Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.


E-mail:

**Table S1:** Non-bonding force field parameters for ions

| system | atom | q(e) | $\sigma$(Å) | $\epsilon(\frac{KJ}{mol})$ |
|---|---|---|---|---|
| Li | Li1 | 1 | 2.34 | 0.6700 |
| $PF_6$ | P1 | 0.580 | 3.94 | 0.8360 |
| - | F1 | -0.263 | 3.12 | 0.2552 |
| - | F2 | -0.263 | 3.12 | 0.2552 |
| - | F3 | -0.263 | 3.12 | 0.2552 |
| - | F4 | -0.263 | 3.12 | 0.2552 |
| - | F5 | -0.263 | 3.12 | 0.2552 |
| - | F6 | -0.263 | 3.12 | 0.2552 |

**Table S2:** Non-bonding force field parameters for EA solvent.

| system | atom | q (e) | $\sigma$(Å) | $\epsilon(\frac{KJ}{mol})$ |
|---|---|---|---|---|
| EA | C1 | -0.295 | 3.50 | 0.2761 |
| - | C2 | 0.299 | 3.50 | 0.2761 |
| - | C3 | 0.783 | 3.75 | 0.4393 |
| - | C4 | -0.553 | 3.50 | 0.2761 |
| - | O1 | -0.458 | 3.00 | 0.7112 |
| - | O2 | -0.571 | 2.96 | 0.8786 |
| - | H1 | 0.088 | 2.50 | 0.1255 |
| - | H2 | 0.088 | 2.50 | 0.1255 |
| - | H3 | 0.088 | 2.50 | 0.1255 |
| - | H4 | 0.021 | 2.42 | 0.0627 |
| - | H5 | 0.021 | 2.42 | 0.0627 |
| - | H6 | 0.163 | 2.50 | 0.1255 |
| - | H7 | 0.163 | 2.50 | 0.1255 |
| - | H8 | 0.163 | 2.50 | 0.1255 |

**Table S3:** Non-bonding force field parameters for EMS solvent

| system | atom | q (e) | $\sigma$(Å) | $\epsilon(\frac{KJ}{mol})$ |
|---|---|---|---|---|
| EMS | C1 | -0.509 | 3.50 | 0.2761 |
| - | C2 | -0.072 | 3.50 | 0.2761 |
| - | C3 | -0.180 | 3.50 | 0.2761 |
| - | O1 | -0.548 | 2.93 | 1.1715 |
| - | O1 | -0.548 | 2.93 | 1.1715 |
| - | S1 | 0.832 | 3.56 | 1.6526 |
| - | H1 | 0.201 | 2.50 | 0.1255 |
| - | H2 | 0.201 | 2.50 | 0.1255 |
| - | H3 | 0.201 | 2.50 | 0.1255 |
| - | H4 | 0.097 | 2.50 | 0.1255 |
| - | H5 | 0.097 | 2.50 | 0.1255 |
| - | H6 | 0.076 | 2.50 | 0.1255 |
| - | H7 | 0.076 | 2.50 | 0.1255 |
| - | H8 | 0.076 | 2.50 | 0.1255 |


**Figure S1:** Preliminary information to use Supporting Information tables.

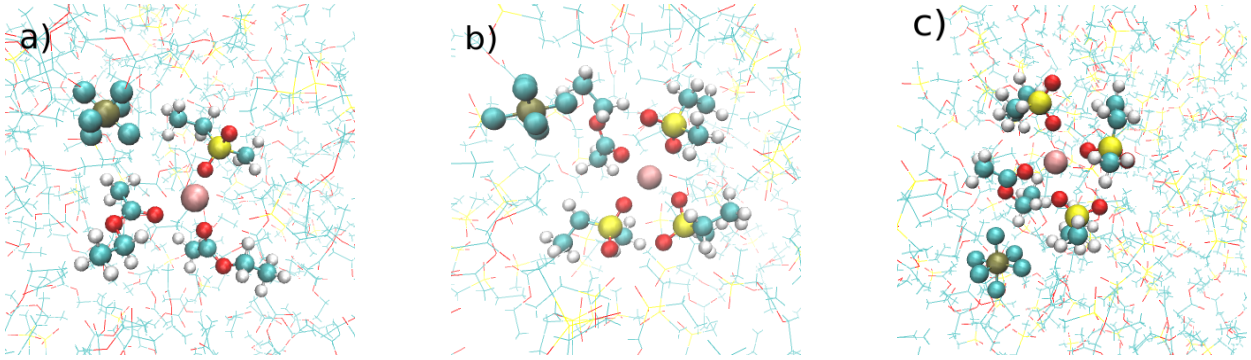


**Figure S2:** Panels (a), (b), and (c) represent the structural snapshot of system 3 (2:1(EA:EMS)), system 4 (1:2(EA:EMS)) and system 5 (1:1(EA:EMS)), respectively in visualizing molecular dynamics (VMD) after the NVE simulation at 45 ns.

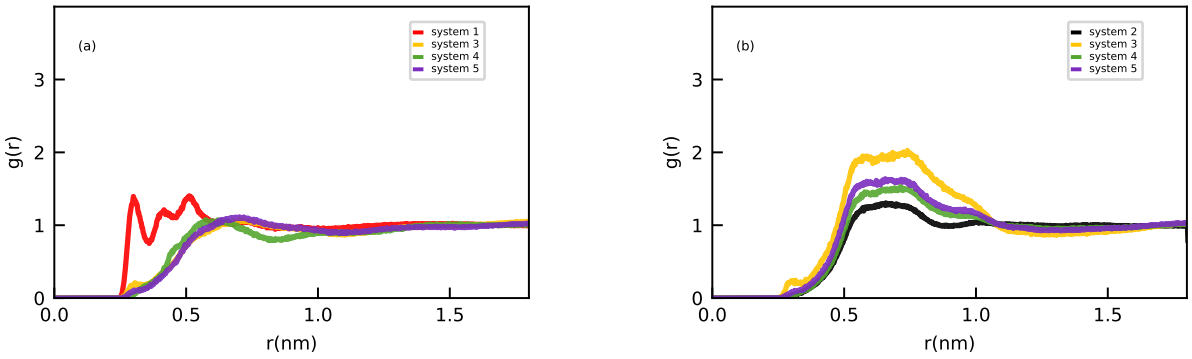


**Figure S3:** Radial distribution functions, g(r) of (a) $PF_6^-$ and oxygen atoms of EA, (b) $PF_6^-$ and oxygen atoms of EMS as a function of different molar ratio of EA and EMS.

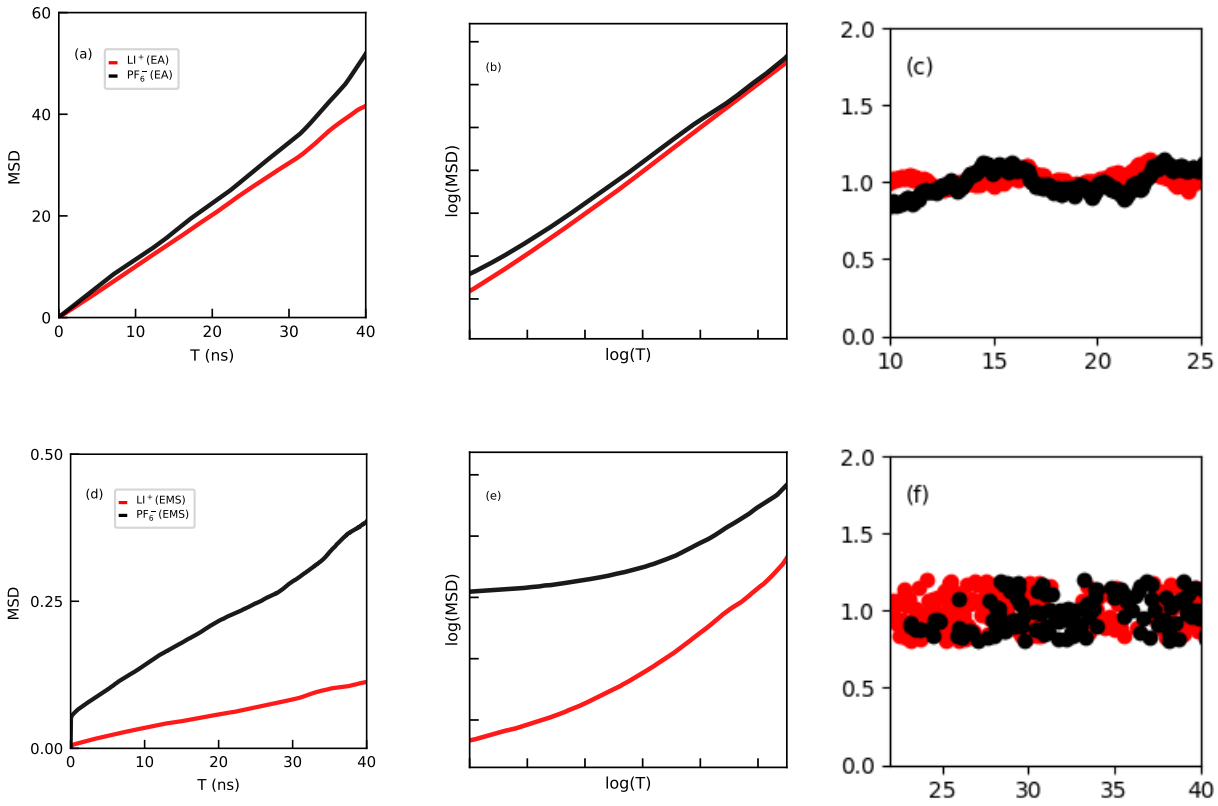


**Figure S4:** The left panels (a) and (d) represent the mean squared displacement, the middle panels (b) and (e) represent the log MSD versus log T plots and the right panels (c) and (f) show the beta value which corresponds to the diffusive regime for the cation and anion in unmixed EA and EMS systems, respectively.

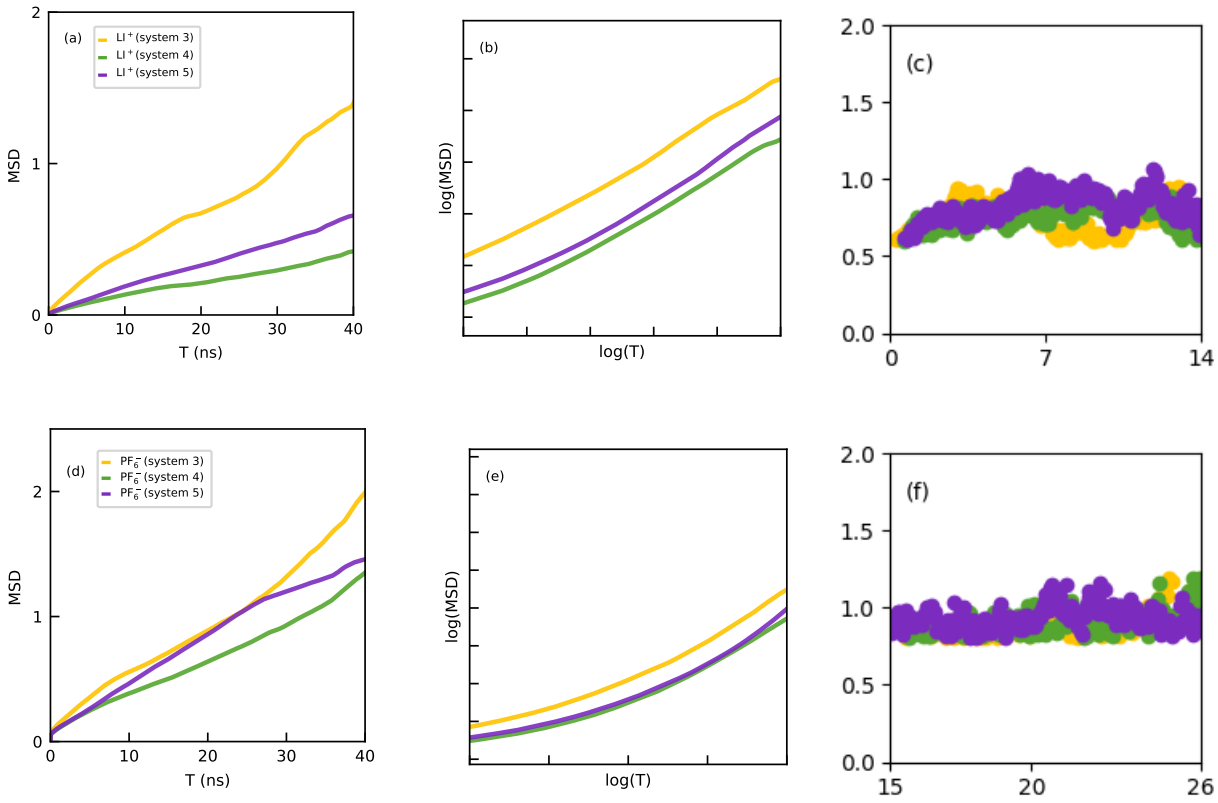


**Figure S5:** Upper panel of figure represents the diffusive motion of cation while the lower panel of figure represents the diffusive motion of anion in different solvent mixtures. (a) and (d) represent the mean square displacement, (b) and (e) represent the log MSD versus log T and (c) and (f) represent the beta value which is shown under diffusive regime.

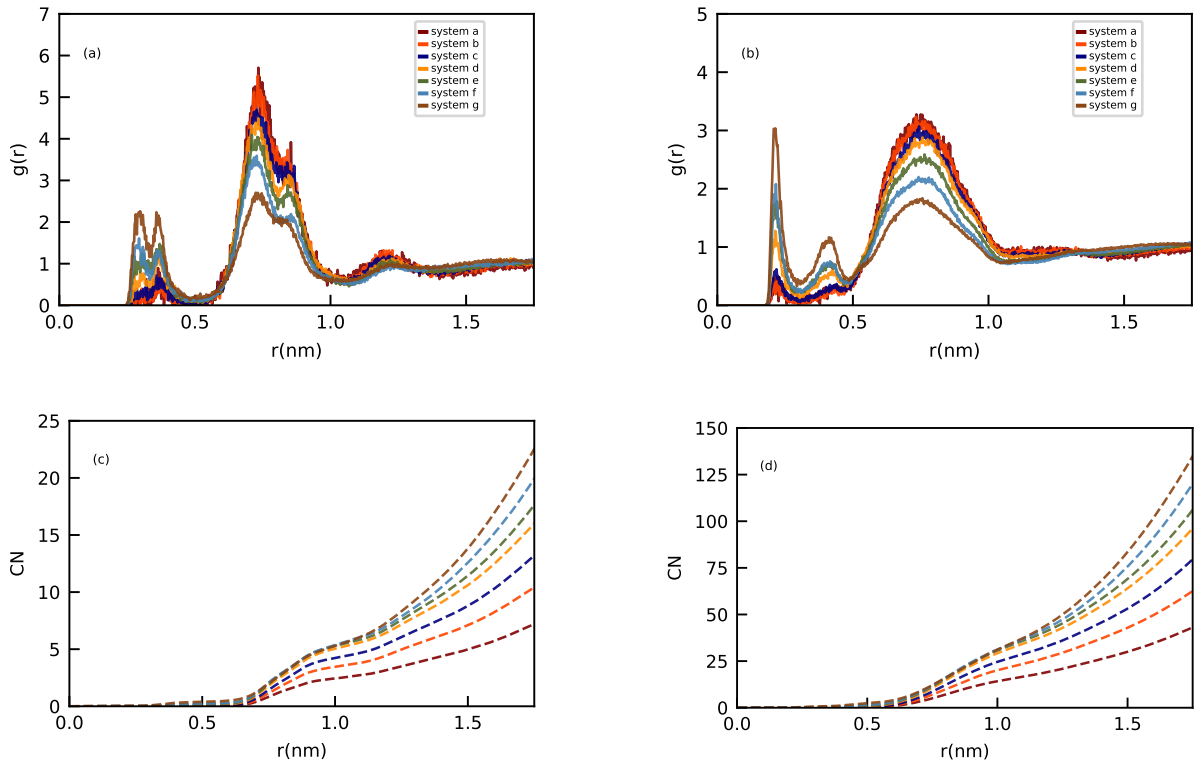


**Figure S6:** Illustrate radial distribution functions, g(r) and number integral where panel (a) represents the correlation of $Li^+$ with phosphorus atoms of anions, (b) represents the correlation of $Li^+$ with fluorine atoms of anions as a function of different salt concentration. The corresponding number distribution functions are shown in panels (c) and (d): (c) number integral of phosphorus atoms of anoins around cation, $CN_{Li\text{-}P}$, (d) number integral of fluorine atoms of anions around cation, $CN_{Li\text{-}F}$ in systems with different salt concentration.

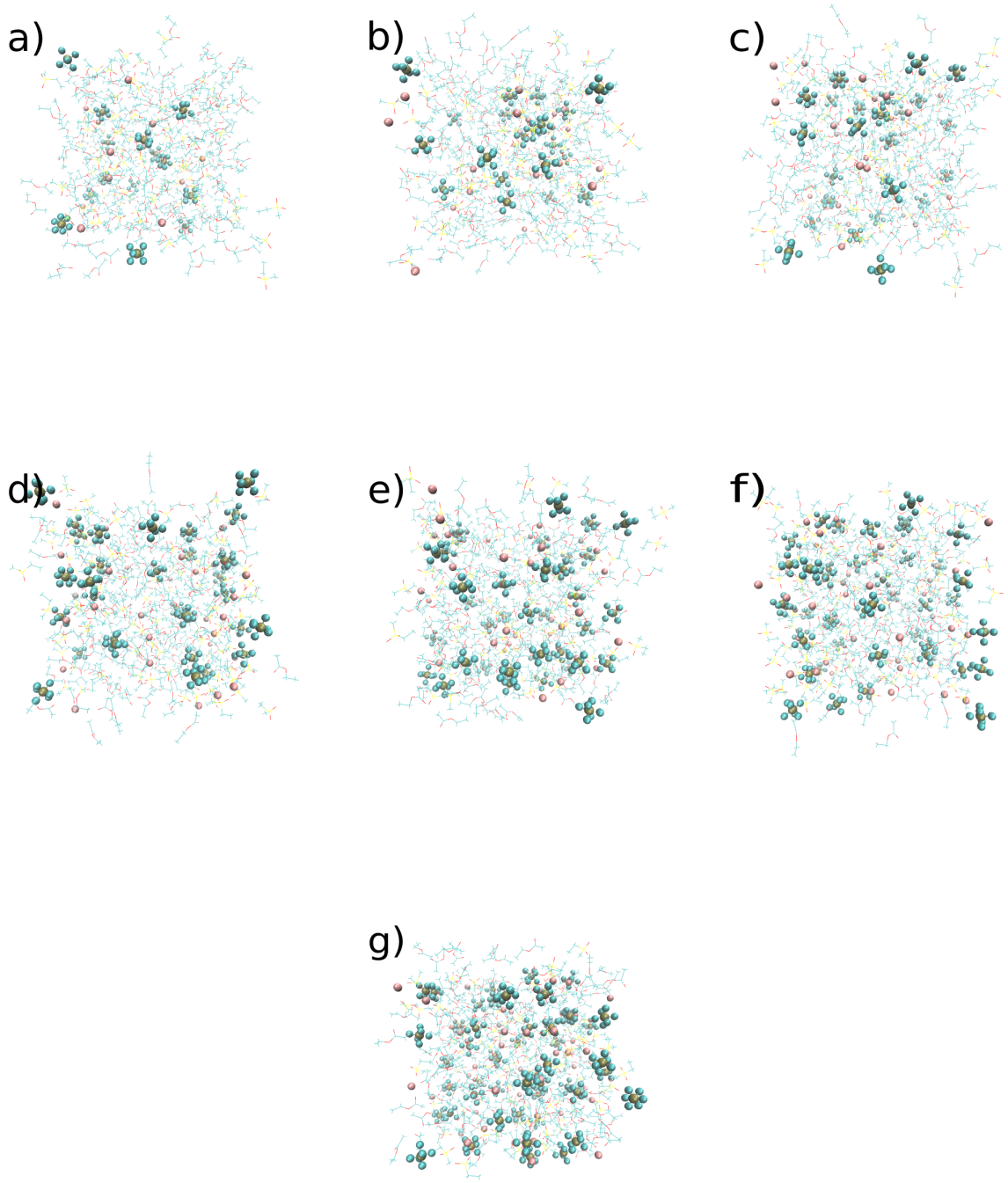


**Figure S7:** Snap shots of systems with different salt concentration from the trajectories. Panels a, b, c, d, e, f, and g represent the system having concentration of 0.485, 0.694, 0.894, 1.084, 1.261, 1.463, and 1.643 M.

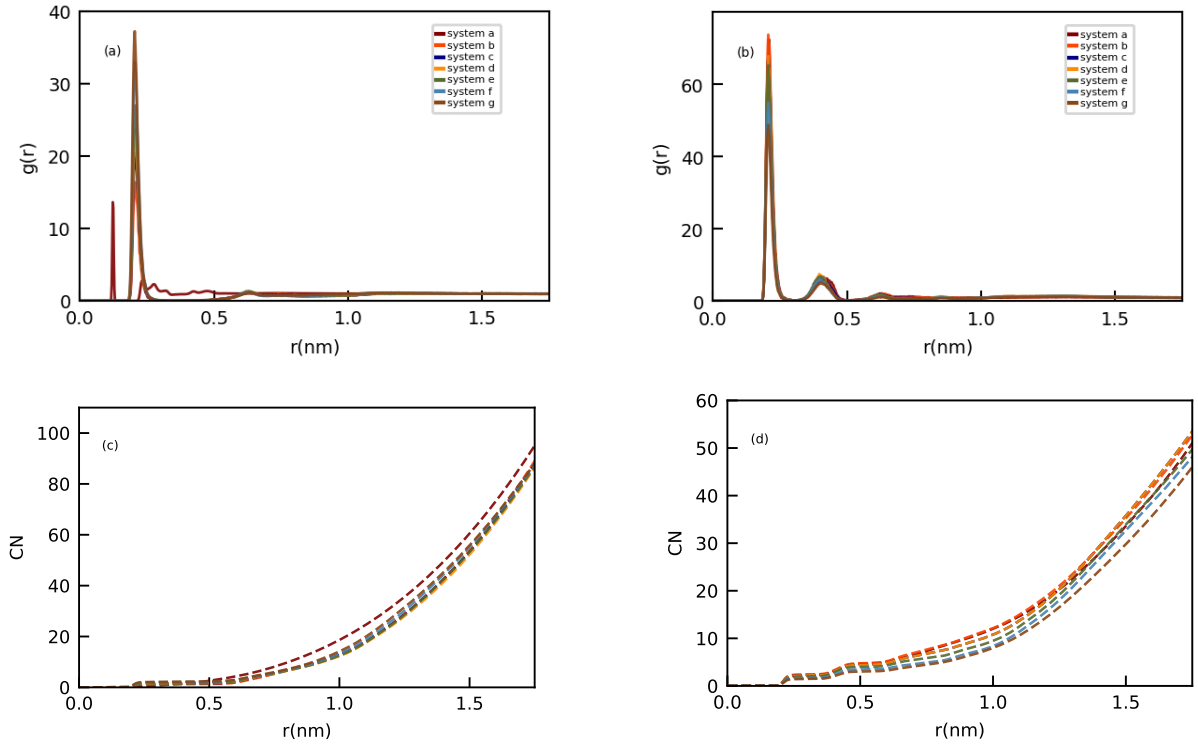


**Figure S8:** Radial distribution functions of $Li^+$-$O_{EA}$ (a) and $Li^+$-$O_{EMS}$ (b) with their integrated profiles, panels (c) and (d), respectively as a function of different salt concentration.

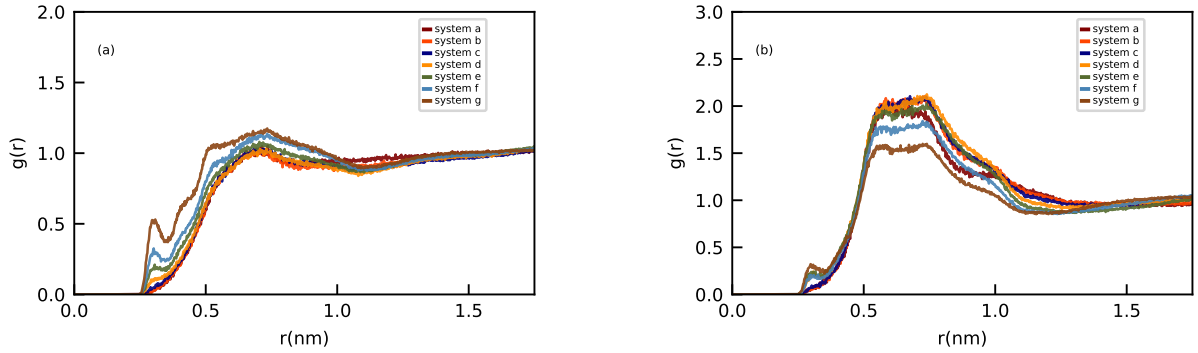


**Figure S9:** Panels (a) and (b) represents the correlation of anion with carbonyl oxygen atom of EA and oxygen atoms of EMS, respectively with varying salt concentration.

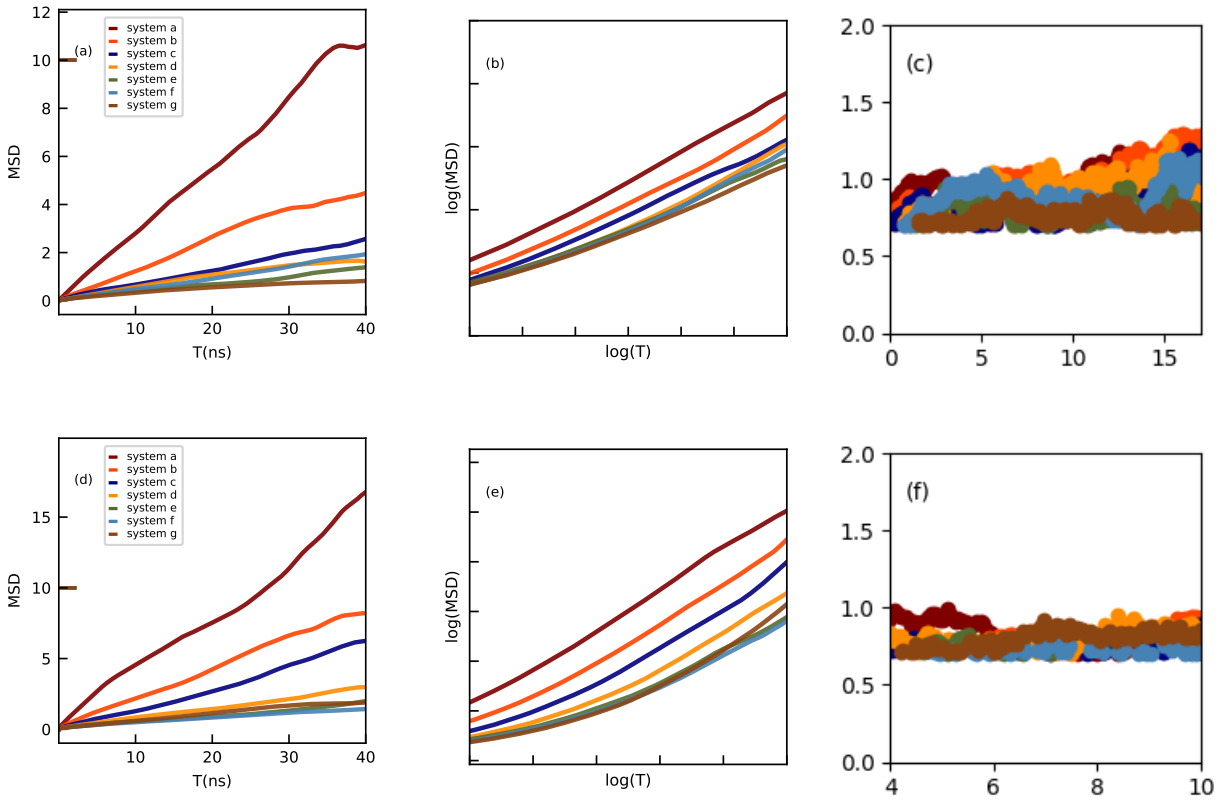


**Figure S10:** Upper panel of figure represents the diffusive motion of cation while the lower panel of figure represents the diffusive motion of anion in systems with different salt concentration. The left panels (a) and (d) represent the mean squared displacement, the middle panels (b) and (e) represent the log MSD versus log T plots and the left panels (c) and (f) show the beta value which corresponds to the diffusive regime.

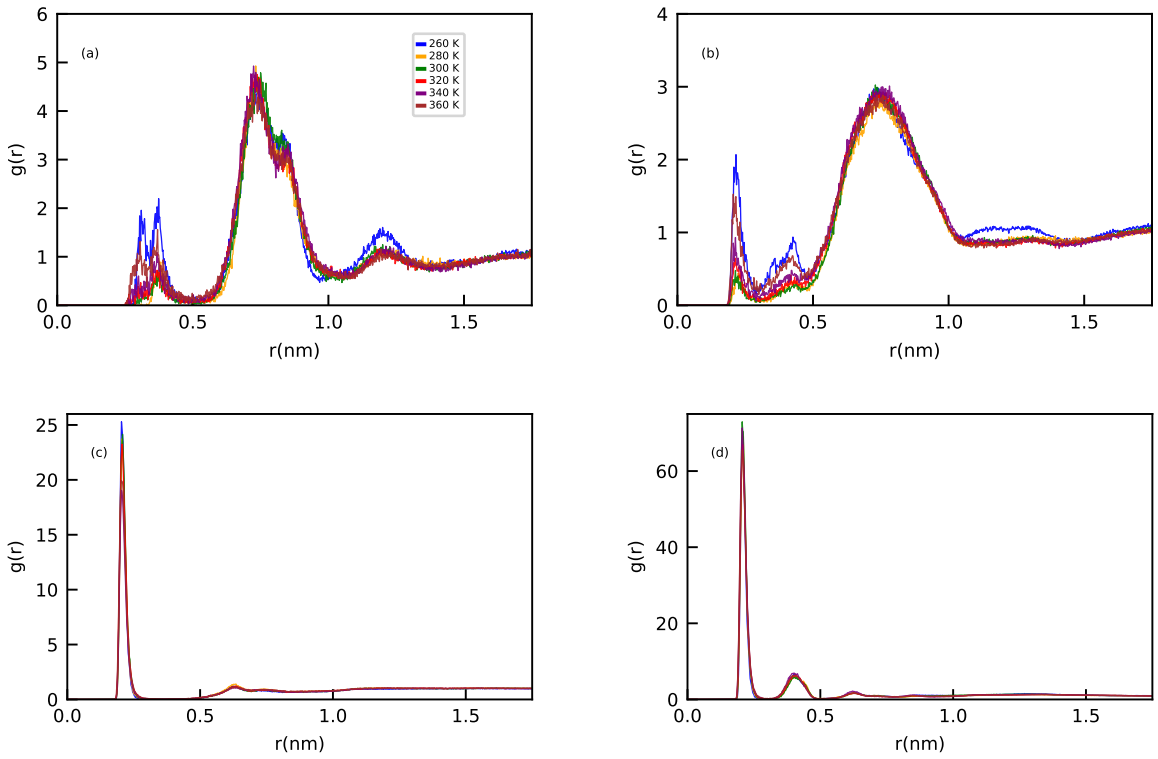


**Figure S11:** Radial distribution functions of (a) $Li^+$-P, (b) $Li^+$-F, (c) $Li^+$-$O_{EA}$, and (d) $Li^+$-$O_{EMS}$ as a function of temperature. We present the data for temperatures with a difference of 20 K for better visualization.

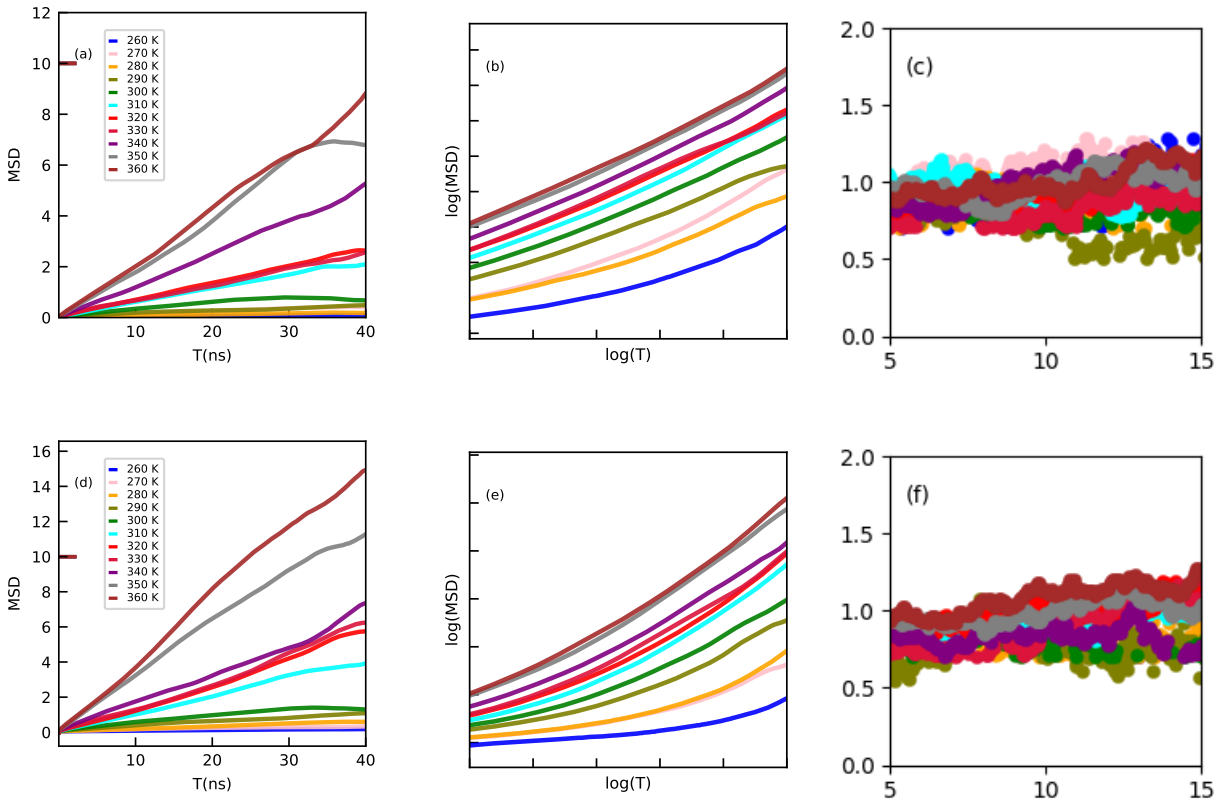


**Figure S12:** Upper panel of figure represents the diffusive motion of cation while the lower panel of figure represents the diffusive motion of anion in systems with different temperature. The left panels (a) and (d) represent the mean squared displacement, the middle panels (b) and (e) represent the log MSD versus log T plots and the left panels (c) and (f) show the beta value which corresponds to the diffusive regime.