Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic supplementary information

Evaluating the Behaviour of Deep Eutectic Solvent Electrolytes on 2D Ca_2C MXene Anode for the Li-Ion Batteries

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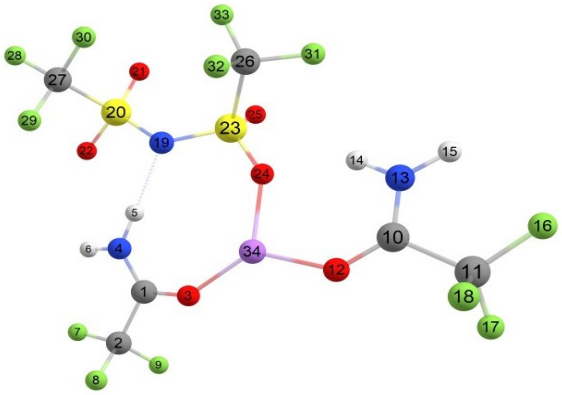
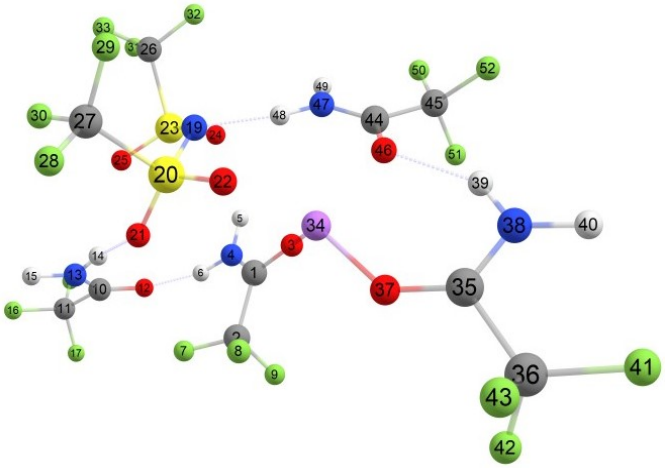
Table S1. Atomic Charges of Li[TFSI]:2TFA



Atoms	Atomic Number	Charge
1	C	0.75513900
2	C	0.65791300
3	O	-0.74033500
4	N	-0.99033000
5	H	0.58637100
6	H	0.43192700
7	F	-0.23570300
8	F	-0.22144200
9	F	-0.22112100
10	C	0.67254500
11	C	0.61472300
12	O	-0.65425600
13	N	-0.80188200
14	H	0.42158900
15	H	0.38405300
16	F	-0.22846800
17	F	-0.20183200
18	F	-0.20643000
19	N	-0.89624200
20	S	1.15961400
21	O	-0.51447800
22	O	-0.53594600
23	S	1.27587600
24	O	-0.78059200
25	O	-0.50632700
26	C	0.38174000
27	C	0.35449900
28	F	-0.14082200
29	F	-0.15432600
30	F	-0.11373600
31	F	-0.15863500
32	F	-0.15372900
33	F	-0.13616600
34	Li	0.89680900

Table S2. Atomic Charges of Li[TFSI]:4TFA.



Atoms	Atomic Number	Charge
1	C	0.841096000
2	C	0.504562000
3	O	-0.742571000
4	N	-0.938602000
5	H	0.487353000
6	H	0.488371000
7	F	-0.184122000
8	F	-0.180297000
9	F	-0.226833000
10	C	0.756786000
11	C	0.604246000
12	O	-0.664593000
13	N	-0.953525000
14	H	0.587095000
15	H	0.381542000
16	F	-0.231345000
17	F	-0.220381000
18	F	-0.214120000
19	N	-0.870456000
20	S	1.099035000
21	O	-0.651124000
22	O	-0.625642000
23	S	1.095087000
24	O	-0.570731000
25	O	-0.549299000
26	C	0.504232000
27	C	0.657919000
28	F	-0.195633000
29	F	-0.202671000
30	F	-0.207359000
31	F	-0.166619000
32	F	-0.176261000
33	F	-0.158357000
34	Li	0.913513000
35	C	0.734918000
36	C	0.607980000
37	O	-0.692708000
38	N	-0.898415000
39	H	0.452195000

40	H	0.405526000
41	F	-0.238896000
42	F	-0.205737000
43	F	-0.199000000
44	C	0.703182000
45	C	0.642179000
46	O	-0.670895000
47	N	-0.940730000
48	H	0.578086000
49	H	0.406331000
50	F	-0.220496000
51	F	-0.224806000
52	F	-0.229010000

Table S3. The Lennard Jones Parameters of Ca_2C.

Ca_2C atoms	**σ/nm**	**ε/kJ. mol^{-1}**	**Charge**
Ca_1	0.302800	0.996500	0.675140
Ca_2	0.302800	0.996500	0.675140
C	0.343100	0.439600	-1.35028

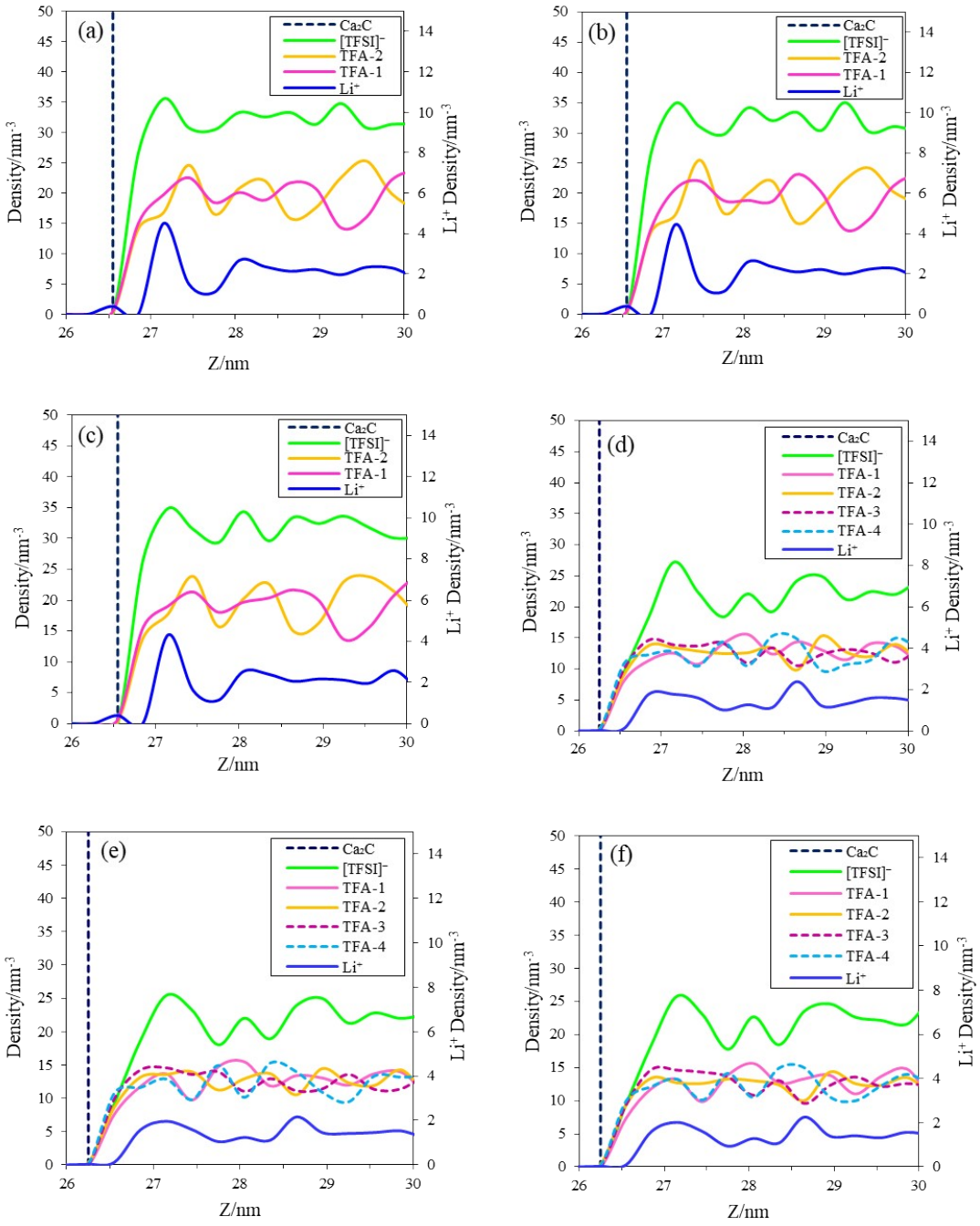


Figure S1. Density profiles of all species in Li[TFSI]:2TFA/Ca_2C at (a) 333.15 K, (b) 353.15 K, and (c) 373.15 K, and Li[TFSI]:4TFA/ Ca_2C at (d) 333.15 K, (e) 353.15 K, and (f) 373.15 K.

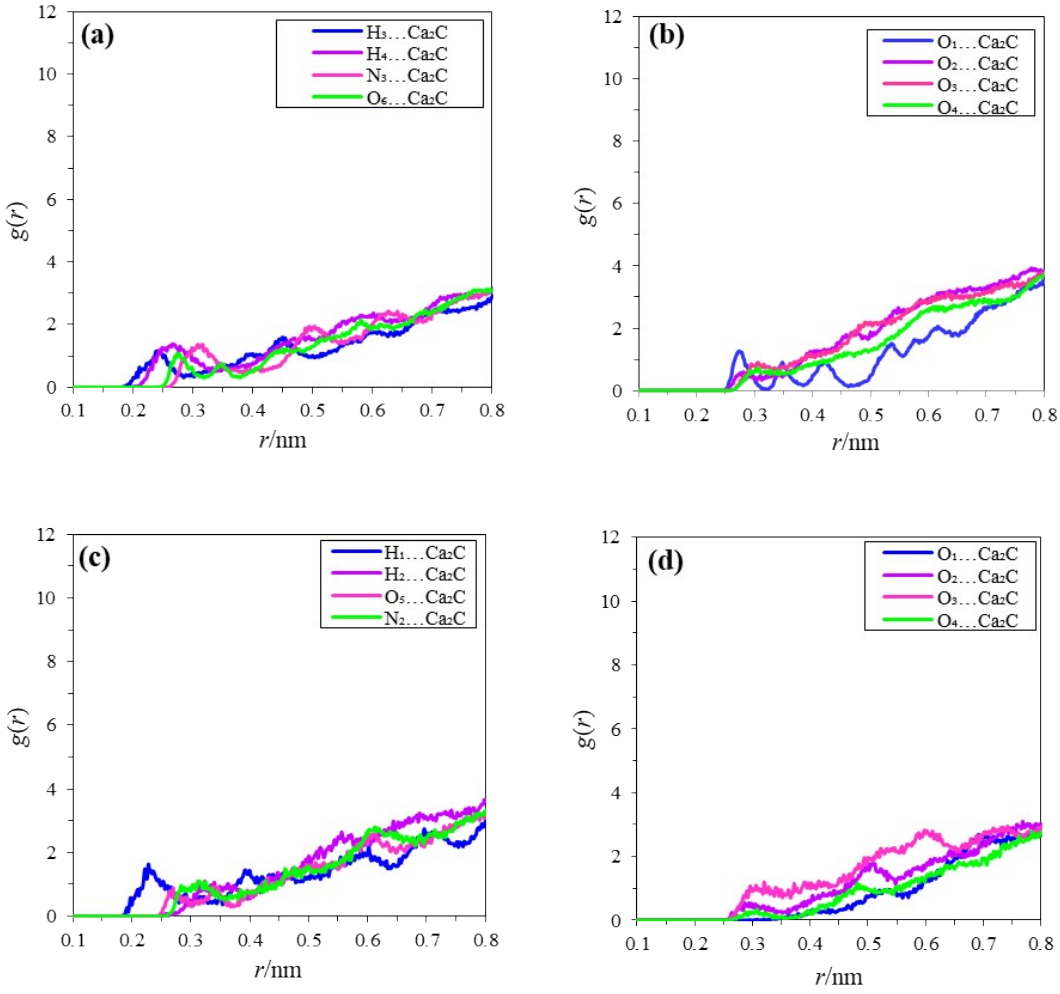


Figure S2. Pair correlation function between Ca_2C and (a) TFA-2 atoms of Li[TFSI]:2TFA, (b) $[TFSI]^-$ atoms of Li[TFSI]:2TFA, (c) TFA-1 atoms of Li[TFSI]:4TFA (d) $[TFSI]^-$ atoms of Li[TFSI]:4TFA at 298.15 K.

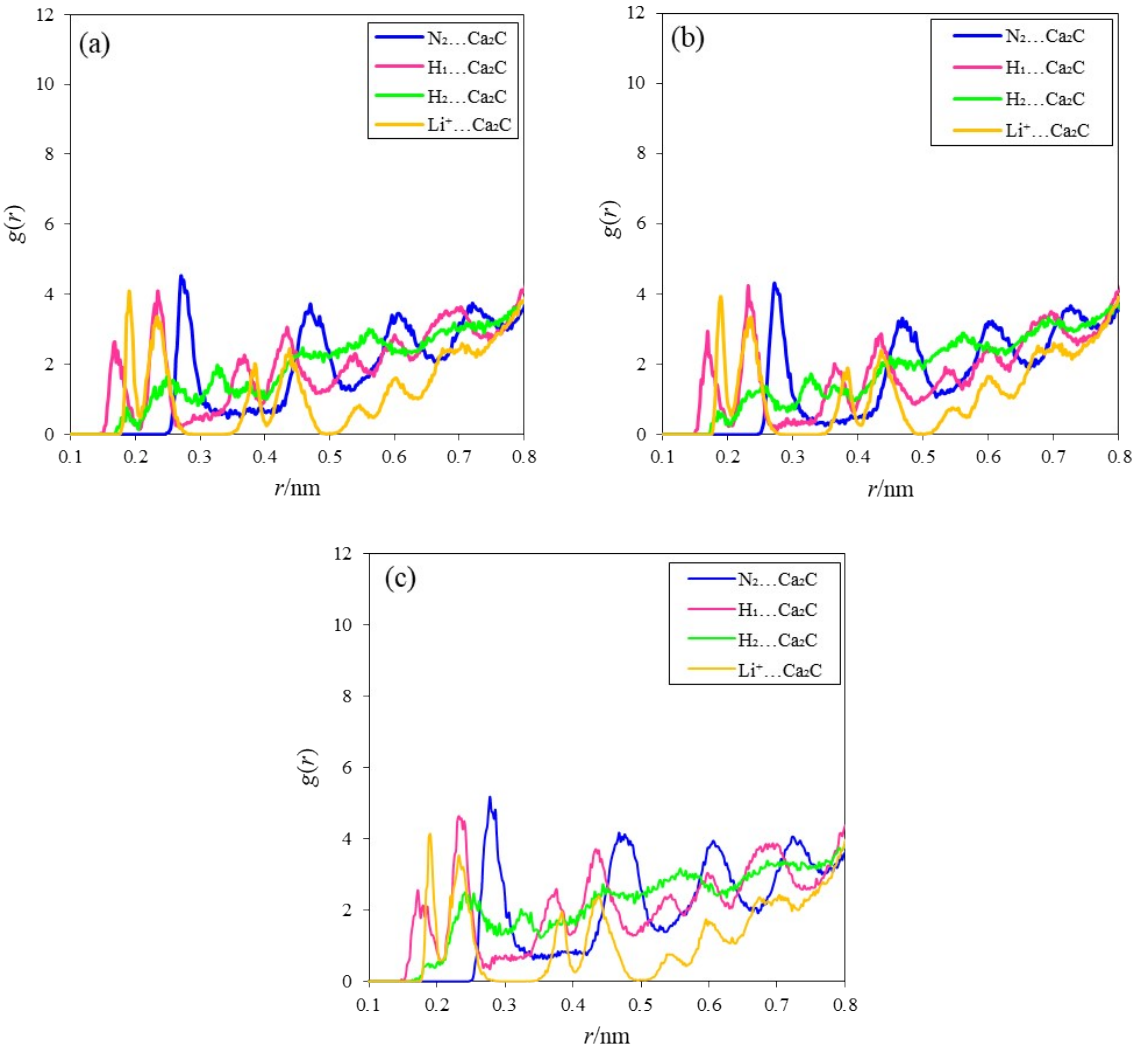


Figure S3. Pair correlation function between Ca_2C and TFA-1 atoms and Li^+ of Li[TFSI]:2TFA at (a) 333.15 K, (b) 353.15 K, and (c) 373.15 K.

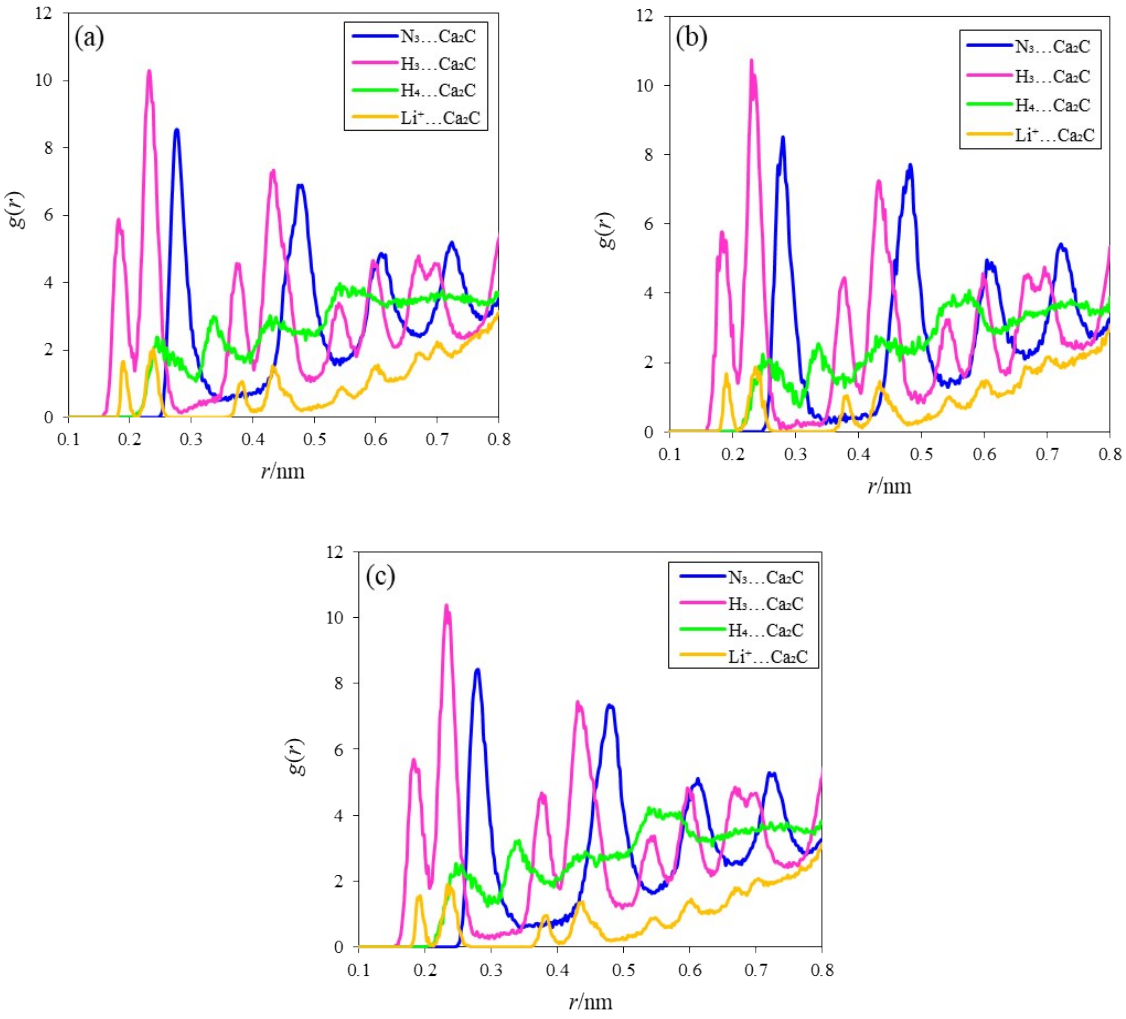


Figure S4. Pair correlation function between Ca_2C and TFA-2 atoms and Li^+ of Li[TFSI]:4TFA at (a) 333.15 K, (b) 353.15 K, and (c) 373.15 K.

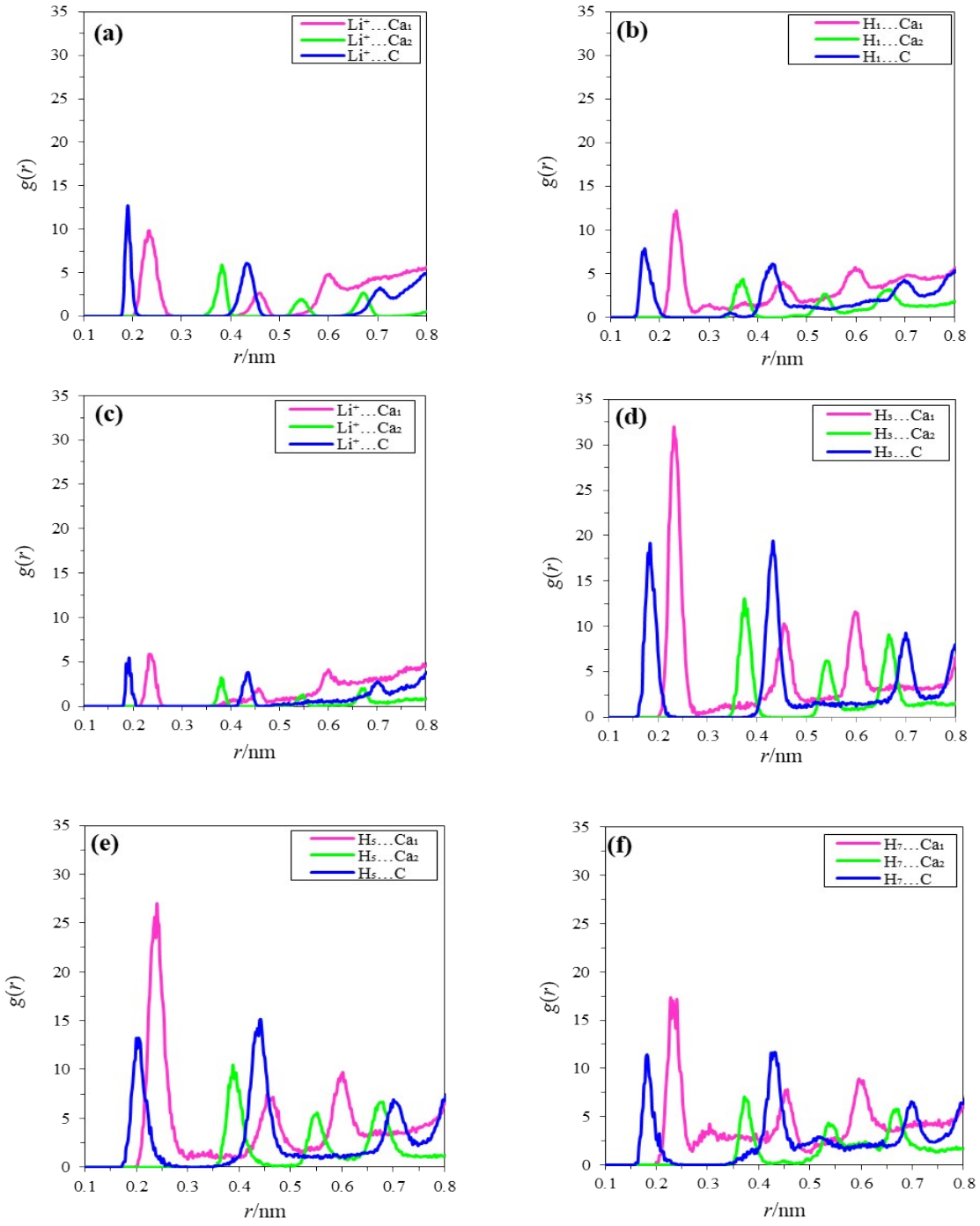


Figure S5. The pair correlation function between Ca_2C atoms and (a) Li^+ of Li[TFSI]:2TFA, (b) H_1 of Li[TFSI]:2TFA, (c) Li^+ of Li[TFSI]:4TFA, (d) H_3 of Li[TFSI]:4TFA, (e) H_5 of Li[TFSI]:4TFA, and (f) H_7 of Li[TFSI]:4TFA at 298.15 K.

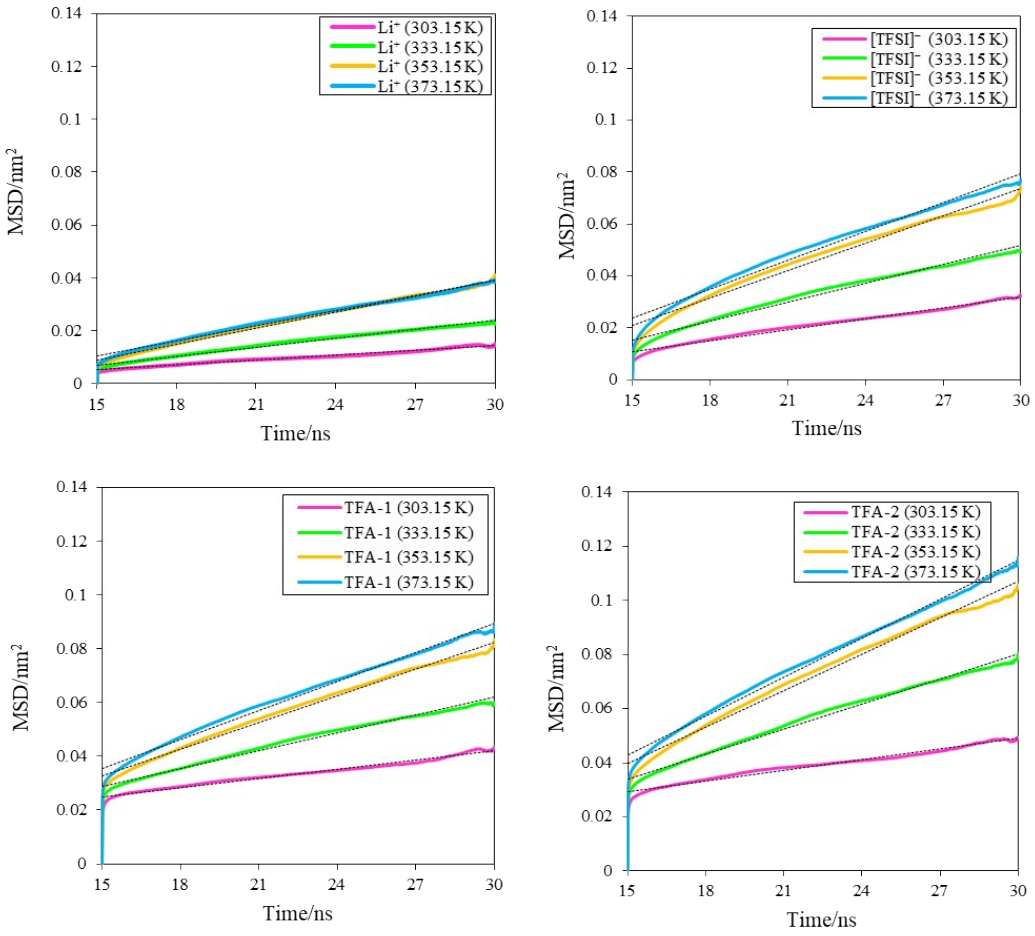


Figure S6. MSD curves of Li[TFSI]:2TFA particles over the last 15 ns of simulation time at 303.15 K., 333.15 K, 353.15 K, and 373.15 K.

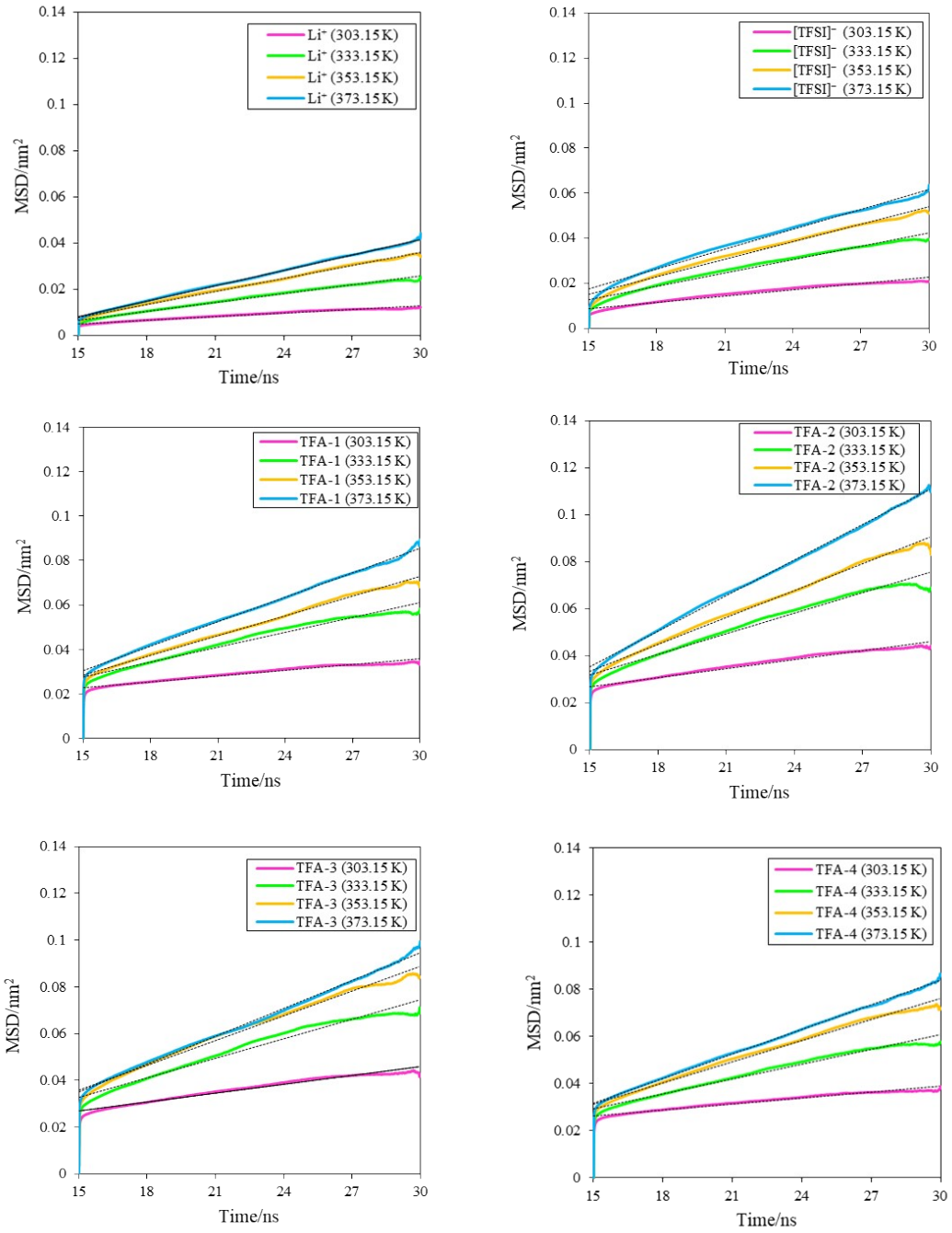


Figure S7. MSD curves of Li[TFSI]:4TFA particles over the last 15 ns of simulation time at 303.15 K., 333.15 K, 353.15 K, and 373.15 K.