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

Supplementary Information

Distinct Effect of Zwitterionic Molecules on Ionic Solvation in (Ethylene Oxide)$_{10}$: a Molecular Dynamics Simulation Study

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Table S1. Force field parameters. Labels as shown in Figure 1.

Label	σ (nm)	ε (kJ/mol)	q (e)
MPC			
C1	0.355	0.317984	-0.1723
C2	0.355	0.317984	-0.1605
C3	0.35	0.276144	-0.2016
C4	0.355	0.29288	0.4866
C5	0.35	0.276144	-0.0058
C6	0.35	0.276144	0.0849
C7	0.35	0.276144	-0.002
C8	0.35	0.276144	-0.0943
C9	0.35	0.276144	-0.1506
CX	0.35	0.276144	-0.1822
CY	0.35	0.276144	-0.1863
H11, and H12	0.25	0.12552	0.1428
H31, H32, and H33	0.25	0.12552	0.0983
H51, and H52	0.25	0.12552	0.1025
H61, and H62	0.25	0.12552	0.0971
H71, and H72	0.25	0.12552	0.0811
H81, and H82	0.25	0.12552	0.1306
H91, H92, and H93	0.25	0.12552	0.1608
HX1, HX2, and HX3	0.25	0.12552	0.1519
HY1, HY2, and HY3	0.25	0.12552	0.139
N	0.325	0.71128	-0.0123
O1	0.296	0.87864	-0.4613
O2	0.29	0.58576	-0.3565
O3	0.29	0.58576	-0.9069
O4, and O5	0.296	0.87864	-1.1686
O6	0.29	0.58576	-0.8125
P	0.374	0.8368	2.7126
CB			
C	0.355	0.29288	0.486

C1	0.35	0.276144	-0.276
C2	0.35	0.276144	0.023
C3	0.355	0.29288	0.198
C4	0.355	0.29288	-0.074
C5	0.355	0.29288	-0.077
C6	0.35	0.276144	0.002
C7	0.35	0.276144	-0.171
C8	0.35	0.276144	-0.29
H11, H12, and H13	0.25	0.12552	0.119
H21, and H22	0.25	0.12552	0.135
H3	0.242	0.12552	0.347
H4	0.242	0.12552	0.234
H5	0.242	0.12552	0.242
H61, and H62	0.25	0.12552	0.145
H71, and H72	0.25	0.12552	0.107
H81, and H82	0.25	0.12552	0.088
N1	0.325	0.71128	-0.324
N2	0.325	0.71128	-0.213
O1, and O2	0.296	0.87864	-0.707
SB			
C1	0.35	0.276144	-0.2595
C2	0.35	0.276144	-0.0352
C3	0.355	0.29288	0.0914
C4	0.355	0.29288	-0.1274
C5	0.355	0.29288	-0.08
C6	0.35	0.276144	-0.066
C7	0.35	0.276144	-0.133
C8	0.35	0.276144	-0.6807
H11, H12, and H13	0.25	0.12552	0.1196
H21, and H22	0.25	0.12552	0.1324
H3	0.242	0.12552	0.2719
H4	0.242	0.12552	0.25
H5	0.242	0.12552	0.2744

H61, and H62	0.25	0.12552	0.1318
H71, and H72	0.25	0.12552	0.1279
H81, and H82	0.25	0.12552	0.1329
N1	0.325	0.71128	-0.1837
N2	0.325	0.71128	-0.087
O1, O2, and O3	0.296	0.71128	-0.7122
S	0.355	1.046	1.4926
$[TFSI]^-$			
N	0.325	0.71128	-0.66
S1 and S2	0.355	1.046	1.02
O11, O12, O21 and O22	0.296	0.87864	-0.53
C1 and C2	0.35	0.27614	0.35
F11, F12 and F13	0.295	0.22175	-0.16
F21, F22 and F23	0.295	0.22175	-0.16
EO_{10}			
C1, and C20	0.35	0.276144	0.11
H1-3, and H40-42	0.25	0.12552	0.03
O1-10	0.29	0.58576	-0.4
C2-19	0.35	0.276144	0.14
H4-39	0.25	0.12552	0.03

Table S2. Details of the simulation systems

#	Li^+	$[TFSI]^-$	EO_{10}	ZW	Li^+: $O(EO_{10})$	Mol. conc. (mol/L)	Total number of atoms
		Case A:					
1	200	200	120		1:6	2.3	11840
2	200	200	120	40 MPC	1:6	2.3	13480
3	200	200	120	40 CB	1:6	2.4	12920
4	200	200	120	40 SB	1:6	2.4	12960
		Case B:					
5	100	100	180		1:18	1.1	14560
6	100	100	180	20 MPC	1:18	1.1	15380
7	100	100	180	20 CB	1:18	1.1	15100
8	100	100	180	20 SB	1:18	1.1	15120

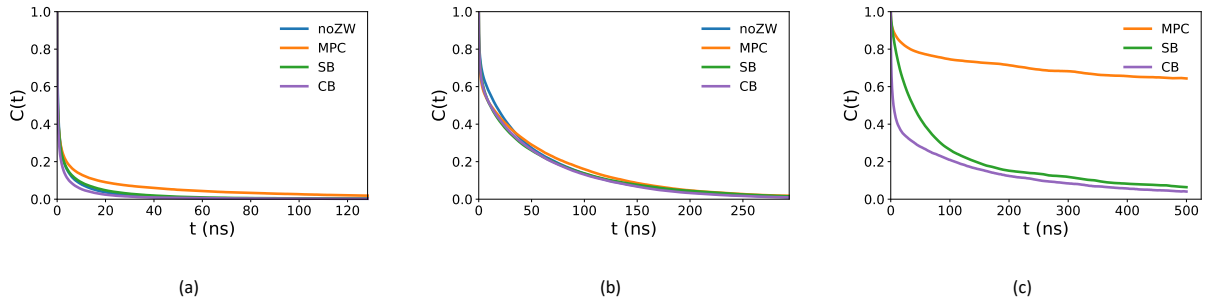


Figure S1. Residence C(t) curves of (a) Li^+-O($[TFSI]^-$) in, (b) Li^+-O(EO_{10}) and (c) Li^+-O(ZW) in case-A systems at 600K. Colors correspond to the presence of ZW molecules, as shown in the legends in Figure S1a.

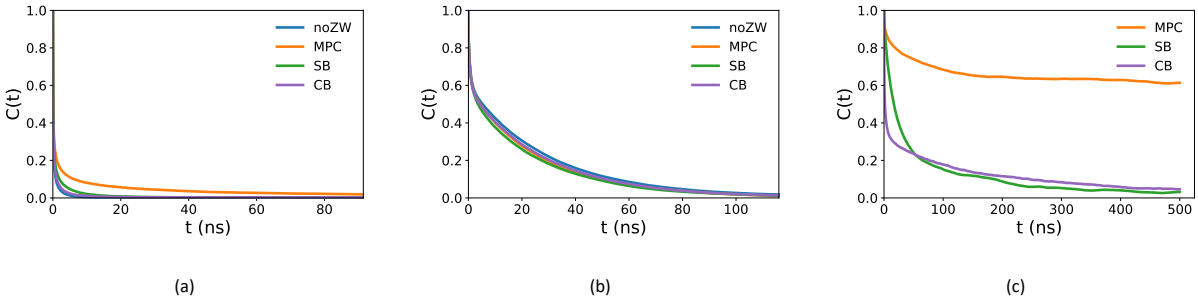
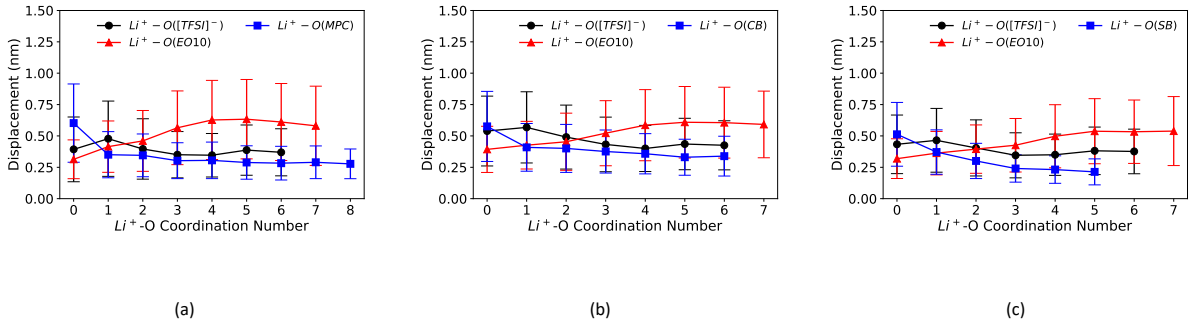
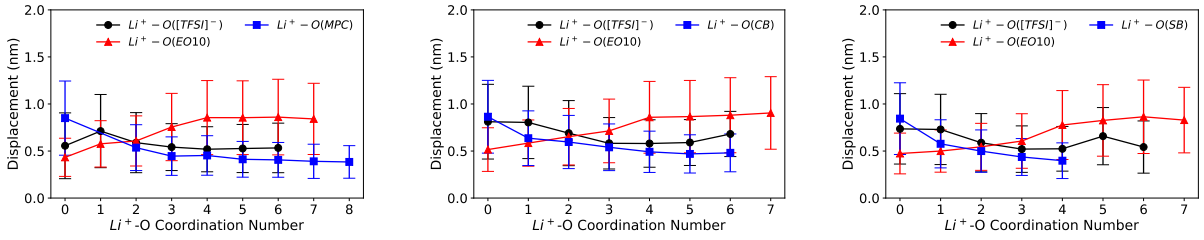


Figure S2. Residence C(t) curves of (a) Li^+-O($[TFSI]^-$), (b) Li^+-O(EO_{10}) and (c) Li^+-O(ZW) in case-B systems at 600K. Colors correspond to the presence of ZW molecules, as shown in the legends in Figure S2a.



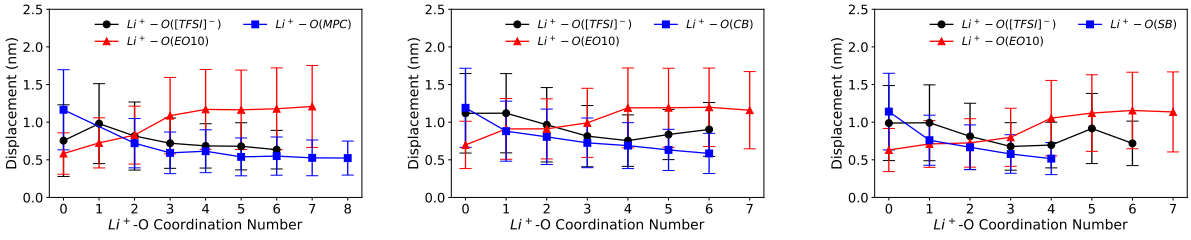
(a) (b) (c)

Figure S3. Distance travelled by Li⁺ ions in a specific O coordination number over 2-ns for case-A systems (a) with MPC, (b) with CB, and (c) with SB at 600K.



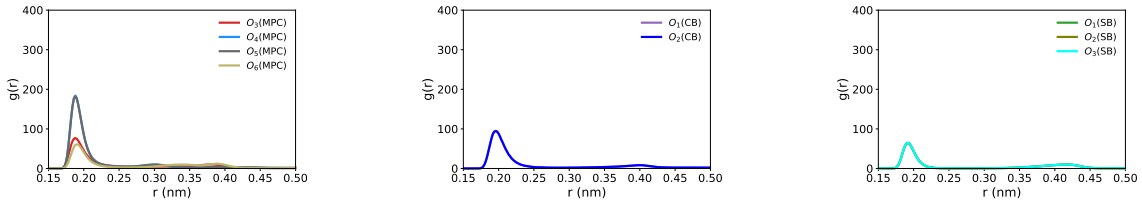
(a) (b) (c)

Figure S4. Distance travelled by Li⁺ ions in a specific O coordination number over 1-ns for case-B systems (a) with MPC, (b) with CB, and (c) with SB at 600K.



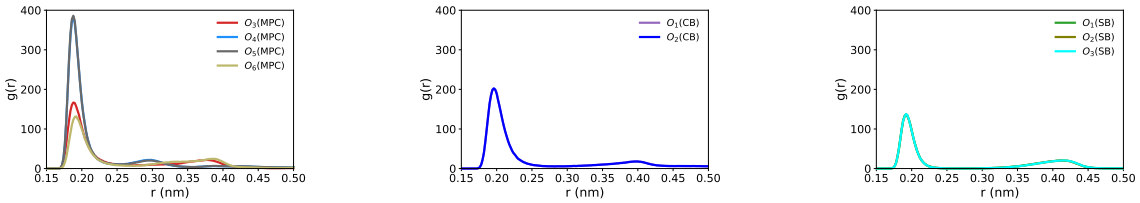
(a) (b) (c)

Figure S5. Distance travelled by Li⁺ ions in a specific O coordination number over 2-ns for case-B systems (a) with MPC, (b) with CB, and (c) with SB at 600K.



(a) (b) (c)

Figure S6. Radial distribution functions of (a) Li⁺-O(MPC), (b) Li⁺-O(CB) , and (c) Li⁺-O(SB) in case-A systems at 600K. Atom names are the same as in Figure 1.



(a) (b) (c)

Figure S7. Radial distribution functions of (a) Li^+-O(MPC), (b) Li^+-O(CB) , and (c) Li^+-O(SB) in case-B systems at 600K. Atom names are the same as in Figure 1.

Table S3. Diffusion coefficient of Li^+ at 600K (nm^2/ns)

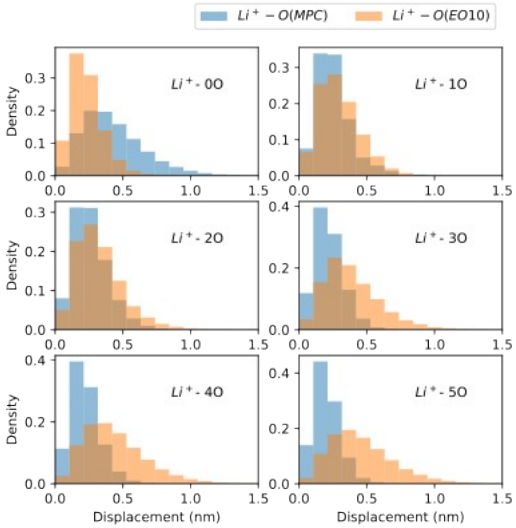
System	noZW	MPC	CB	SB
A	0.019± 0.001	0.019 ± 0.003	0.019 ± 0.001	0.015 ± 0.003
B	0.128 ± 0.018	0.081 ± 0.004	0.099 ± 0.006	0.090 ± 0.005

Table S4. Diffusion coefficient of $[TFSI]^-$ at 600K (nm^2/ns)

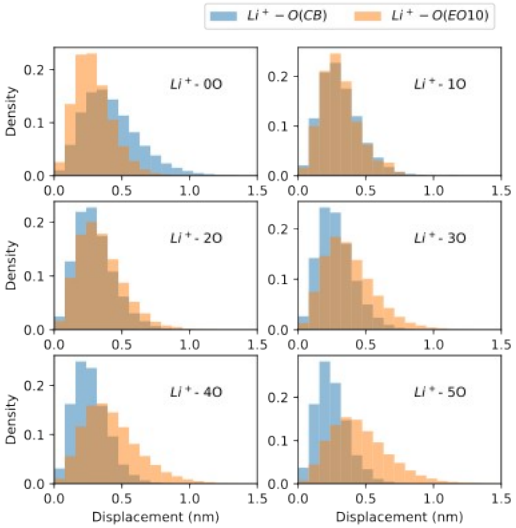
System	noZW	MPC	CB	SB
A	0.027 ± 0.002	0.023 ± 0.003	0.030 ± 0.001	0.024 ± 0.004
B	0.161 ± 0.032	0.102 ± 0.003	0.131 ± 0.014	0.131 ± 0.007

Table S5. Diffusion coefficients of ZW at 600K (nm^2/ns)

System	MPC	CB	SB
A	0.007 ± 0.002	0.007 ± 0.001	0.006 ± 0.001
B	0.025 ± 0.008	0.048 ± 0.009	0.045 ± 0.006



(a)



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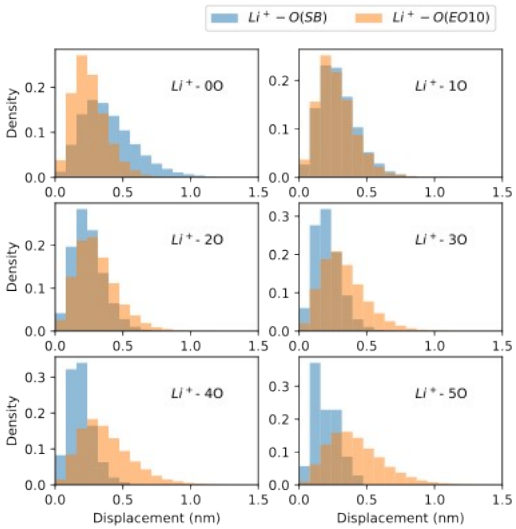
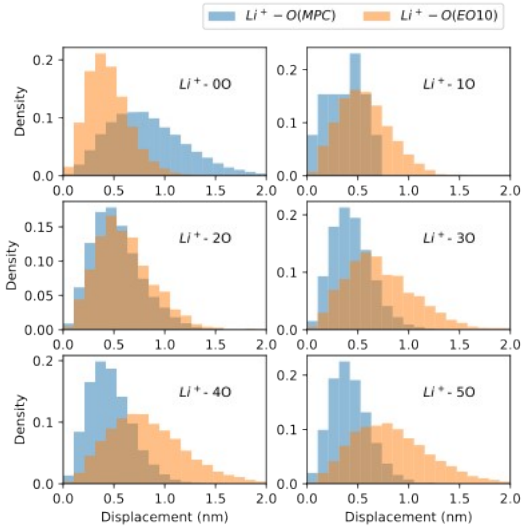
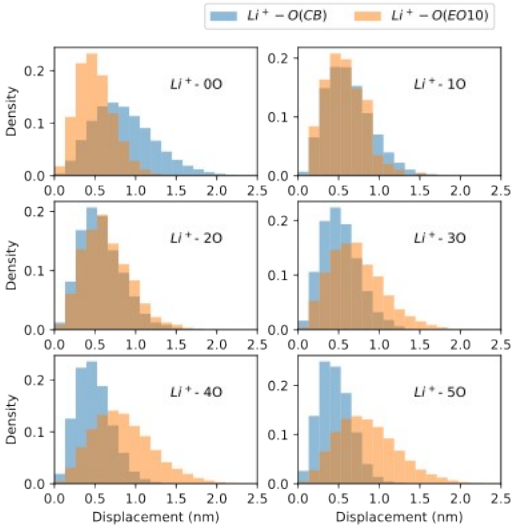


(c)

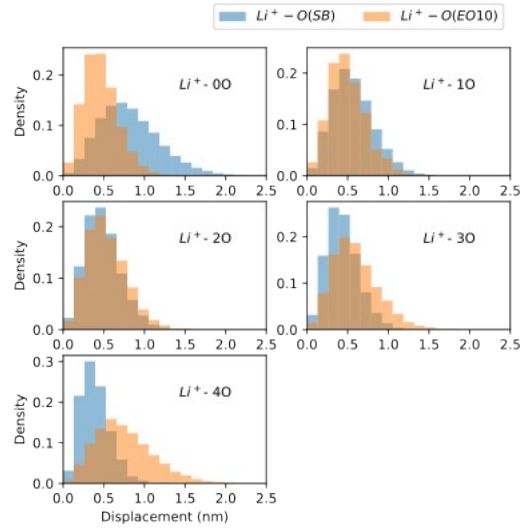
Figure S8. Distribution of distance traveled by Li^+ ions in a specific O coordination number over 1-ns for systems (a) with MPC, (b) with CB, and (c) with SB in case-A systems at 600K.



(a)

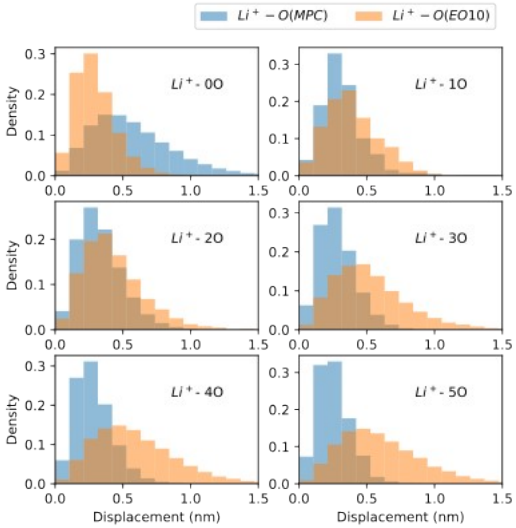


(b)

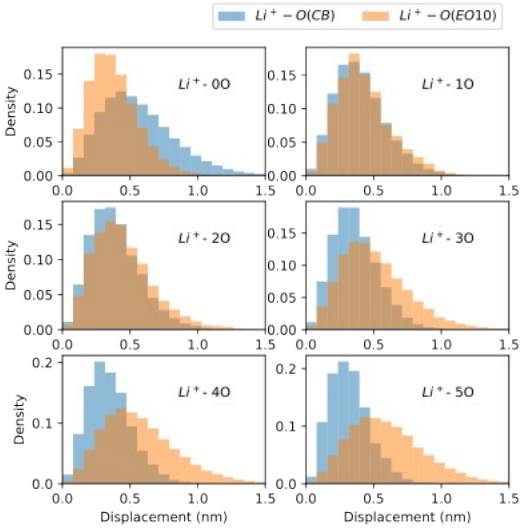


(c)

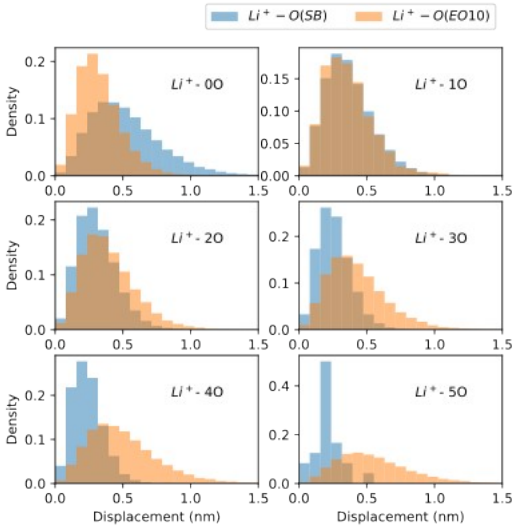
Figure S9. Distribution of distance traveled by Li^+ ions in a specific O coordination number over 1-ns for systems (a) with MPC, (b) with CB, and (c) with SB in case-B systems at 600K.



(a)

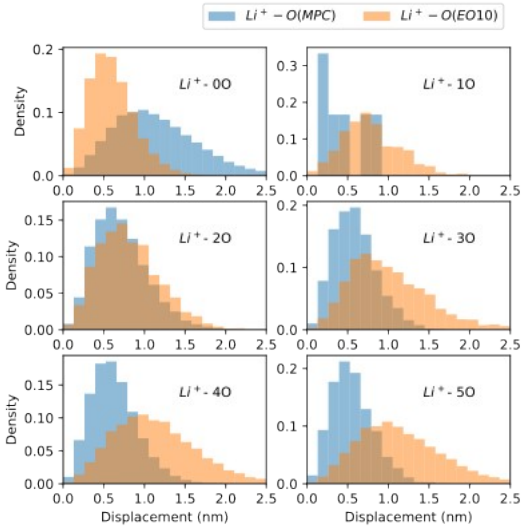


(b)

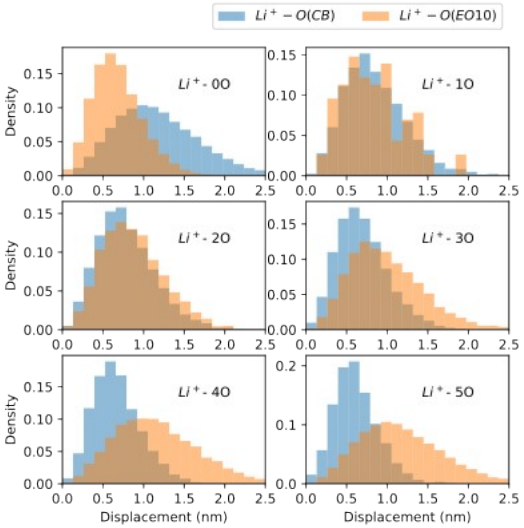


(c)

Figure S10. Distribution of distance traveled by Li^+ ions in a specific O coordination number over 2-ns for systems (a) with MPC, (b) with CB, and (c) with SB in case-A systems at 600K.



(a)



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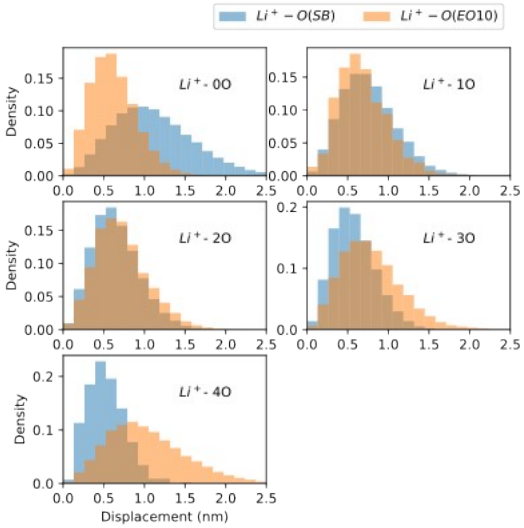
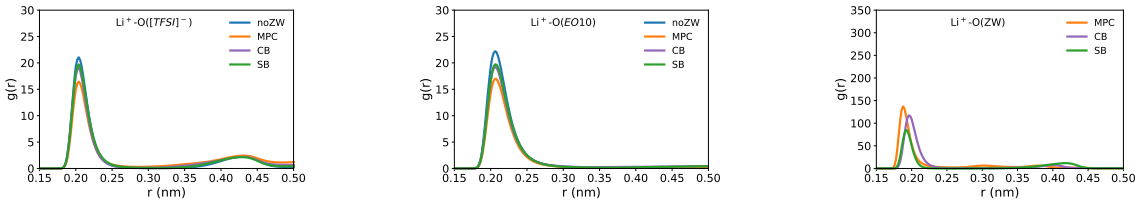


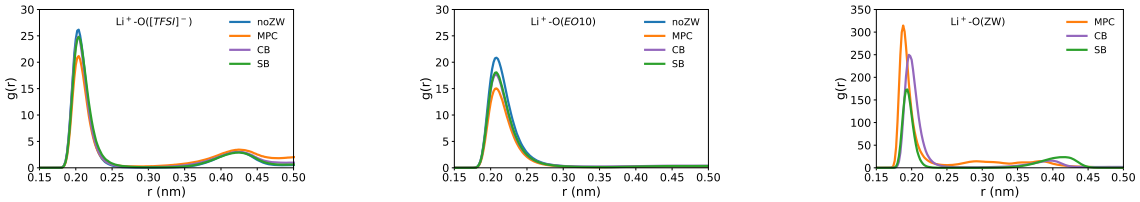
(c)

Figure S11. Distribution of distance traveled by Li^+ ions in a specific O coordination number over 2-ns for systems (a) with MPC, (b) with CB, and (c) with SB in case-B systems at 600K.



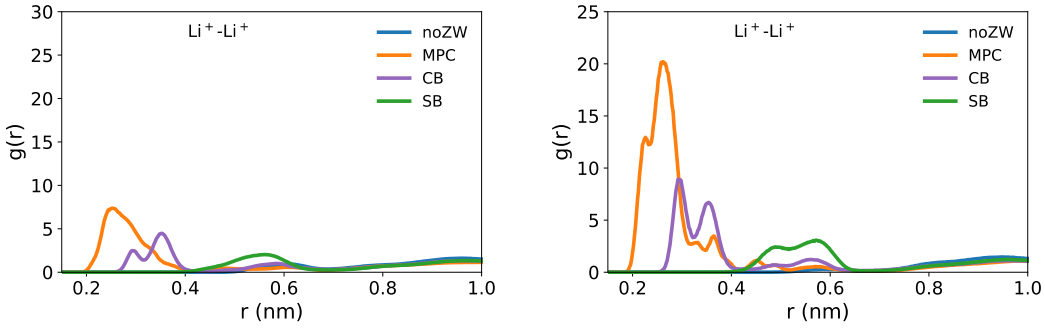
(a) (b) (c)

Figure S12. Radial distribution functions of (a) Li^+-O([TFSI]$^-$), (b) Li^+-O(EO_{10}) and (c) Li^+-O(ZW) in case-A systems at 353K.



(a) (b) (c)

Figure S13. Radial distribution functions of (a) Li^+-O([TFSI]$^-$), (b) Li^+-O(EO_{10}) and (c) Li^+-O(ZW) in case-B systems at 353K.



(a) (b)

Figure S14. Radial distribution functions of Li^+-Li^+ in (a) case-A and (b) case-B systems at 353K.

Table S6. Association numbers of Li^+-O in case-A systems at 353K

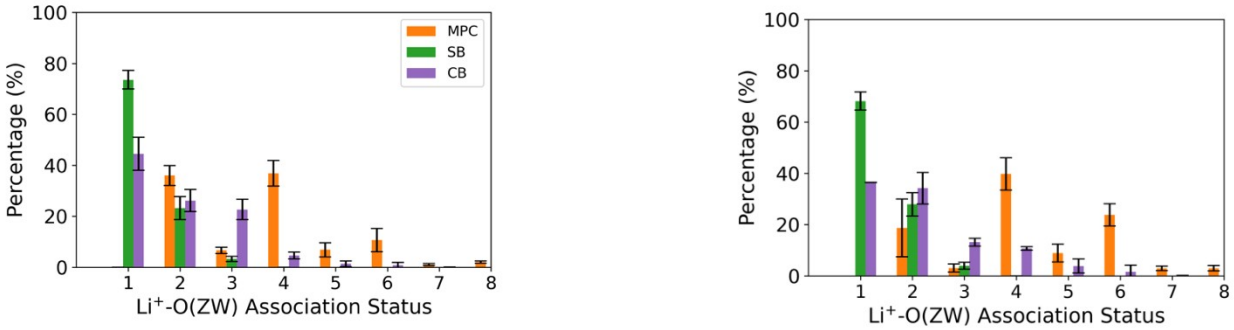
	No ZW	MPC	SB	CB
Total	6.42 ± 0.01	6.18 ± 0.03	6.09 ± 0.01	6.17 ± 0.02
Li^+-O(ZW)	N/A	1.51 ± 0.05	0.60 ± 0.01	0.78 ± 0.03
Li^+-O($[TFSI]^-$)	1.94 ± 0.03	1.42 ± 0.03	1.72 ± 0.04	1.64 ± 0.02
Li^+-O(EO_{10})	4.47 ± 0.03	3.24 ± 0.02	3.77 ± 0.05	3.75 ± 0.05

Table S7. Association numbers of Li^+-O in case-B systems at 353K

	No ZW	MPC	SB	CB
Total	6.75 ± 0.01	6.42 ± 0.08	6.37 ± 0.01	6.47 ± 0.03
Li^+-O(ZW)	N/A	1.46 ± 0.09	0.58 ± 0.01	0.76 ± 0.03
Li^+-O($[TFSI]^-$)	0.95 ± 0.02	0.74 ± 0.04	0.98 ± 0.04	0.95 ± 0.04
Li^+-O(EO_{10})	5.80 ± 0.03	4.22 ± 0.19	4.81 ± 0.04	4.76 ± 0.08

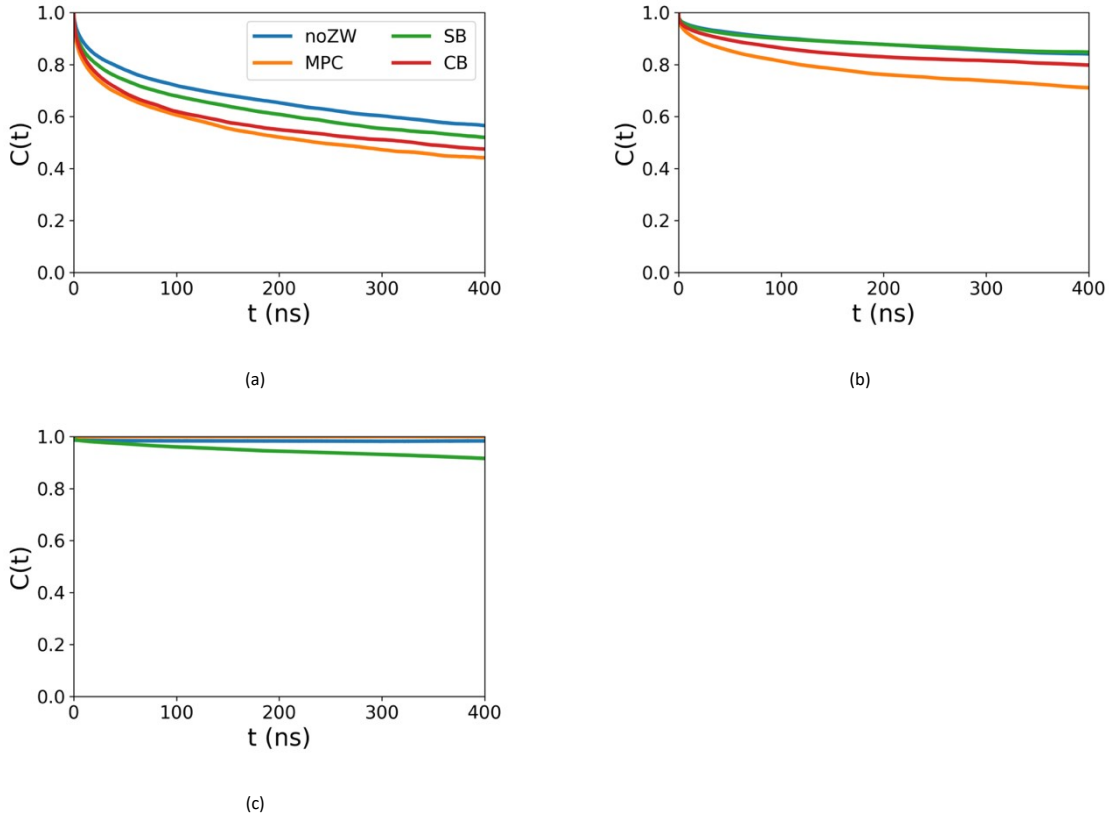
Table S8. Percentage of Li^+ not coordinating with EO_{10} for systems at 353K

System	CB	MPC	noZW	SB
A	21 ± 3 %	35 ± 1 %	8 ± 1 %	20 ± 2 %
B	10 ± 3 %	23 ± 5 %	0	7 ± 1 %



(a) (b)

Figure S15. Association statuses of Li^+-O(ZW) in (a) case-A, and (b) case-B systems 353K. Colors correspond to the presence of ZW molecules, as shown in the legends in Figure S15a.



(a) (b)

(c)

Figure S16. Residence C(t) curves of (a) Li^+-O($[TFSI]^-$) in, (b) Li^+-O(EO_{10}) and (c) Li^+-O(ZW) in case-A systems at 353K. Colors correspond to the presence of ZW molecules, as shown in the legends in Figure S16a.

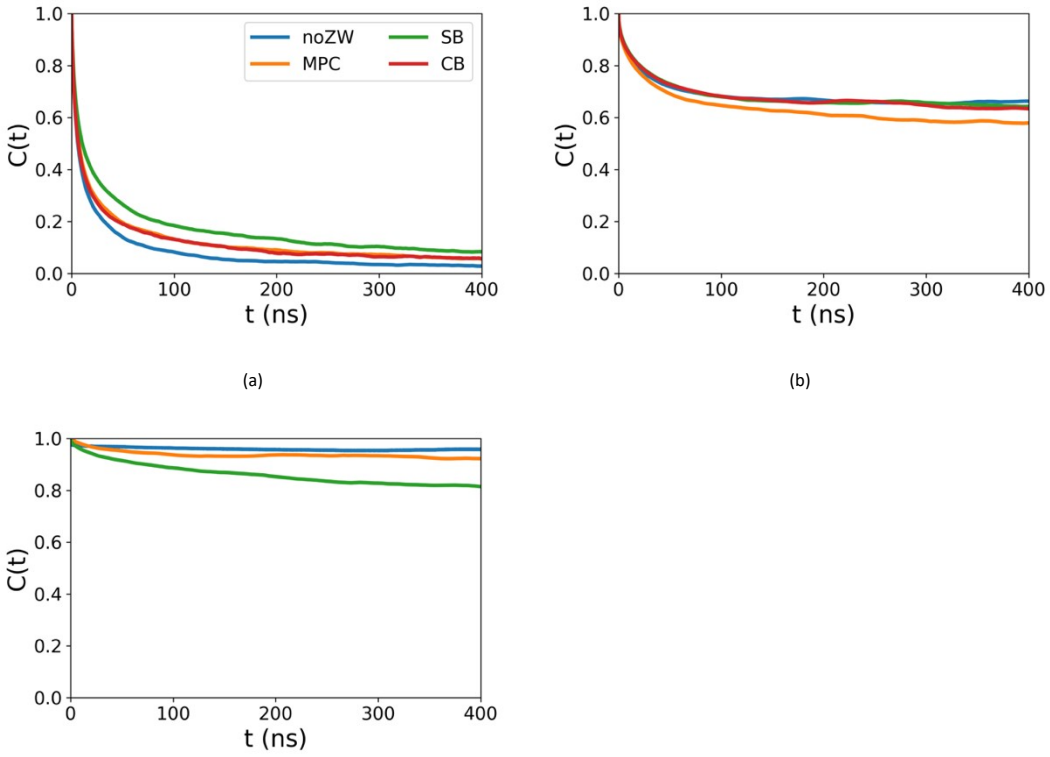


Figure S17. Residence C(t) curves of (a) Li^+-O($[TFSI]^-$), (b) Li^+-O(EO_{10}) and (c) Li^+-O(ZW) in case-B systems at 353K. Colors correspond to the presence of ZW molecules, as shown in the legends in Figure S17a.

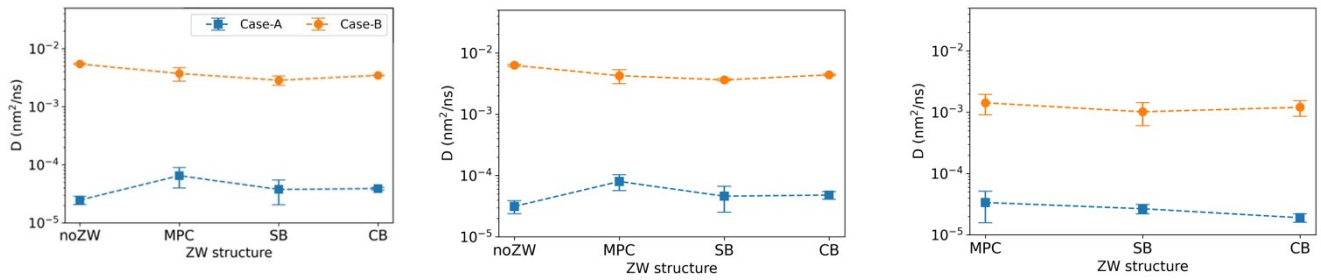


Figure S18. Diffusion coefficients of (a) Li^+, (b) $[TFSI]^-$, and (c) ZW for systems at 353K. Colors correspond to the Li^+:O(EO_{10}) molar ratios - r, as shown in the legends in Figure S18a.