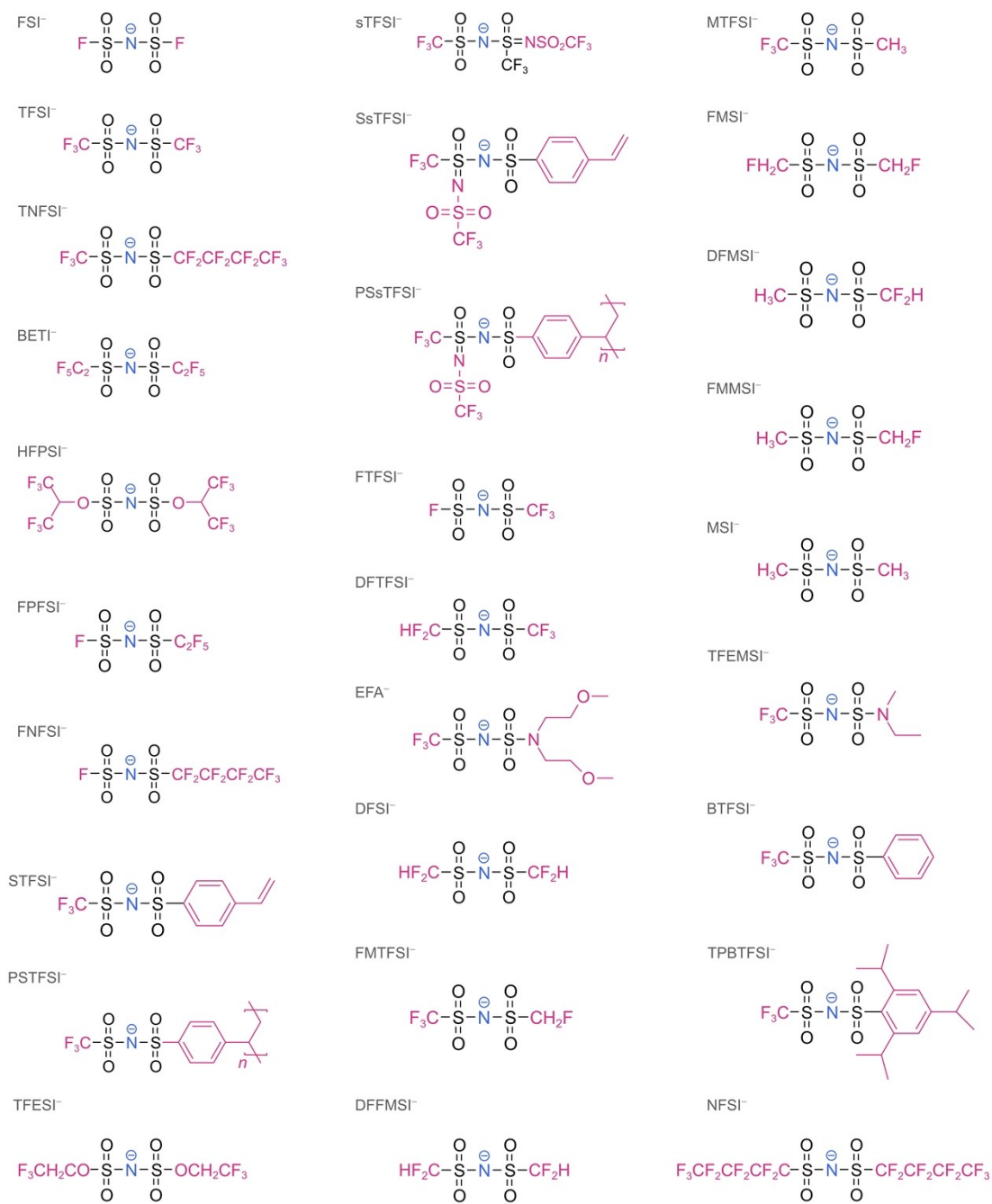


Fig. S1 Chemical structures of the sulfonimide anions utilized as electrolyte materials.

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