S1. Calculated Diffusivity Values

Cross Diffusivity Terms (D_{ij}) computed from Self Diffusivity Values (D_{ii}) using Equation 2. Self-Diffusivity values are calculated from molecular dynamics trajectories using Equation 1. Standard deviations are shown in parenthesis.

System A	EC	EMC	Li+	PF6-
EC	3.80E-10 (1.97E-12)	3.75E-10	1.30E-10	2.05E-10
EMC	3.75E-10	3.64E-10 (3.35e-12)	1.26E-10	2.03E-10
Li+	1.30E-10	1.26E-10	1.23E-10 (8.58E-12)	1.62E-10
PF6-	2.05E-10	2.03E-10	1.62E-10	2.00E-10 (1.83e-11)

System B	EC	EMC	Li+	PF6-
EC	2.47E-10 (2.36E-12)	2.31E-10	1.01E-10	1.52E-10
EMC	2.31E-10	1.98E-10 (1.44E-12)	8.87E-11	1.43E-10
Li+	1.01E-10	8.87E-11	8.10E-11 (1.16E-12)	1.10E-10
PF6-	1.52E-10	1.43E-10	1.10E-10	1.39E-10 (7.71E-12)

System C	EC	EMC	Li+	PF6-
EC	1.33E-10 (3.26E-12)	1.20E-10	6.19E-11	9.50E-11
EMC	1.20E-10	9.41E-11 (9.21E-13)	4.83E-11	8.55E-11
Li+	6.19E-11	4.83E-11	4.18E-11 (1.16E-12)	6.31E-11
PF6-	9.50E-11	8.55E-11	6.31E-11	8.43E-11 (2.83E-12)

System D	EC	EMC	Li+	PF6-
EC	2.87E-11 (1.47E-12)	2.48E-11	1.62E-11	2.04E-11
EMC	2.48E-11	1.71E-11 (1.73E-12)	1.09E-11	1.60E-11
Li+	1.62E-11	1.09E-11	9.14E-12 (4.59E-13)	1.24E-11
PF6-	2.04E-11	1.60E-11	1.24E-11	1.57E-11 (7.04E-13)

Standard deviations were calculated using block averaging the mean squared displacement from PyLAT across 20 different intervals of 5 ns each. For the 25 ns long simulation with NVT ensemble, the slope of MSD was obtained for 0 to 5 ns, 1 to 6 ns, 2 to 7 ns etc.

S2. Amber format prep files obtained from Antechamber

EC.prep

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-------------------------------------------------------------

    0    0    2

This is a remark line
molecule.res
EC   INT  0
CORRECT     OMIT DU   BEG
  0.0000
   1  DUMM  DU    M    0  -1  -2     0.000      .0        .0      .00000
   2  DUMM  DU    M    1   0  -1     1.449      .0        .0      .00000
   3  DUMM  DU    M    2   1   0     1.523   111.21       .0      .00000
   4  O1    os    M    3   2   1     1.540   111.208  -180.000 -0.424941
   5  C1    c3    M    4   3   2     1.437    97.800   105.315  0.089081
   6  H1    h1    E    5   4   3     1.093   108.651  -167.677  0.075335
   7  H2    h1    E    5   4   3     1.089   108.731   -48.090  0.075335
   8  C2    c3    M    5   4   3     1.531   102.619    72.889  0.089081
   9  H3    h1    E    8   5   4     1.089   113.925   140.746  0.075335
  10  H4    h1    E    8   5   4     1.093   112.613   -93.229  0.075335
  11  O2    os    M    8   5   4     1.437   102.619    23.403 -0.424941
  12  C3    c2    M   11   8   5     1.362   109.447   -19.883  0.944461
  13  O3    o     M   12  11   8     1.188   124.951  -171.725 -0.574083


LOOP
   C3   O1

IMPROPER
   O3   O2   C3   O1

DONE
STOP
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EMC.prep

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    0    0    2

This is a remark line
molecule.res
EMC   INT  0
CORRECT     OMIT DU   BEG
  0.0000
   1  DUMM  DU    M    0  -1  -2     0.000      .0        .0      .00000
   2  DUMM  DU    M    1   0  -1     1.449      .0        .0      .00000
   3  DUMM  DU    M    2   1   0     1.523   111.21       .0      .00000
   4  C3    c3    M    3   2   1     1.540   111.208  -180.000 -0.345795
   5  H3    hc    E    4   3   2     1.093    35.013  -180.000  0.091106
   6  H4    hc    E    4   3   2     1.092    88.636    54.316  0.091106
   7  H5    hc    E    4   3   2     1.093    88.584   -54.200  0.091106
   8  C1    c3    M    4   3   2     1.514   144.568  -179.869  0.580567
   9  H1    h1    E    8   4   3     1.092   112.024   -60.873 -0.068488
  10  H2    h1    E    8   4   3     1.092   112.052    60.710 -0.068488
  11  O1    os    M    8   4   3     1.450   107.358   179.917 -0.619903
  12  C2    c2    M   11   8   4     1.336   115.669   179.873  1.116925
  13  O3    o     E   12  11   8     1.207   126.178     0.052 -0.657736
  14  O2    os    M   12  11   8     1.340   108.090  -179.993 -0.431308
  15  C4    c3    M   14  12  11     1.439   115.215  -179.955 -0.045680
  16  H6    h1    E   15  14  12     1.087   105.155  -179.836  0.088863
  17  H7    h1    E   15  14  12     1.091   110.513   -60.467  0.088863
  18  H8    h1    E   15  14  12     1.091   110.546    60.740  0.088863


LOOP

IMPROPER
   O3   O1   C2   O2

DONE
STOP
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```

PF6.pepi

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    0    0    2

This is a remark line
molecule.res
PF6   INT  0
CORRECT     OMIT DU   BEG
  0.0000
   1  DUMM  DU    M    0  -1  -2     0.000      .0        .0      .00000
   2  DUMM  DU    M    1   0  -1     1.449      .0        .0      .00000
   3  DUMM  DU    M    2   1   0     1.523   111.21       .0      .00000
   4  F1    f1    M    3   2   1     1.540   111.208  -180.000 -0.409967
   5  P1    p5    M    4   3   2     1.622   117.868   -38.941  1.459802
   6  F3    f2    E    5   4   3     1.626    89.956  -112.483 -0.409967
   7  F4    f1    E    5   4   3     1.626   179.531   -53.746 -0.409967
   8  F5    f3    E    5   4   3     1.627    89.893   -22.795 -0.409967
   9  F6    f3    E    5   4   3     1.621    90.360   157.473 -0.409967
  10  F2    f2    M    5   4   3     1.622    90.290    67.101 -0.409967


LOOP

IMPROPER

DONE
STOP
---------------------------------------------------------------
```