Supplementary materials

Understanding the role of additive in solvation structure and interfacial reactions on lithium metal anode

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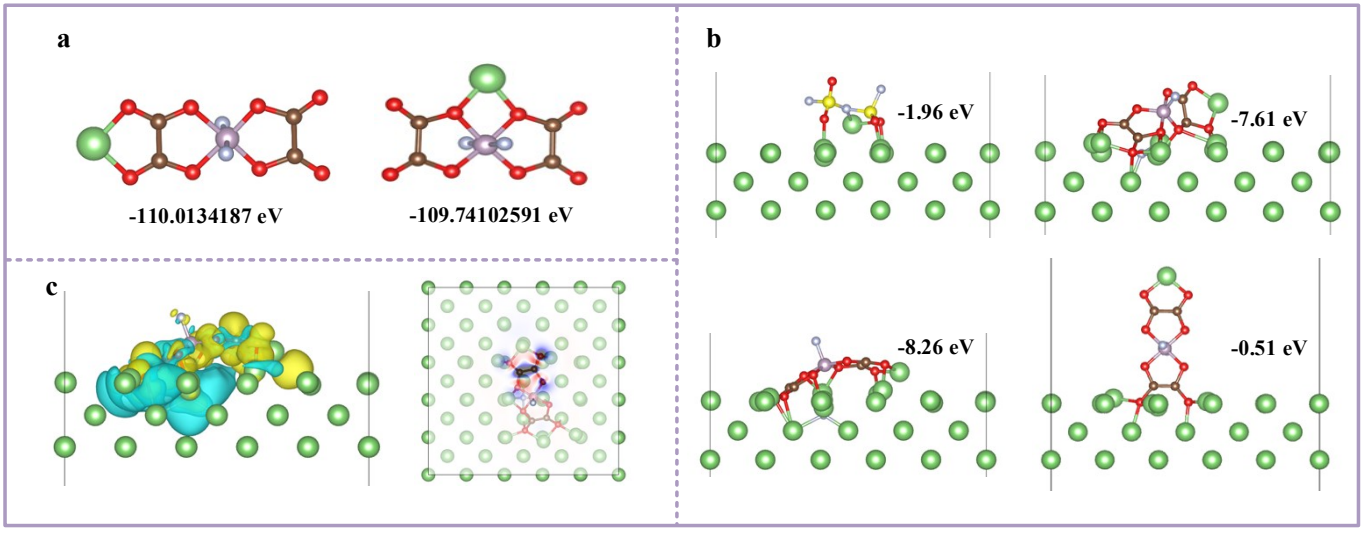

Fig. S1 (a) The energy contrast between the two LiDFBOP structures, (b) adsorption energy of LiDFBOP on Li surface, (c) charge difference density of LiDFBOP on Li surface.

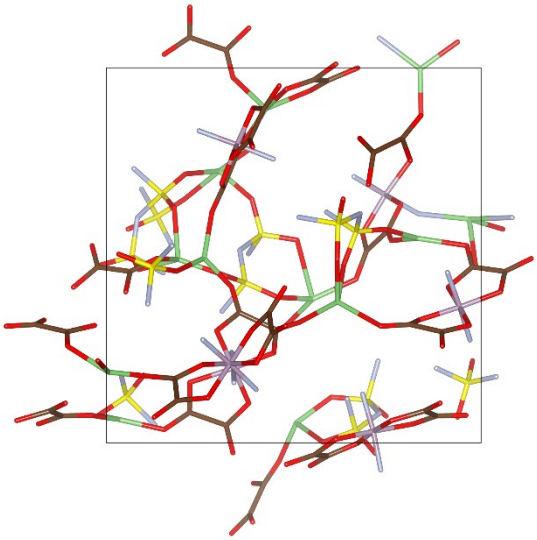

Fig. S2 Snapshots of LiFSI and LiDFBOP uniformly mixed model at 5 ps.

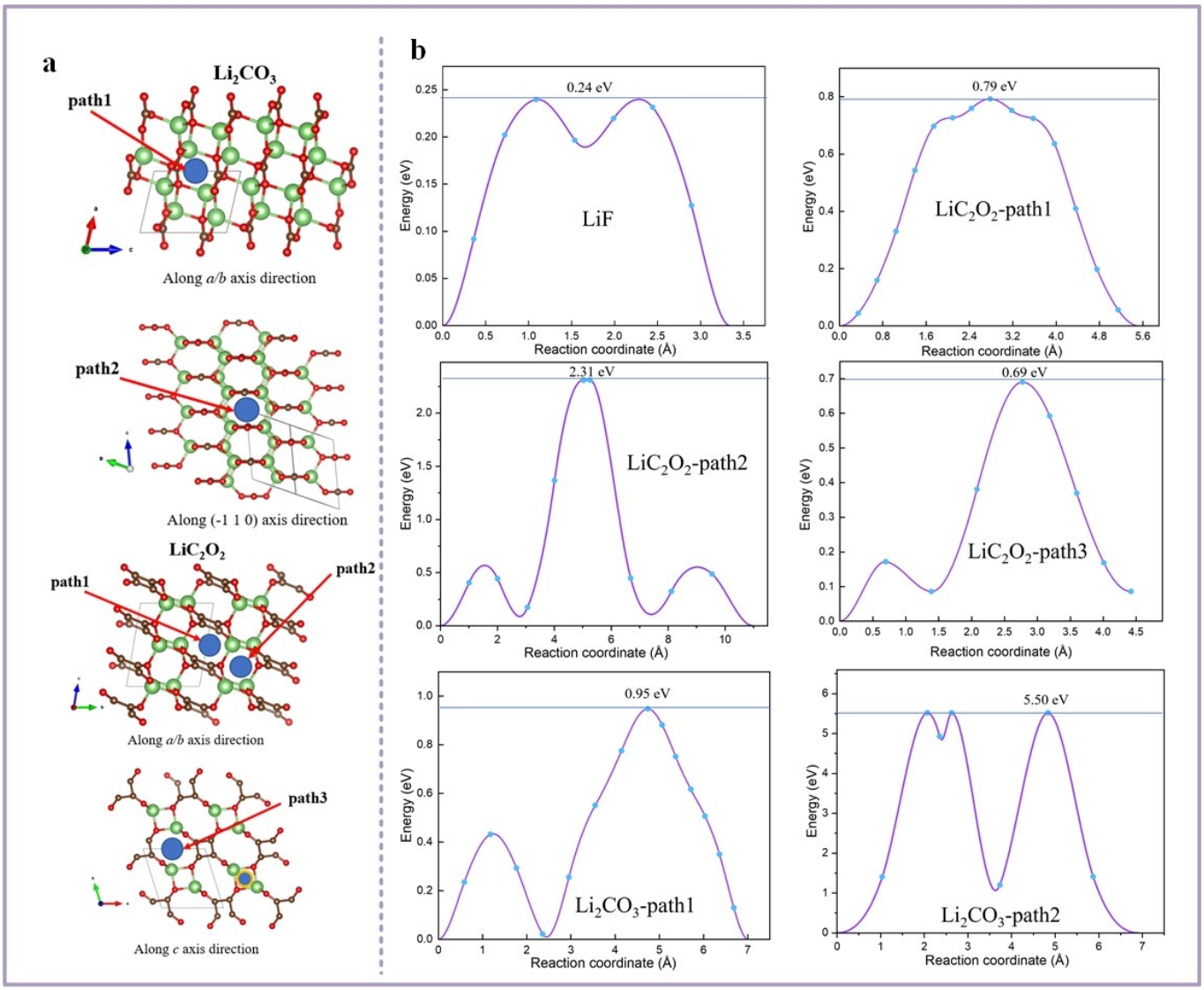

Fig. S3 (a) Schematic diagram of different ion diffusion paths in Li_2CO_3 and LiC_2O_2, (b) diffusion energy barrier of Li ion on the surface of LiF and in bulk of Li_2CO_3 and LiC_2O_2.

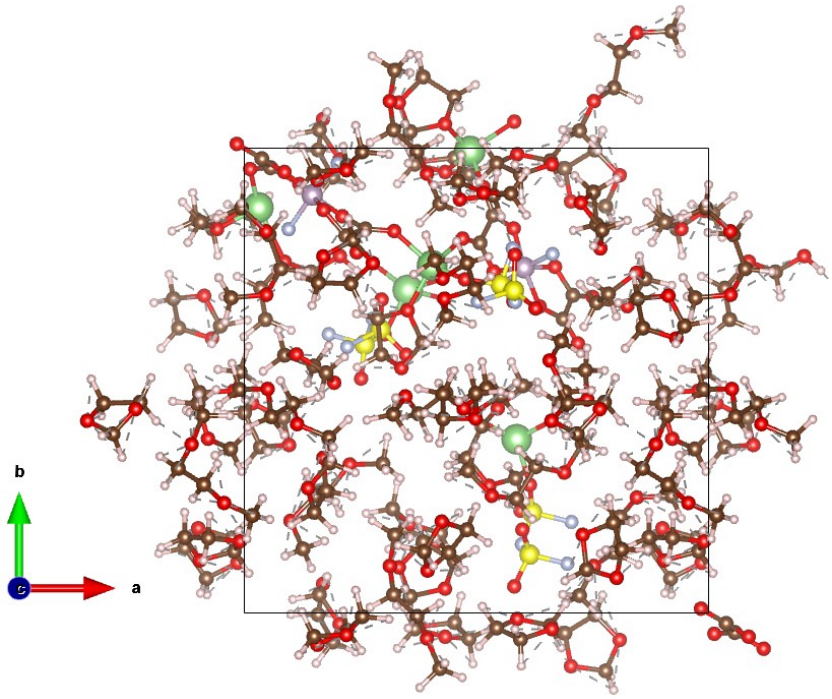

Fig. S4 Snapshot of electrolyte model in AIMD calculation at 4 ps.

A 6 ps (6000-time steps) NVT calculation was performed. The temperature of this calculation was set to 310 K, and time step was set to 1 fs. Fig. S4 is a snapshot at 4 ps. The ratio of number of LiFSI, DOL, and DME in this module was 3 to 22 to 14, which is approximately equal to the experiment ratio. It is very difficult to calculate AIMD for a system with a large number of atoms. However, in such a small model, it is impossible to add LiDFBOP in actual proportion, so two LiDFBOP molecules were added to represent a local environment. The final ratio of LiDFBOP, LiFSI, DOL, and DME is 2 to 3 to 22 to 14.

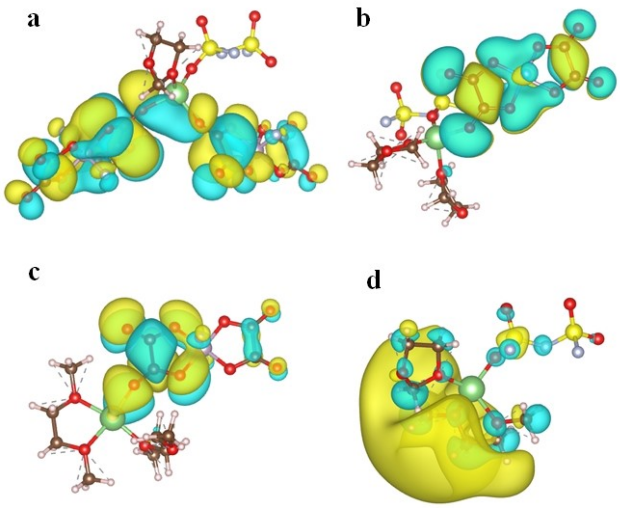

Fig. S5 The spatial distribution diagram of LUMO, (a) structure A, (b) structure B, (c) structure C, (d) structure D.

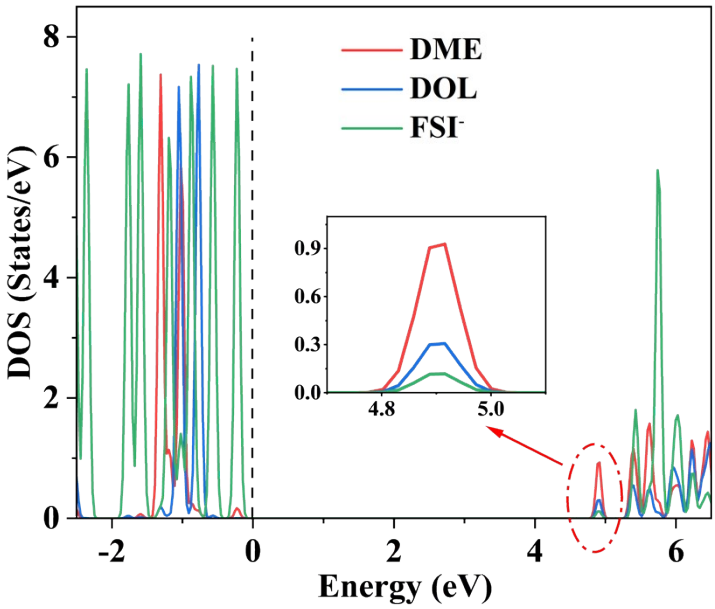

Fig. S6 Density of stats of solvent structure D (Li/FSI/DOL/DME complex).

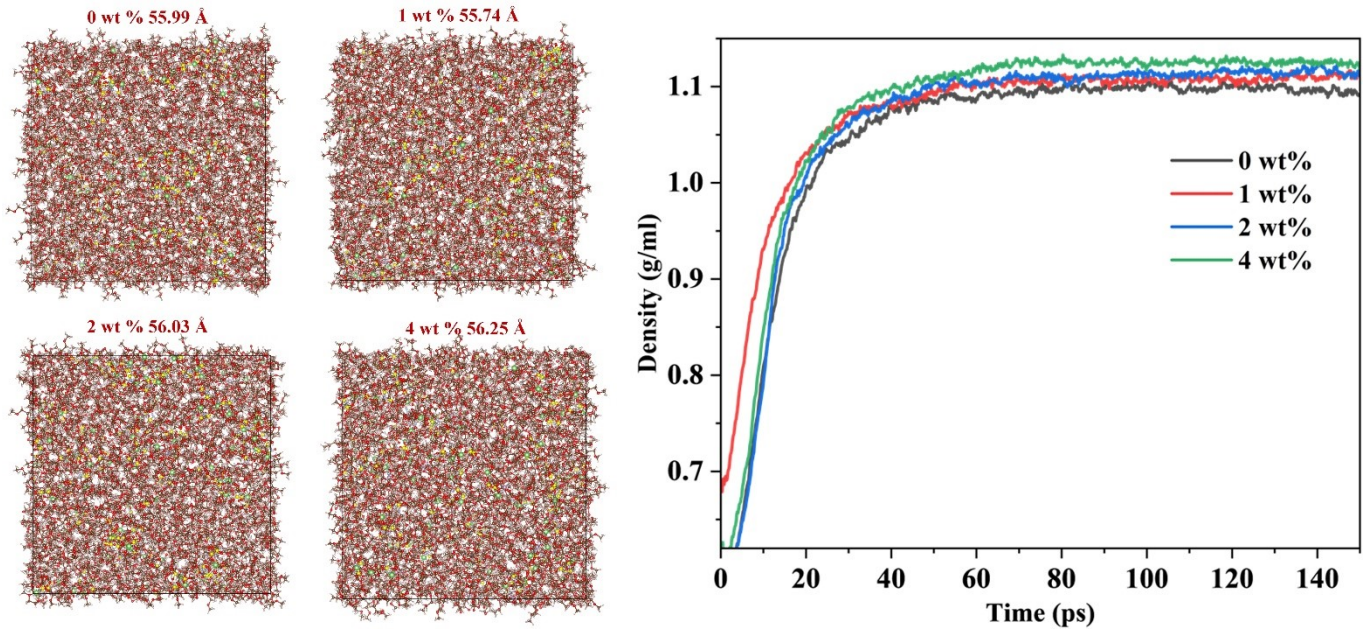

Fig. S7 Four electrolyte models with 0, 1, 2, and 4 wt% LiDFBOP content, and evolution of system density in NPT calculation. All models are cubes with sides of 55.99, 55.74, 56.03, and 56.25 Å, respectively.

For small molecule systems, 100 ps is usually sufficient to describe the diffusion behavior, except for large molecules such as DNA, proteins, which need to judge the diffusion equilibrium at ns scale according to relevant data. A 150 ps NPT (fixed atomic number N, pressure P, temperature T) was prebalanced to relax the initial modeling to a reasonable structure at 310K. According to the density change trend in Fig. S7, it can be seen that it has basically reached the equilibrium state at about 80ps. On the basis of this pretreatment, a 300 ps NVT (fixed atom number N, volume V, temperature T) of 300 ps at 310K was carried

out. The time step was set to 1fs.

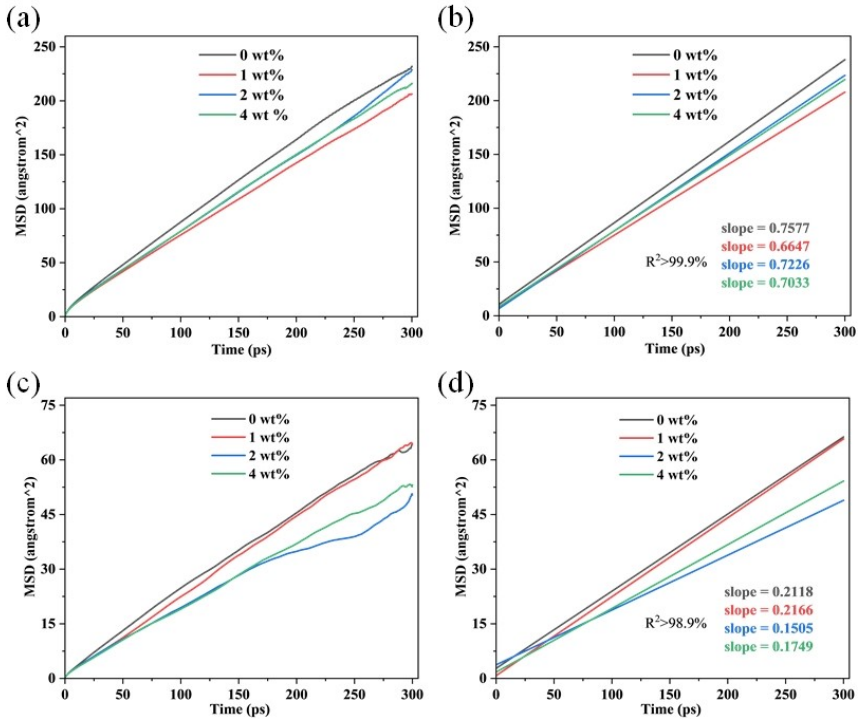

Fig. S8 MSD of (a) solution and (c) Li ions, and their corresponding linear fitting results. (b) and (d) are linear fitting results of (a) and (c), respectively

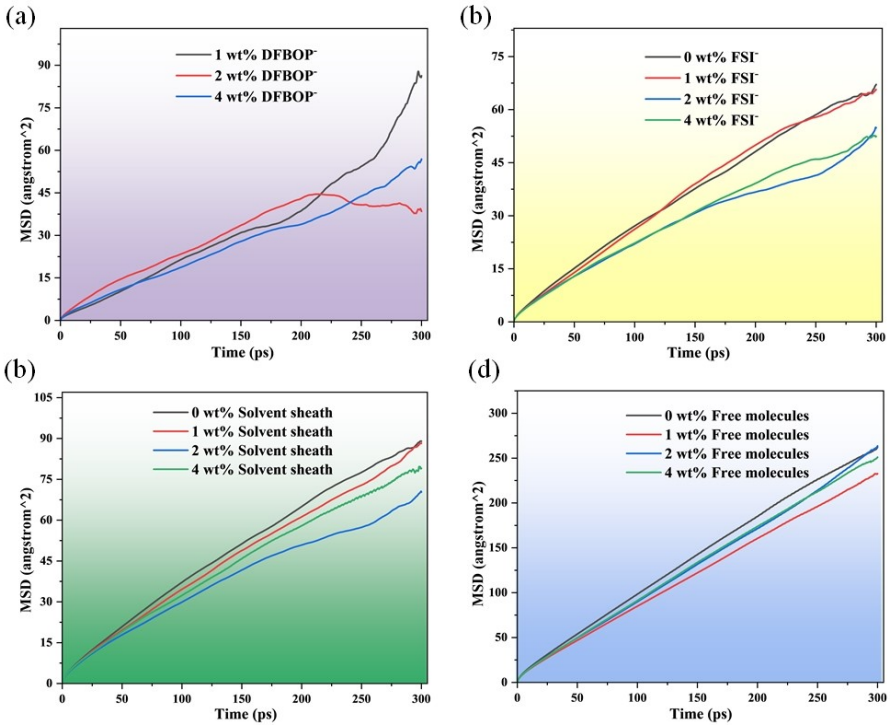

Fig. S9 MSD of (a) $DFBOP^-$, (b) FSI^-, (c) solvent sheath, and (d) free molecules

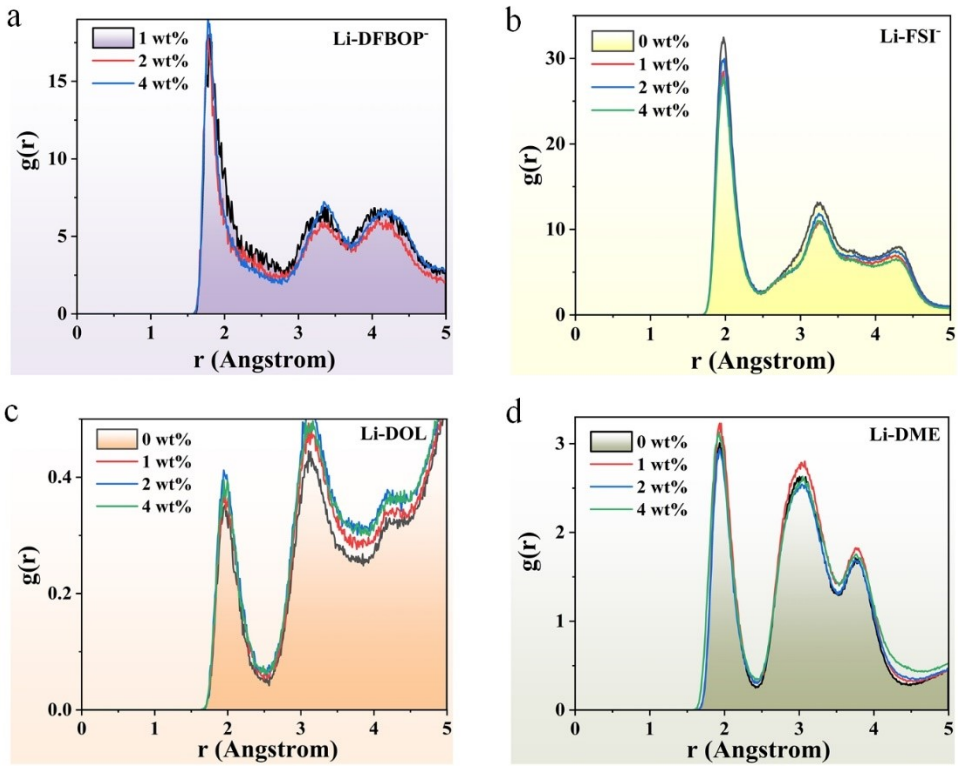

Fig. S10 The radial distribution function (RDF) of (a) DFBOP anion, (b) FSI anion, (c) DOL, (d) MDE, in 300 ps.

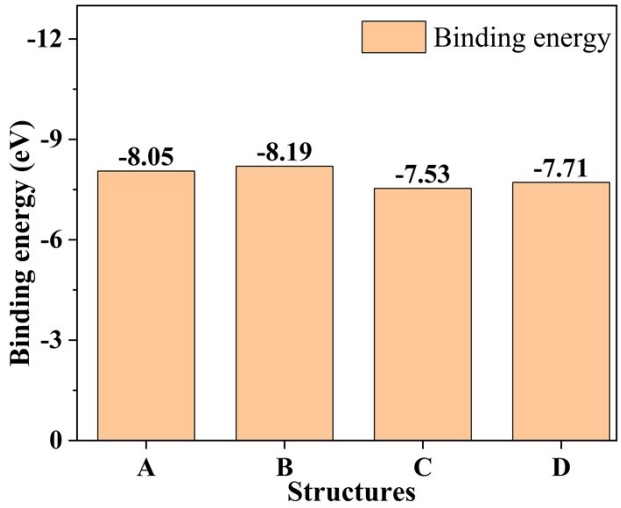

Fig. S11 Total binding energy of the four solvated structures

The total binding energy of the four solvated structures is about 750 KJ/mol. Theoretically there are many different solvated structures. For the convenience of analysis, the de-solvation energy of FSI^-, DOL and DME was calculated by structure D, and the de-solvation energy of $DFBOP^-$ was calculated by structure C.

Table. S1 Vacuum layer thickness convergence test (based on LiF(0 0 1) slab)

Thickness (Å)	9	11	13	15	17	19
Total energy (eV)	-42.628894	-42.694150	-42.748644	-42.748663	-42.755535	-42.760871
Energy difference /atom(meV)	/	2.719	2.271	0.001	0.286	0.222

NOTE. S1 POSCAR (structure input file for VASP) parameters for the Li Slab

Li (1 0 0)

1.000

0.0000000000000000 6.8632580000000001 0.0000000000000000

0.0000000000000000 0.0000000000000000 6.8632580000000001

25.1474435000000014 0.0000000000000000 0.0000000000000000

Li

24

Selective Dynamics

Direct

0.0000000000000000	0.0000000000000000	0.4016936568211612	T	T	T	Li1
0.0000000000000000	0.0000000000000000	0.5330189053409730	F	F	F	Li2
0.0000000000000000	0.0000000000000000	0.6694792542701965	F	F	F	Li3
0.2500000000000000	0.2500000000000000	0.3305207457298035	T	T	T	Li4
0.2500000000000000	0.2500000000000000	0.4647887308763560	F	F	F	Li5
0.2500000000000000	0.2500000000000000	0.6012490798055846	F	F	F	Li6
0.5000000000000000	0.0000000000000000	0.4016936568211612	T	T	T	Li7
0.5000000000000000	0.0000000000000000	0.5330189053409730	F	F	F	Li8
0.5000000000000000	0.0000000000000000	0.6694792542701965	F	F	F	Li9
0.7500000000000000	0.2500000000000000	0.3305207457298035	T	T	T	Li10
0.7500000000000000	0.2500000000000000	0.4647887308763560	F	F	F	Li11
0.7500000000000000	0.2500000000000000	0.6012490798055846	F	F	F	Li12
0.0000000000000000	0.5000000000000000	0.4016936568211612	T	T	T	Li13
0.0000000000000000	0.5000000000000000	0.5330189053409730	F	F	F	Li14
0.0000000000000000	0.5000000000000000	0.6694792542701965	F	F	F	Li15
0.2500000000000000	0.7500000000000000	0.3305207457298035	T	T	T	Li16
0.2500000000000000	0.7500000000000000	0.4647887308763560	F	F	F	Li17
0.2500000000000000	0.7500000000000000	0.6012490798055846	F	F	F	Li18
0.5000000000000000	0.5000000000000000	0.4016936568211612	T	T	T	Li19
0.5000000000000000	0.5000000000000000	0.5330189053409730	F	F	F	Li20
0.5000000000000000	0.5000000000000000	0.6694792542701965	F	F	F	Li21
0.7500000000000000	0.7500000000000000	0.3305207457298035	T	T	T	Li22
0.7500000000000000	0.7500000000000000	0.4647887308763560	F	F	F	Li23
0.7500000000000000	0.7500000000000000	0.6012490798055846	F	F	F	Li24

NOTE. S2 POSCAR (structure input file for VASP) parameters for the $H_2(CO_2)_2$ slab

H2C2O4

1.0

12.000000 0.000000 0.000000

0.000000 12.000000 0.000000

0.000000 0.000000 8.000000

H C O

2 2 4

Selective Dynamics
Direct
-0.731824 0.441758 -0.525492 T T T
-0.266888 0.523834 -0.549892 T T T
-0.552589 0.446942 -0.524916 T T T
-0.444711 0.516697 -0.519653 T T T
-0.664324 0.504831 -0.526001 T T T
-0.332117 0.460485 -0.524411 T T T
-0.547186 0.321192 -0.529335 T T T
-0.451704 0.642234 -0.513535 T T T

NOTE. S3 POSCAR (structure input file for VASP) parameters for the Li_2CO_3 crystal

Li4 C2 O6
1.0
4.9069232941 0.0000000000 0.0000000000
2.3141082148 4.3269850224 0.0000000000
2.2351958747 1.3393736144 5.7883017225
Li C O
4 2 6
Direct
0.749758005 0.647944987 0.161044002
0.352055013 0.250241995 0.338955998
0.250241995 0.352055013 0.838955998
0.647944987 0.749758005 0.661044002
0.934962988 0.065036997 0.750000000
0.065036997 0.934962988 0.250000000
0.680145979 0.319853991 0.750000000
0.319853991 0.680145979 0.250000000
0.211668000 0.082082003 0.685253024
0.917918026 0.788331985 0.814746976
0.788332999 0.917918026 0.314747006
0.082082003 0.211667001 0.185252994

NOTE. S4 POSCAR (structure input file for VASP) parameters for the LiC_2O_2 crystal

Li2 C4 O4
1.0
6.0392227173 0.0000000000 0.0000000000
-1.6893012106 5.7981438796 0.0000000000
0.4219164004 0.5623853192 3.3065219036
Li C O
2 4 4
Direct
0.352717012 0.647283018 0.000000000
0.647283018 0.352717012 0.000000000
0.107823998 0.892175972 0.500000000

0.861252010	0.861252010	0.664785981
0.892175972	0.107823998	0.500000000
0.138748005	0.138748005	0.335213989
0.306528002	0.306528002	0.137349993
0.761061013	0.238939002	0.500000000
0.238939002	0.761061013	0.500000000
0.693472028	0.693472028	0.862649977

NOTE. S5 POSCAR (structure input file for VASP) parameters for the LiFSI binding on Li surface

LiBulk

1.00000000000000

17.1174999999999997	0.0000000000000000	0.0000000000000000
0.0000000000000000	17.1174999999999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	33.4234999999999971

Li	N	O	F	S
76	1	4	2	2

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.4456539999999976	F	F	F
0.9999706861229284	0.0000523828857034	0.5547556864264224	T	T	T
0.1000000000000014	0.1000000000000014	0.5000000000000000	F	F	F
0.2000000000000028	0.0000000000000000	0.4456539999999976	F	F	F
0.2005921487325856	0.0000298956872662	0.5549657250847365	T	T	T
0.2999999999999972	0.1000000000000014	0.5000000000000000	F	F	F
0.3999999999999986	0.0000000000000000	0.4456539999999976	F	F	F
0.3995239893196282	0.0000269497739443	0.5541266725104564	T	T	T
0.5000000000000000	0.1000000000000014	0.5000000000000000	F	F	F
0.6000000000000014	0.0000000000000000	0.4456539999999976	F	F	F
0.6004426287147969	0.0001709194844731	0.5546272446026014	T	T	T
0.7000000000000028	0.1000000000000014	0.5000000000000000	F	F	F
0.7999999999999972	0.0000000000000000	0.4456539999999976	F	F	F
0.7996377099455925	0.9999697109239528	0.5546875915053046	T	T	T
0.8999999999999986	0.1000000000000014	0.5000000000000000	F	F	F
0.0000000000000000	0.2000000000000028	0.4456539999999976	F	F	F
0.0009716424185111	0.1997594350328874	0.5547249111643076	T	T	T
0.1000000000000014	0.2999999999999972	0.5000000000000000	F	F	F
0.2000000000000028	0.2000000000000028	0.4456539999999976	F	F	F
0.2005939501943460	0.2004697471169420	0.5546974355600882	T	T	T
0.2999999999999972	0.2999999999999972	0.5000000000000000	F	F	F
0.3999999999999986	0.2000000000000028	0.4456539999999976	F	F	F
0.4042767417854187	0.1991721441776694	0.5546896006824363	T	T	T
0.5000000000000000	0.2999999999999972	0.5000000000000000	F	F	F
0.6000000000000014	0.2000000000000028	0.4456539999999976	F	F	F

0.5963934900661887	0.2056992130816811	0.5560838530705415	T	T	T
0.7000000000000028	0.2999999999999972	0.5000000000000000	F	F	F
0.7999999999999972	0.2000000000000028	0.4456539999999976	F	F	F
0.7993398104648884	0.2001173766053724	0.5547634354085949	T	T	T
0.8999999999999986	0.2999999999999972	0.5000000000000000	F	F	F
0.0000000000000000	0.3999999999999986	0.4456539999999976	F	F	F
0.9999144820147863	0.4000319261389463	0.5551867514255088	T	T	T
0.1000000000000014	0.5000000000000000	0.5000000000000000	F	F	F
0.2000000000000028	0.3999999999999986	0.4456539999999976	F	F	F
0.1954823294182944	0.3985075595901396	0.5536483759399476	T	T	T
0.2999999999999972	0.5000000000000000	0.5000000000000000	F	F	F
0.3999999999999986	0.3999999999999986	0.4456539999999976	F	F	F
0.3875083187037877	0.3930252620270980	0.5547094775576575	T	T	T
0.5000000000000000	0.5000000000000000	0.5000000000000000	F	F	F
0.6000000000000014	0.3999999999999986	0.4456539999999976	F	F	F
0.6057513347540714	0.3956133476388604	0.5468169904748807	T	T	T
0.7000000000000028	0.5000000000000000	0.5000000000000000	F	F	F
0.7999999999999972	0.3999999999999986	0.4456539999999976	F	F	F
0.7995759886662719	0.3985235642361722	0.5546350167413957	T	T	T
0.8999999999999986	0.5000000000000000	0.5000000000000000	F	F	F
0.0000000000000000	0.6000000000000014	0.4456539999999976	F	F	F
0.0000836259005655	0.6003101279355864	0.5540581542159644	T	T	T
0.1000000000000014	0.7000000000000028	0.5000000000000000	F	F	F
0.2000000000000028	0.6000000000000014	0.4456539999999976	F	F	F
0.1978269752824263	0.6005726564225158	0.5540063941277698	T	T	T
0.2999999999999972	0.7000000000000028	0.5000000000000000	F	F	F
0.3999999999999986	0.6000000000000014	0.4456539999999976	F	F	F
0.3982730640323601	0.6006877387291608	0.5625555863640246	T	T	T
0.5000000000000000	0.7000000000000028	0.5000000000000000	F	F	F
0.6000000000000014	0.6000000000000014	0.4456539999999976	F	F	F
0.6072177647580580	0.5982925876330688	0.5633230377745060	T	T	T
0.7000000000000028	0.7000000000000028	0.5000000000000000	F	F	F
0.7999999999999972	0.6000000000000014	0.4456539999999976	F	F	F
0.8040505608551336	0.6011944097578514	0.5536536927387679	T	T	T
0.8999999999999986	0.7000000000000028	0.5000000000000000	F	F	F
0.0000000000000000	0.7999999999999972	0.4456539999999976	F	F	F
0.9999676954345392	0.7989519922315793	0.5543682296767326	T	T	T
0.1000000000000014	0.8999999999999986	0.5000000000000000	F	F	F
0.2000000000000028	0.7999999999999972	0.4456539999999976	F	F	F
0.2004746433611205	0.7995403752400450	0.5546751006569300	T	T	T
0.2999999999999972	0.8999999999999986	0.5000000000000000	F	F	F
0.3999999999999986	0.7999999999999972	0.4456539999999976	F	F	F
0.3990954821331278	0.8020767789308241	0.5543326930916566	T	T	T
0.5000000000000000	0.8999999999999986	0.5000000000000000	F	F	F
0.6000000000000014	0.7999999999999972	0.4456539999999976	F	F	F

0.6005443730374784 0.8021074749121007 0.5545746395221262 T T T
0.7000000000000028 0.8999999999999986 0.5000000000000000 F F F
0.7999999999999972 0.7999999999999972 0.4456539999999976 F F F
0.8003414310646563 0.8003749695579269 0.5546567674603374 T T T
0.8999999999999986 0.8999999999999986 0.5000000000000000 F F F
0.5015092335141607 0.3383972882928734 0.6093747740057985 T T T
0.5234904097558092 0.4547944035393576 0.6395911209981430 T T T
0.4186338871081369 0.5528770672500261 0.6157001661446854 T T T
0.4014103923500911 0.4078692456072026 0.6140279188676558 T T T
0.5755827216917884 0.5518068242608695 0.6916836601651684 T T T
0.6048373965298454 0.5737292501246122 0.6200047763803932 T T T
0.3959119909388920 0.4800655069502997 0.6760168769496335 T T T
0.6593875141433579 0.4629322491211146 0.6544101011261806 T T T
0.4356769401836967 0.4772782135404757 0.6327005122173330 T T T
0.5870796694438198 0.5211285284133377 0.6525098407212215 T T T

NOTE. S6(a) POSCAR (structure input file for VASP) parameters for the LiDFBOP binding on Li surface

Adsorption1
1.00000000000000
17.1174999999999997 0.0000000000000000 0.0000000000000000
0.0000000000000000 17.1174999999999997 0.0000000000000000
0.0000000000000000 0.0000000000000000 33.4234999999999971
Li C O F P
76 4 8 2 1
Selective dynamics
Direct
0.0000000000000000 0.0000000000000000 0.4456539999999976 F F F
0.0023441210061660 0.9976684359122115 0.5557868004964003 T T T
0.1000000000000014 0.1000000000000014 0.5000000000000000 F F F
0.2000000000000028 0.0000000000000000 0.4456539999999976 F F F
0.2002508262310278 0.9978668487846555 0.5558118317242172 T T T
0.2999999999999972 0.1000000000000014 0.5000000000000000 F F F
0.3999999999999986 0.0000000000000000 0.4456539999999976 F F F
0.4022771260759923 0.0008067915586430 0.5557646307199194 T T T
0.5000000000000000 0.1000000000000014 0.5000000000000000 F F F
0.6000000000000014 0.0000000000000000 0.4456539999999976 F F F
0.5985151834087626 -0.0070444021848957 0.5527012653272123 T T T
0.7000000000000028 0.1000000000000014 0.5000000000000000 F F F
0.7999999999999972 0.0000000000000000 0.4456539999999976 F F F
0.8001065874122320 0.9984233173452691 0.5545050143198470 T T T
0.8999999999999986 0.1000000000000014 0.5000000000000000 F F F
0.0000000000000000 0.2000000000000028 0.4456539999999976 F F F
0.0032237155895119 0.1978390898923259 0.5550095414514762 T T T

0.1000000000000014	0.2999999999999972	0.5000000000000000	F	F	F
0.2000000000000028	0.2000000000000028	0.4456539999999976	F	F	F
0.1999170640364949	0.1969848356972588	0.5546829876733597	T	T	T
0.2999999999999972	0.2999999999999972	0.5000000000000000	F	F	F
0.3999999999999986	0.2000000000000028	0.4456539999999976	F	F	F
0.3958166940030102	0.1944435182256950	0.5540428337409941	T	T	T
0.5000000000000000	0.2999999999999972	0.5000000000000000	F	F	F
0.6000000000000014	0.2000000000000028	0.4456539999999976	F	F	F
0.5875815450718705	0.1673046944676798	0.5728985964721589	T	T	T
0.7000000000000028	0.2999999999999972	0.5000000000000000	F	F	F
0.7999999999999972	0.2000000000000028	0.4456539999999976	F	F	F
0.7567833726214189	0.1944029421220082	0.5723753807742713	T	T	T
0.8999999999999986	0.2999999999999972	0.5000000000000000	F	F	F
0.0000000000000000	0.3999999999999986	0.4456539999999976	F	F	F
0.0025161025264151	0.4039189796701487	0.5537067964701519	T	T	T
0.1000000000000014	0.5000000000000000	0.5000000000000000	F	F	F
0.2000000000000028	0.3999999999999986	0.4456539999999976	F	F	F
0.2007561264495450	0.3987279229166907	0.5547862118040370	T	T	T
0.2999999999999972	0.5000000000000000	0.5000000000000000	F	F	F
0.3999999999999986	0.3999999999999986	0.4456539999999976	F	F	F
0.4219926449679673	0.4052265891291458	0.5723336321071050	T	T	T
0.5000000000000000	0.5000000000000000	0.5000000000000000	F	F	F
0.6000000000000014	0.3999999999999986	0.4456539999999976	F	F	F
0.5902243821139858	0.3977727623693580	0.5500314482541435	T	T	T
0.7000000000000028	0.5000000000000000	0.5000000000000000	F	F	F
0.7999999999999972	0.3999999999999986	0.4456539999999976	F	F	F
0.8011088724507228	0.4041085899426060	0.5547823554178499	T	T	T
0.8999999999999986	0.5000000000000000	0.5000000000000000	F	F	F
0.0000000000000000	0.6000000000000014	0.4456539999999976	F	F	F
0.0020395256892131	0.6017454270816287	0.5554483196796597	T	T	T
0.1000000000000014	0.7000000000000028	0.5000000000000000	F	F	F
0.2000000000000028	0.6000000000000014	0.4456539999999976	F	F	F
0.2003211277534346	0.6017947626638279	0.5557883269414055	T	T	T
0.2999999999999972	0.7000000000000028	0.5000000000000000	F	F	F
0.3999999999999986	0.6000000000000014	0.4456539999999976	F	F	F
0.4035118271221237	0.5959197330327768	0.5598683496196677	T	T	T
0.5000000000000000	0.7000000000000028	0.5000000000000000	F	F	F
0.6000000000000014	0.6000000000000014	0.4456539999999976	F	F	F
0.5714689512841988	0.6010632172738360	0.5696893543574830	T	T	T
0.7000000000000028	0.7000000000000028	0.5000000000000000	F	F	F
0.7999999999999972	0.6000000000000014	0.4456539999999976	F	F	F
0.8053359245369081	0.6040778550255436	0.5542853000549017	T	T	T
0.8999999999999986	0.7000000000000028	0.5000000000000000	F	F	F
0.0000000000000000	0.7999999999999972	0.4456539999999976	F	F	F
0.0000085443779061	0.7981957429394823	0.5557640735780208	T	T	T

0.1000000000000014	0.8999999999999986	0.5000000000000000	F	F	F
0.2000000000000028	0.7999999999999972	0.4456539999999976	F	F	F
0.1991577151669876	0.7985808044114506	0.5561758688163680	T	T	T
0.2999999999999972	0.8999999999999986	0.5000000000000000	F	F	F
0.3999999999999986	0.7999999999999972	0.4456539999999976	F	F	F
0.3989096553247303	0.8018964477319256	0.5551531585852564	T	T	T
0.5000000000000000	0.8999999999999986	0.5000000000000000	F	F	F
0.6000000000000014	0.7999999999999972	0.4456539999999976	F	F	F
0.6005063230881946	0.8019403946401404	0.5546010284496977	T	T	T
0.7000000000000028	0.8999999999999986	0.5000000000000000	F	F	F
0.7999999999999972	0.7999999999999972	0.4456539999999976	F	F	F
0.8016662567236008	0.8000154025993154	0.5547193453560612	T	T	T
0.8999999999999986	0.8999999999999986	0.5000000000000000	F	F	F
0.4269899824169852	0.6073754321899755	0.6466342957891439	T	T	T
0.4910689935832420	0.4828657277186323	0.6531233727666385	T	T	T
0.4898610639782828	0.4958576526701641	0.6109020366410908	T	T	T
0.6968680450610354	0.3240464573463011	0.5831695396657424	T	T	T
0.6574981362825933	0.2761771448353919	0.6078322210833660	T	T	T
0.4484515855036318	0.5180080893045333	0.6779014994637511	T	T	T
0.4795106550760822	0.5739507659493984	0.5993995458545837	T	T	T
0.5459551737331964	0.4291928967148220	0.6650364913903837	T	T	T
0.6088710967054662	0.3213698684498227	0.6354171170188682	T	T	T
0.6856875460745909	0.4044981854327815	0.5916977234225878	T	T	T
0.6596087867797075	0.2000232765546149	0.6097327838219703	T	T	T
0.7502498066892398	0.3057373755699354	0.5552525381767588	T	T	T
0.5696935807750444	0.4679983439690693	0.5976597963450637	T	T	T
0.4973759995816169	0.3436884499730972	0.5503407649809360	T	T	T
0.6809167170648472	0.4540032874399735	0.6580921543204959	T	T	T
0.6168899808165014	0.4143772337415292	0.6303545255575264	T	T	T

NOTE. S6(b) POSCAR (structure input file for VASP) parameters for the LiDFBOP binding on Li surface

Adsorption2

1.00000000000000

17.1174999999999997 0.0000000000000000 0.0000000000000000

0.0000000000000000 17.1174999999999997 0.0000000000000000

0.0000000000000000 0.0000000000000000 33.4234999999999971

Li C O F P

76 4 8 2 1

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.4456539999999976	F	F	F
0.0003513333935891	0.9962614639486523	0.5556300260263479	T	T	T

0.1000000000000014	0.1000000000000014	0.5000000000000000	F	F	F
0.2000000000000028	0.0000000000000000	0.4456539999999976	F	F	F
0.2000490586493945	0.9978205545215090	0.5555769257132198	T	T	T
0.2999999999999972	0.1000000000000014	0.5000000000000000	F	F	F
0.3999999999999986	0.0000000000000000	0.4456539999999976	F	F	F
0.3982129147483166	0.9977844169921872	0.5537722743067938	T	T	T
0.5000000000000000	0.1000000000000014	0.5000000000000000	F	F	F
0.6000000000000014	0.0000000000000000	0.4456539999999976	F	F	F
0.6014203811204332	0.9956757836382849	0.5528328813163444	T	T	T
0.7000000000000028	0.1000000000000014	0.5000000000000000	F	F	F
0.7999999999999972	0.0000000000000000	0.4456539999999976	F	F	F
0.7993034059382903	0.0028040485018378	0.5559767857179309	T	T	T
0.8999999999999986	0.1000000000000014	0.5000000000000000	F	F	F
0.0000000000000000	0.2000000000000028	0.4456539999999976	F	F	F
0.9964183581427336	0.1979851540149016	0.5547102804066688	T	T	T
0.1000000000000014	0.2999999999999972	0.5000000000000000	F	F	F
0.2000000000000028	0.2000000000000028	0.4456539999999976	F	F	F
0.2016923334738291	0.1979938010483712	0.5546394865731059	T	T	T
0.2999999999999972	0.2999999999999972	0.5000000000000000	F	F	F
0.3999999999999986	0.2000000000000028	0.4456539999999976	F	F	F
0.4062406597974931	0.1994516135985192	0.5571626483511506	T	T	T
0.5000000000000000	0.2999999999999972	0.5000000000000000	F	F	F
0.6000000000000014	0.2000000000000028	0.4456539999999976	F	F	F
0.6053552921302503	0.1773608751319710	0.5540886281156393	T	T	T
0.7000000000000028	0.2999999999999972	0.5000000000000000	F	F	F
0.7999999999999972	0.2000000000000028	0.4456539999999976	F	F	F
0.7746789256955132	0.2149429925623513	0.5618026261853722	T	T	T
0.8999999999999986	0.2999999999999972	0.5000000000000000	F	F	F
0.0000000000000000	0.3999999999999986	0.4456539999999976	F	F	F
-0.0000892776261214	0.4026296134948096	0.5546617491989694	T	T	T
0.1000000000000014	0.5000000000000000	0.5000000000000000	F	F	F
0.2000000000000028	0.3999999999999986	0.4456539999999976	F	F	F
0.2046748671038679	0.4015435796146194	0.5545923787075752	T	T	T
0.2999999999999972	0.5000000000000000	0.5000000000000000	F	F	F
0.3999999999999986	0.3999999999999986	0.4456539999999976	F	F	F
0.4206939254716215	0.4065402798656751	0.5696119578001694	T	T	T
0.5000000000000000	0.5000000000000000	0.5000000000000000	F	F	F
0.6000000000000014	0.3999999999999986	0.4456539999999976	F	F	F
0.6020916974198866	0.4110365313391032	0.5432160437504416	T	T	T
0.7000000000000028	0.5000000000000000	0.5000000000000000	F	F	F
0.7999999999999972	0.3999999999999986	0.4456539999999976	F	F	F
0.7956840546610554	0.4086008491821499	0.5564286875809574	T	T	T
0.8999999999999986	0.5000000000000000	0.5000000000000000	F	F	F
0.0000000000000000	0.6000000000000014	0.4456539999999976	F	F	F
0.0000595822949593	0.6008177864267371	0.5544957042904829	T	T	T

0.1000000000000014	0.7000000000000028	0.5000000000000000	F	F	F
0.2000000000000028	0.6000000000000014	0.4456539999999976	F	F	F
0.1890711776013470	0.6009113512630393	0.5538603987888148	T	T	T
0.2999999999999972	0.7000000000000028	0.5000000000000000	F	F	F
0.3999999999999986	0.6000000000000014	0.4456539999999976	F	F	F
0.3660052577080163	0.6091046644419386	0.5677352136847990	T	T	T
0.5000000000000000	0.7000000000000028	0.5000000000000000	F	F	F
0.6000000000000014	0.6000000000000014	0.4456539999999976	F	F	F
0.6421427241418342	0.6248808653913527	0.5755112852292782	T	T	T
0.7000000000000028	0.7000000000000028	0.5000000000000000	F	F	F
0.7999999999999972	0.6000000000000014	0.4456539999999976	F	F	F
0.8125037685320994	0.6002968462652220	0.5536097215548322	T	T	T
0.8999999999999986	0.7000000000000028	0.5000000000000000	F	F	F
0.0000000000000000	0.7999999999999972	0.4456539999999976	F	F	F
0.9997225726847340	0.7970379659175012	0.5566626190062259	T	T	T
0.1000000000000014	0.8999999999999986	0.5000000000000000	F	F	F
0.2000000000000028	0.7999999999999972	0.4456539999999976	F	F	F
0.2003126723407020	0.7983796486028996	0.5562443940272070	T	T	T
0.2999999999999972	0.8999999999999986	0.5000000000000000	F	F	F
0.3999999999999986	0.7999999999999972	0.4456539999999976	F	F	F
0.3972931516926139	0.8072118855312590	0.5520623376811677	T	T	T
0.5000000000000000	0.8999999999999986	0.5000000000000000	F	F	F
0.6000000000000014	0.7999999999999972	0.4456539999999976	F	F	F
0.5996800117609407	0.8055022115288195	0.5526672056981022	T	T	T
0.7000000000000028	0.8999999999999986	0.5000000000000000	F	F	F
0.7999999999999972	0.7999999999999972	0.4456539999999976	F	F	F
0.7993691663582426	0.7992463134776404	0.5559969359694280	T	T	T
0.8999999999999986	0.8999999999999986	0.5000000000000000	F	F	F
0.4948258936563172	0.6860730677972058	0.6093746416292614	T	T	T
0.4796887191685918	0.5475942403952239	0.6224436649723833	T	T	T
0.5560536455231219	0.5641857946703912	0.6281073192928212	T	T	T
0.6214101331475379	0.3039588207139926	0.5819872268240206	T	T	T
0.5439533063214663	0.2881679237733384	0.5797235678694673	T	T	T
0.4248678867012626	0.5965876188379554	0.6111343264597502	T	T	T
0.5898778641295265	0.6329598110550659	0.6233163524518398	T	T	T
0.4681789768508473	0.4652536828830553	0.6183604442941800	T	T	T
0.4982630543728085	0.3398538342805674	0.6021971883914824	T	T	T
0.6351865131498176	0.3737866643775391	0.6041578246165491	T	T	T
0.5076477783553351	0.2359891841434342	0.5569643232220129	T	T	T
0.6811320690559060	0.2681155668831496	0.5639735831490800	T	T	T
0.6027615239793970	0.4957022285412202	0.6293834466195330	T	T	T
0.4988220743113931	0.4112641184833727	0.5295413277747528	T	T	T
0.5503154044462637	0.3834457001584019	0.6670733418541868	T	T	T
0.5520243033540376	0.4149781861551167	0.6228045841257172	T	T	T

NOTE. S7 POSCAR (structure input file for VASP) parameters for the LiDFBOP molecule

LiDFBOP

1.00000000000000

20.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

O C P F Li

8 4 1 2 1

Direct

0.3051867269535222 0.5470730037503273 0.5131144703150952

0.3198046979019580 0.4178309636092550 0.4662528867361928

0.4183219821114434 0.5562591232712890 0.5069626062410677

0.5392180321377040 0.5694692575844087 0.5025513691101366

0.5523689133878662 0.4542193158054175 0.4606761423100707

0.6499571853446113 0.5949869320338976 0.5044369212604352

0.6658439598199166 0.4558706398161760 0.4544408721598714

0.4317847189261741 0.4372698642085524 0.4636831157010946

0.3619916411497144 0.5251490427117389 0.5006650017724539

0.3701191043528524 0.4533499600356876 0.4745945840632686

0.6139300925055480 0.4834311890299432 0.4673388166224726

0.6056739803060935 0.5557626229272969 0.4934455800474211

0.4891073264851471 0.5047739675970746 0.4832943889594787

0.4892448597574415 0.4769151203279449 0.5598057124912117

0.4777714196889278 0.5311265035654529 0.4071637884085817

0.2483052971711146 0.4742924917255422 0.4922436758011557

NOTE. S8 POSCAR (structure input file for VASP) parameters for the LiFSI molecule

LiFSI

1.00000000000000

10.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 10.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 10.0000000000000000

F S N O Li

2 2 1 4 1

Direct

0.2438102234441999 0.5200000586425375 0.5588678074578866

0.7024775893958122 0.5596905795207121 0.5478928226206889

0.3413808420070765 0.4192695192140761 0.4807034409171322

0.5673234877227884 0.5901328788135061 0.4656277819740211

0.4873816667036621 0.4606896223922234 0.5271656907245301

0.3060520943143104 0.4318506839295679 0.3433560269344227

0.3219147484651188 0.2918080819773721 0.5506455067840790

0.5174001360148779 0.7139714206062493 0.5168231212841192

0.6009071672368762 0.5742137001701906 0.3277221473635663
0.4940120636952798 0.2960333897335730 0.6326756249395658