Electronic supplementary information (ESI) for: Impact of anion shape on Li^+ solvation and on transport properties for lithium-air batteries: a molecular dynamics study

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The information contained in this material is described as:

- Section 1 comprises the time correlation functions for shear viscosity, self-diffusivity and ionic conductivity.
- Section 2 presents the system size effect analyses on transport properties.
- Section 3 has the information of structural arrangement for different molalities and temperatures.
- Section 4 consists on simulation details of initial configurations, force fields and LAMMPS running files.

1 Time correlation functions

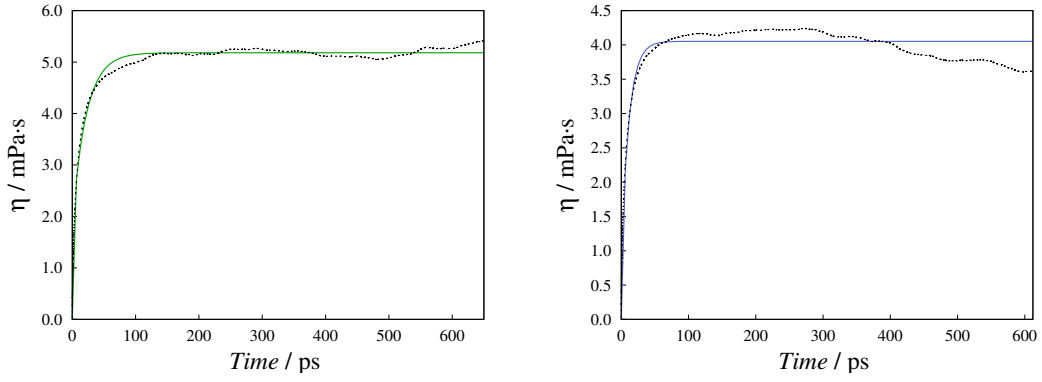

Figure S1: The shear viscosity corresponding to the running integral (Eq. 2) averaged over 30 trajectories (dashed line) and the fitting empirical function (Eq. 3) (solid line) at 1 mol·kg^{-1} and 298 K for: (a) $LiPF_6$, and (b) LiPyr.

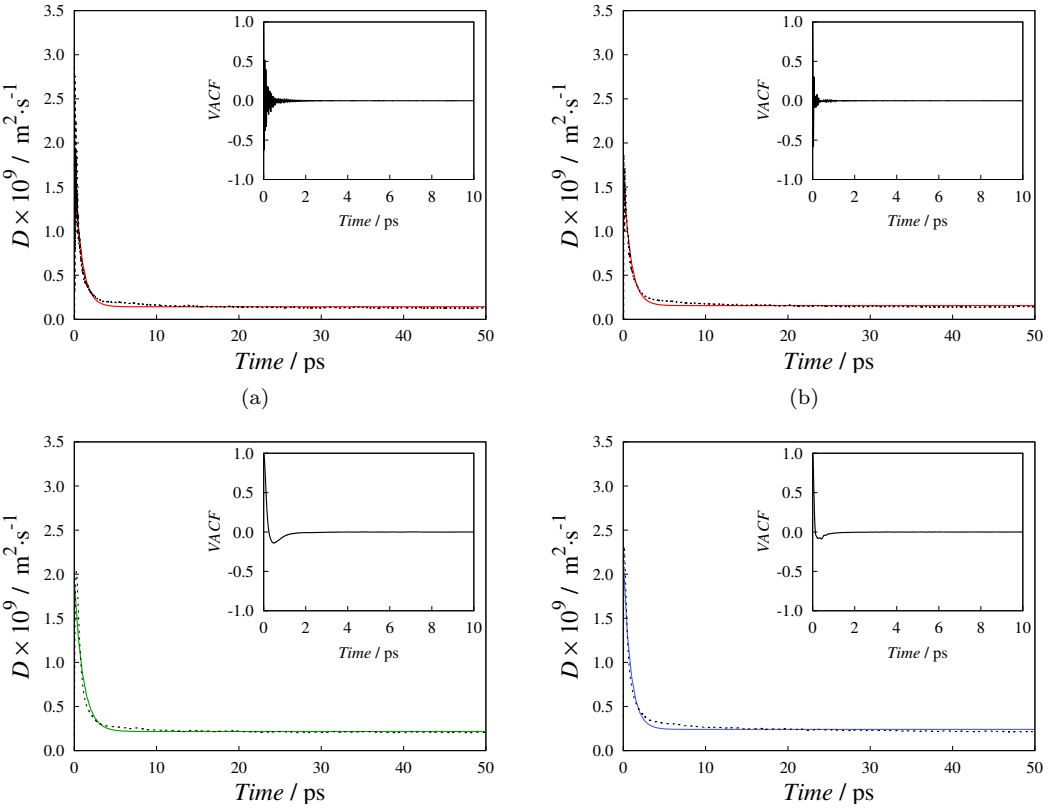

Figure S2: Self-diffusion corresponding to the running integral (Eq. 6) averaged over 10 trajectories (dashed line) and the fitting empirical function (Eq. 7) (solid line) at 1 mol·kg^{-1} and 298 K for: (a) Li^+ in solution with PF_6^-, (b) Li^+ in solution with Pyr^-, (c) PF_6^-, and (d) Pyr^-, The insets show the normalized velocity autocorrelation function (VACF).

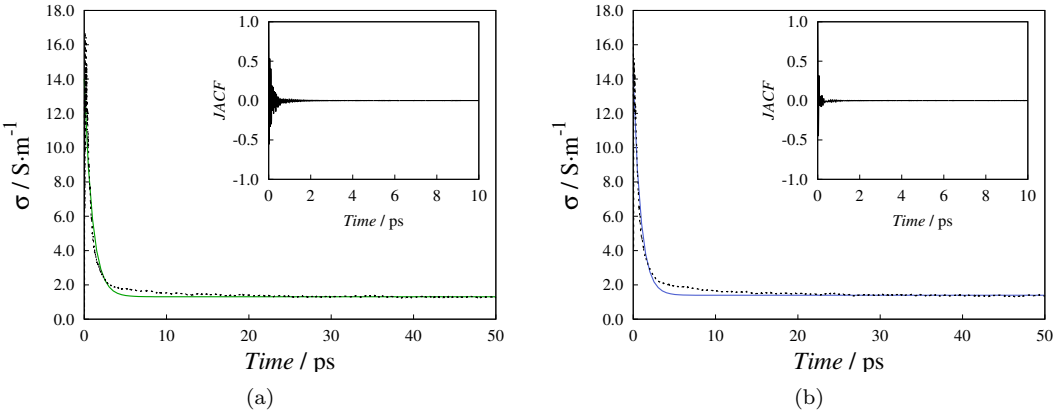

Figure S3: Ionic conductivity corresponding to the running integral (Eq. 9) averaged over 10 trajectories (dashed line) and the fitting empirical function (analogous to Eq. 7) (solid line) at 1 mol·kg^{-1} and 298 K for: (a) $LiPF_6$, and (b) LiPyr. The insets show the normalized electrical current autocorrelation function (JACF).

2 System size analysis

System size effect at collective properties must be taken into account in molecular simulations. Several authors have discussed such an effect considering error propagation and poor statistics caused by the influence of periodic boundary conditions in small box size and limited number of molecules. [1, 2, 3, 4,

5, 6].

Although larger system sizes improve the accuracy, they also increase the computational cost. To counterbalance computation cost and good accuracy of results, three set of systems were considered. We evaluated the system size effect on the self-diffusion coefficients and the ionic conductivities; viscosity seems to be unaffected by the system size [2, 5, 7, 6, 8]. $LiPF_6$ and LiPyr in DMSO solutions with 1 mol·kg^{-1} at 298 K were simulated with the following number of lithium ions and number of DMSO molecules: 40/512, 60/768, and 80/1024 (the number of anions is equal to the number of lithium ions).

Figure S4 (a) and (c) presents results of transport coefficients as a function of the inverse of number of cations. Even though we notice decrease of uncertainties for larger systems, almost the same average trend is observed for the value of each property. However, in order to increase the accuracy of self-diffusivity coefficient, we implemented the system-size correction (Eq. 9). Figure S4 (b) illustrates the improvement on this property with correction when compared with larger systems.

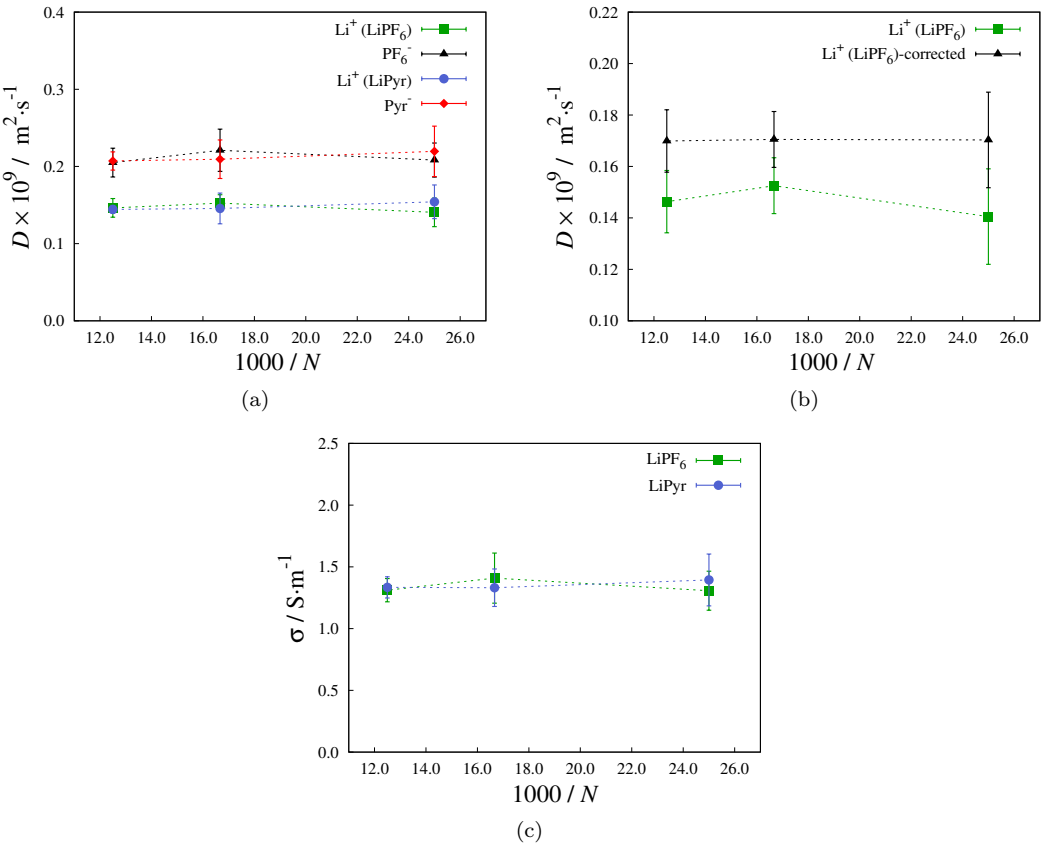

Figure S4: System size effect on the transport properties of $LiPF_6$ in DMSO and LiPyr in DMSO both at 1 mol·kg^{-1} and 298 K: (a) Self-diffusion coefficients without size effect correction, (b) Self-diffusion coefficients of Li^+ of $LiPF_6$ in DMSO without correction and corrected and, (c) Ionic conductivity coefficients.

3 Structural arrangement

Table S1: Coordination numbers of the first solvation shell for Li–O (DMSO), Li–F(PF_6) and Li–N(Pyr) at 1 atm for different salt molalities and at different temperatures.

	Temperature / K			
	298			
Salt molality / mol·kg^{-1}	0.25	0.50	0.75	1.00
$n_{Li\text{-}O}$ for $LiPF_6$ in DMSO	4.00	3.91	3.83	3.74
$n_{Li\text{-}F}$ for $LiPF_6$ in DMSO	0.01	0.09	0.19	0.29
$n_{Li\text{-}O}$ for LiPyr in DMSO	4.00	3.85	3.58	3.32
$n_{Li\text{-}N}$ for LiPyr in DMSO	0.44	0.58	0.70	0.87
	Salt molality / mol·kg^{-1}			
	1.00			
Temperature / K	298	330	360	
$n_{Li\text{-}O}$ for $LiPF_6$ in DMSO	3.74	3.93	3.99	
$n_{Li\text{-}F}$ for $LiPF_6$ in DMSO	0.29	0.08	0.01	
$n_{Li\text{-}O}$ for LiPyr in DMSO	3.32	3.08	2.80	
$n_{Li\text{-}N}$ for LiPyr in DMSO	0.87	1.00	1.14	

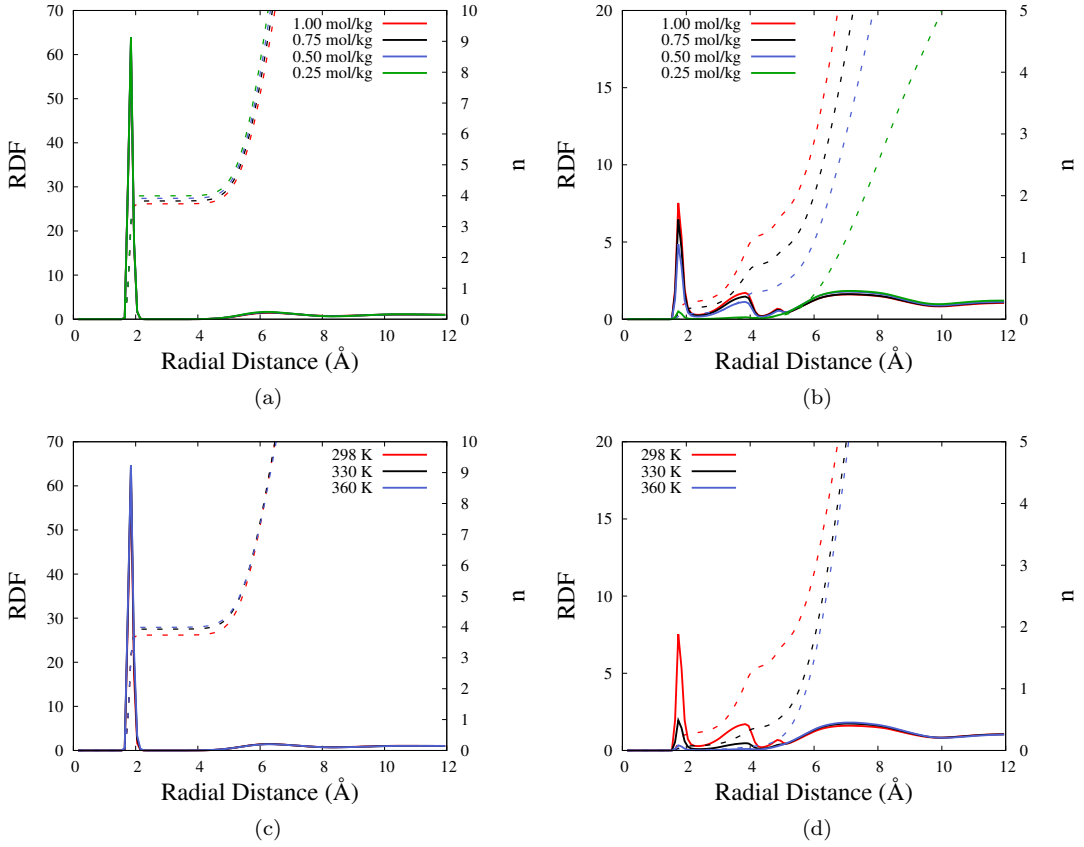

Figure S5: Radial distribution functions (RDF) (solid lines, left y axis), and coordination numbers (dashed lines, right y axis) for $LiPF_6$ in solution with DMSO as function of: (a) concentration at 298 K for Li–O (DMSO), (b) concentration at 298 K for Li–F (PF_6), (c) temperature at 1.0 mol·kg^{-1} for Li–O (DMSO), and (d) temperature at 1.0 mol·kg^{-1} for Li–F (PF_6).

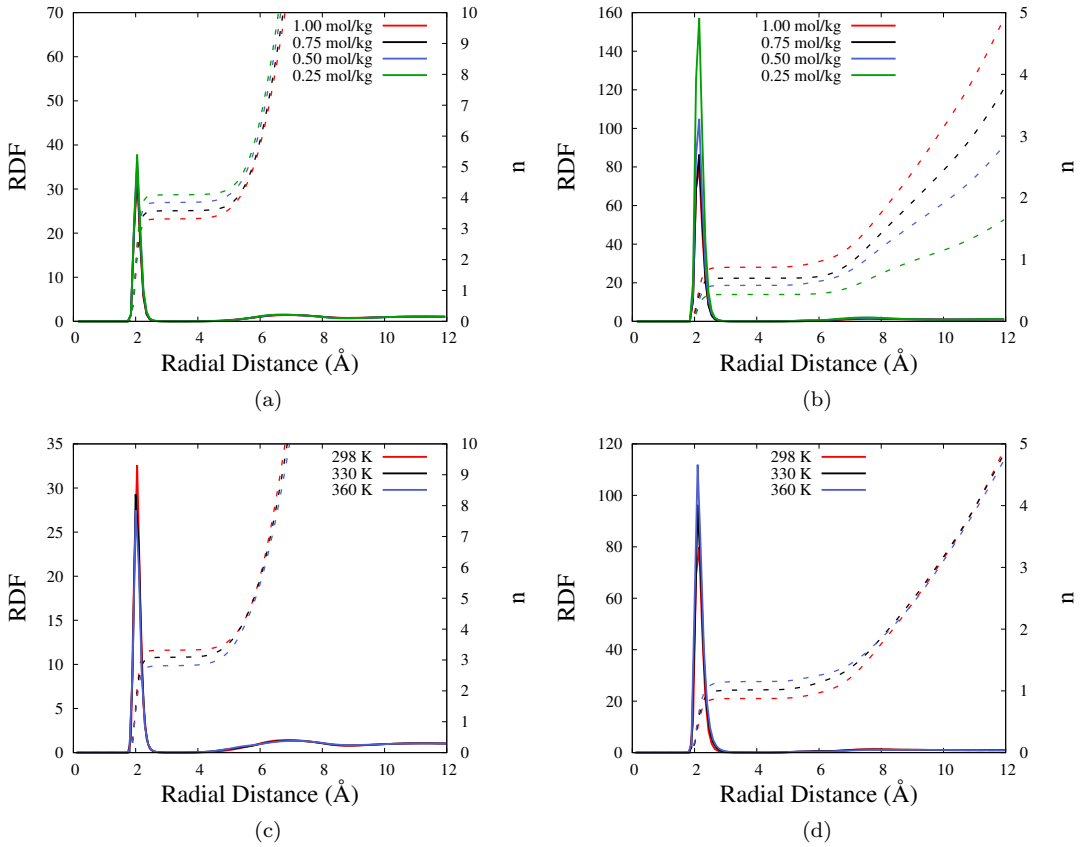

Figure S6: Radial distribution functions (RDF) (solid lines, left y axis), and coordination numbers (dashed lines, right y axis) for LiPyr in solution with DMSO as function of: (a) concentration at 298 K for Li–O (DMSO), (b) concentration at 298 K for Li–N (Pyr), (c) temperature at 1.0 mol·kg^{-1} for Li–O (DMSO), and (d) temperature at 1.0 mol·kg^{-1} for Li–N (Pyr).

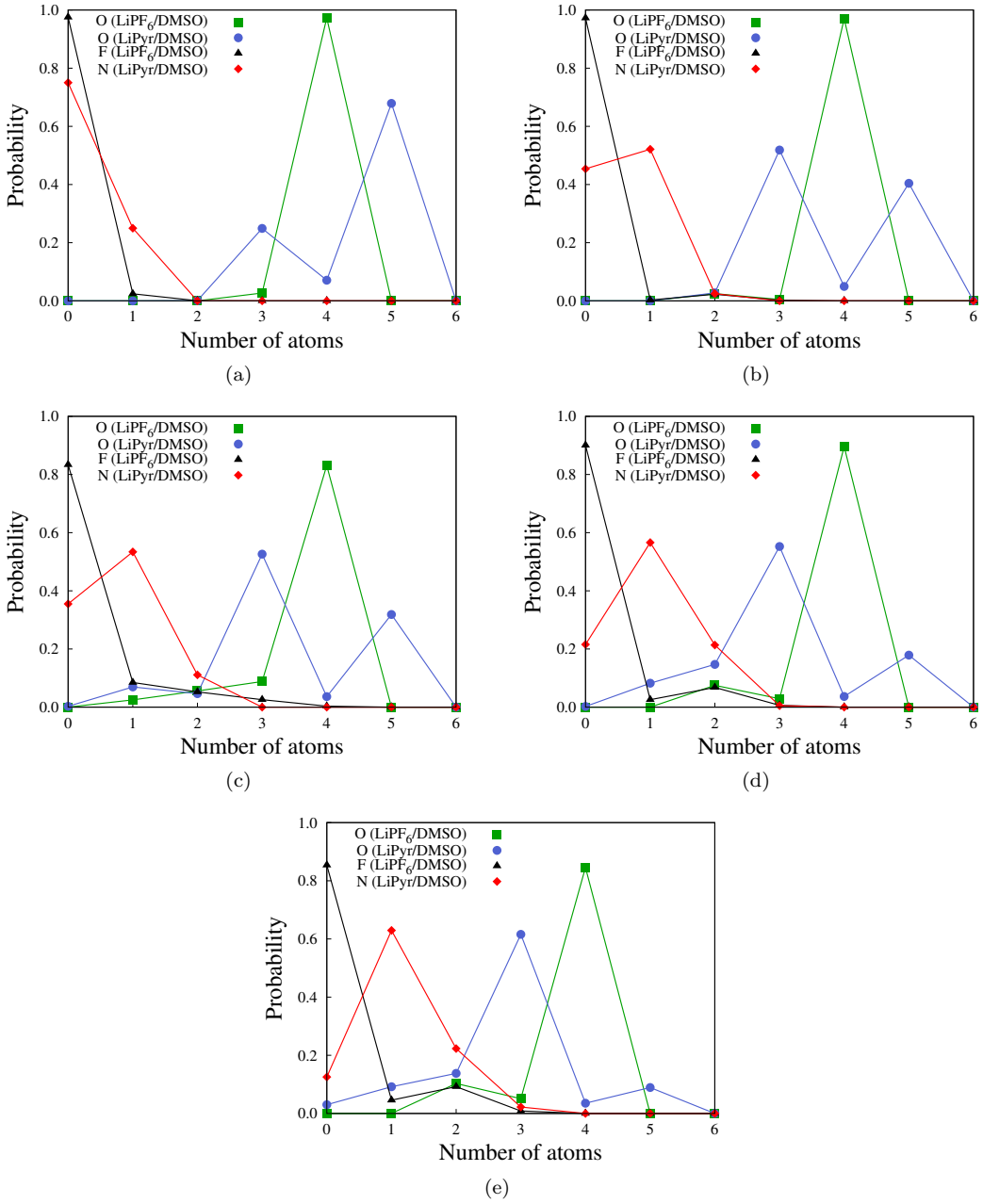

Figure S7: Solvation probability distribution of the first shell layer at: (a) 0.25 mol·kg^{-1} and 298 K, (b) 0.50 mol·kg^{-1} and 298 K, (c) 0.75 mol·kg^{-1} and 298 K, (d) 1.00 mol·kg^{-1} and 330 K, (e) 1.00 mol·kg^{-1} and 360 K,

4 Simulation details

4.1 Molecular sketches

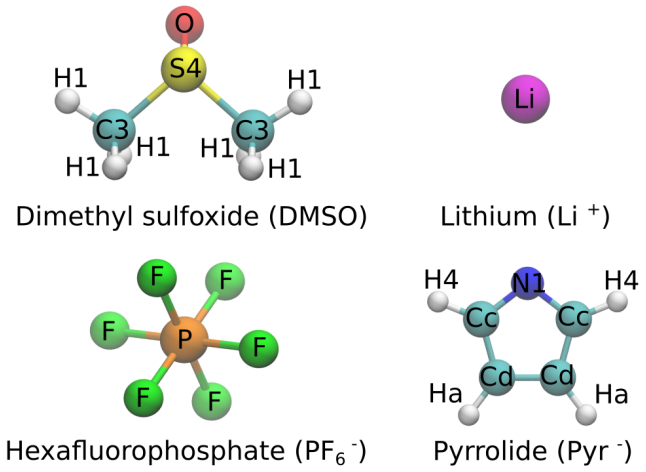

Figure S8: Schematic illustrations of molecular structures for DMSO, PF_6^-, Li^+, and Pyr^- with assignment of atom types.

4.2 Dimethyl sulfoxide Molecule

```
! ATOM:
!! index (int): atom index
!! name (str): atom name (required)
!! type (str): atomtype name
!! charge (float, e): partial atomic charge
!! x (float, angstrom): atom coordinate
!! y (float, angstrom): atom coordinate
!! z (float, angstrom): atom coordinate
ATOM name type charge x y z ! 10
S1    s4   0.359151    0.03900    0.26600    0.62000  ! 1
O1     o  -0.485225    0.55900    1.49000   -0.10400  ! 2
C1    c3  -0.498374   -1.71300    0.05400    0.11500  ! 3
H1    h1   0.187137   -1.77400    0.06600   -0.97400  ! 4
H2    h1   0.187137   -2.10400   -0.87800    0.52700  ! 5
H3    h1   0.187137   -2.26000    0.90200    0.52700  ! 6
C2    c3  -0.498374    0.69300   -1.19800   -0.27200  ! 7
H4    h1   0.187137    0.25900   -2.10800    0.14700  ! 8
H5    h1   0.187137    0.46500   -1.09900   -1.33400  ! 9
H6    h1   0.187137    1.77200   -1.19600   -0.12100  ! 10

! BOND:
BOND   ! 9
O1    S1    ! 1    1.514
C1    S1    ! 2    1.836
C2    S1    ! 3    1.835
C1    H1    ! 4    1.091
C1    H2    ! 5    1.091
C1    H3    ! 6    1.090
C2    H4    ! 7    1.092
C2    H5    ! 8    1.091
C2    H6    ! 9    1.090
```

```
! ANGLE:
ANGLE   ! 15
H1    C1    S1    ! 1   109.073
H2    C1    S1    ! 2   109.676
H3    C1    S1    ! 3   106.567
H4    C2    S1    ! 4   109.681
H5    C2    S1    ! 5   109.052
H6    C2    S1    ! 6   106.508
C1    S1    O1    ! 7   106.834
C2    S1    O1    ! 8   106.865
C1    S1    C2    ! 9    96.563
H1    C1    H2    ! 10   111.483
H1    C1    H3    ! 11   109.923
H2    C1    H3    ! 12   109.991
H4    C2    H5    ! 13   111.483
H4    C2    H6    ! 14   110.000
H5    C2    H6    ! 15   109.987

! DIHEDRAL:
DIHEDRAL   ! 12
H1    C1    S1    O1    ! 1    51.617
H1    C1    S1    C2    ! 2   -58.255
H2    C1    S1    O1    ! 3   173.971
H2    C1    S1    C2    ! 4    64.099
H3    C1    S1    O1    ! 5   -67.004
H3    C1    S1    C2    ! 6  -176.877
H4    C2    S1    O1    ! 7  -173.946
H4    C2    S1    C1    ! 8   -64.101
H5    C2    S1    O1    ! 9   -51.602
H5    C2    S1    C1    ! 10    58.244
H6    C2    S1    O1    ! 11    67.051
H6    C2    S1    C1    ! 12   176.897
```

4.3 Hexafluorophosphate Molecule

```
! ATOM:
!! index (int): atom index
!! name (str): atom name (required)
!! type (str): atomtype name
!! charge (float, e): partial atomic charge
!! x (float, angstrom): atom coordinate
!! y (float, angstrom): atom coordinate
!! z (float, angstrom): atom coordinate
ATOM name type charge x y z ! 7
P1     p   1.07     0.18051     0.87394     0.02384   ! 1
F1     f  -0.345    0.16559     0.88898     1.66961   ! 2
F2     f  -0.345    0.19542     0.85891    -1.62194   ! 3
F3     f  -0.345    1.35402     2.02802     0.02393   ! 4
F4     f  -0.345   -0.99301    -0.28013     0.02374   ! 5
F5     f  -0.345   -0.97348     2.04736     0.00265   ! 6
F6     f  -0.345    1.33449    -0.29947     0.04502   ! 7

! BOND:
BOND   ! 6
P1    F1    ! 1
P1    F2    ! 2
P1    F3    ! 3
P1    F4    ! 4
P1    F5    ! 5
```

```
P1    F6    ! 6

! ANGLE:
ANGLE   ! 12
F1    P1    F3    ! 1
F1    P1    F4    ! 1
F1    P1    F5    ! 1
F1    P1    F6    ! 1
F2    P1    F3    ! 1
F2    P1    F4    ! 1
F2    P1    F5    ! 1
F2    P1    F6    ! 1
F3    P1    F5    ! 1
F3    P1    F6    ! 1
F4    P1    F5    ! 1
```

4.4 Lithium Molecule

```
! ATOM:
!! index (int): atom index
!! name (str): atom name (required)
!! type (str): atomtype name
!! charge (float, e): partial atomic charge
!! x (float, angstrom): atom coordinate
!! y (float, angstrom): atom coordinate
!! z (float, angstrom): atom coordinate
ATOM name type charge x y z ! 1
Li1    li   1.000000    0.00000    0.00000    0.00000   ! 1
```

4.5 Pyrrolide Molecule

```
! ATOM:
!! index (int): atom index
!! name (str): atom name (required)
!! type (str): atomtype name
!! charge (float, e): partial atomic charge
!! x (float, angstrom): atom coordinate
!! y (float, angstrom): atom coordinate
!! z (float, angstrom): atom coordinate
ATOM name type charge x y z ! 9
C1    cc   0.102030   -14.18600     7.64900    -0.31800   ! 1
C2    cc  -0.328829   -12.77900     7.60400    -0.31800   ! 2
C3    cd  -0.328829   -12.35800     8.96400    -0.31800   ! 3
C4    cd   0.102030   -13.54500     9.72200    -0.31800   ! 4
N1    n1  -0.672421   -14.65900     8.93000    -0.31800   ! 5
H1    h4  -0.004135   -14.87600     6.80100    -0.31800   ! 6
H2    ha   0.067145   -12.14700     6.71400    -0.31800   ! 7
H3    ha   0.067145   -11.33400     9.34200    -0.31800   ! 8
H4    h4  -0.004135   -13.63600    10.81100    -0.31800   ! 9

! BOND:
BOND   ! 9
C1    C2    ! 1     1.408
C1    N1    ! 2     1.366
C1    H1    ! 3     1.093
C2    C3    ! 4     1.424
C2    H2    ! 5     1.092
C3    C4    ! 6     1.408
C3    H3    ! 7     1.092
```

```
C4    N1    ! 8     1.367
C4    H4    ! 9     1.093

! ANGLE:
ANGLE   ! 13
C1    C2    C3    ! 1   105.369
C1    C2    H2    ! 2   127.211
C1    N1    C4    ! 3   105.145
C2    C1    N1    ! 4   112.098
C2    C1    H1    ! 5   127.303
C2    C3    C4    ! 6   105.361
C2    C3    H3    ! 7   127.462
C3    C2    H2    ! 8   127.421
C3    C4    N1    ! 9   112.027
C3    C4    H4    ! 10   127.338
C4    C3    H3    ! 11   127.177
H1    C1    N1    ! 12   120.599
H4    C4    N1    ! 13   120.634

! DIHEDRAL:
DIHEDRAL   ! 16
N1    C1    C2    C3    ! 1
H1    C1    C2    C3    ! 2   180.000
N1    C1    C2    H2    ! 3   180.000
H1    C1    C2    H2    ! 4
C2    C1    N1    C4    ! 5
H1    C1    N1    C4    ! 6   180.000
C1    C2    C3    C4    ! 7
H2    C2    C3    C4    ! 8  -180.000
C1    C2    C3    H3    ! 9   180.000
H2    C2    C3    H3    ! 10
C2    C3    C4    N1    ! 11
H3    C3    C4    N1    ! 12   180.000
C2    C3    C4    H4    ! 13   180.000
H3    C3    C4    H4    ! 14
C3    C4    N1    C1    ! 15
H4    C4    N1    C1    ! 16   180.000

! IMPROPER:
IMPROPER   ! 4
C2    H1    C1    N1    ! 1  -180.000
C1    C3    C2    H2    ! 2   180.000
C2    C4    C3    H3    ! 3   180.000
C3    H4    C4    N1    ! 4   180.000
```

4.6 Force Field for DMSO/$LiPF_6$

```
Masses

1    32.060   # s4 DMS
2    16.000   # o DMS
3    12.010   # c3 DMS
4     1.008   # h1 DMS
5     6.941   # li LI
6    31.000   # p PF6
7    19.000   # f PF6

Pair Coeffs # lj/charmm/coul/long
```

```
1 0.35 3.564 0.35 3.564
2 0.12 3.029 0.12 3.029
3 0.078 3.635 0.078 3.635
4 0.024 2.388 0.024 2.388
5 0.10314 1.4424 0.10314 1.4424
6 0.13169 3.695 0.13169 3.695
7 0.028716 2.9347 0.028716 2.9347

Bond Coeffs # harmonic

1 540 1.53
2 240 1.8
3 322 1.11
4 370.8 1.606

Angle Coeffs # harmonic

1 46.1 111.3
2 79 106.75
3 34 95
4 35.5 108.4
5 139.4 90

Dihedral Coeffs # charmm

1 0.2 3 0 0
2 0.2 3 0 0
```

4.7 Force Field for DMSO/LiPyr

```
Masses

1    32.060  # s4 DMS
2    16.000  # o DMS
3    12.010  # c3 DMS
4     1.008  # h1 DMS
5     6.941  # li LI
6    12.010  # cc PYR
7    12.010  # cd PYR
8    14.010  # n1 PYR
9     1.008  # h4 PYR
10     1.008  # ha PYR

Pair Coeffs

1 0.350 3.564  # s4 DMS
2 0.120 3.029  # o DMS
3 0.078 3.635  # c3 DMS
4 0.024 2.388  # h1 DMS
5 0.0182660800896 2.126  # li LI
6 0.0859427210304 3.400  # cc PYR
7 0.0859427210304 3.400  # cd PYR
8 0.169885665734 3.250  # n1 PYR
9 0.0149893860096 2.511  # h4 PYR
10 0.0149893860096 2.600  # ha PYR

Bond Coeffs

1 540 1.53  # harmonic DMS o s4
```

```
2 240 1.80  # harmonic DMS c3 s4
3 322 1.11  # harmonic DMS c3 h1
4 418.018786099  1.429  # harmonic PYR cc cc
5 539.937622253  1.309  # harmonic PYR cc n1
6 349.86553511  1.083  # harmonic PYR cc h4
7 503.661639974  1.371  # harmonic PYR cc cd
8 346.968143194  1.085  # harmonic PYR cc ha
9 418.018786099  1.429  # harmonic PYR cd cd
10 346.968143194  1.085  # harmonic PYR cd ha
11 539.937622253  1.309  # harmonic PYR cd n1
12 349.86553511  1.083  # harmonic PYR cd h4

Angle Coeffs

1 46.1 111.3  # harmonic DMS h1 c3 s4
2 79.0 106.75  # harmonic DMS c3 s4 o
3 34.0 95.0  # harmonic DMS c3 s4 c3
4 35.5 108.4  # harmonic DMS h1 c3 h1
5 68.1135334848  114.19  # harmonic PYR cc cc cd
6 47.4286574016  119.26  # harmonic PYR cc cc ha
7 0.0  0.00  # harmonic PYR cc n1 cd
8 71.6424337152  122.98  # harmonic PYR cc cc n1
9 45.5301607104  129.47  # harmonic PYR cc cc h4
10 68.1135334848  114.19  # harmonic PYR cc cd cd
11 48.3183294912  122.89  # harmonic PYR cc cd ha
12 48.3183294912  122.89  # harmonic PYR cd cc ha
13 71.6424337152  122.98  # harmonic PYR cd cd n1
14 45.5301607104  129.47  # harmonic PYR cd cd h4
15 46.9877931072  121.51  # harmonic PYR cd cd ha
16 52.6137775488  116.36  # harmonic PYR h4 cc n1
17 52.6137775488  116.36  # harmonic PYR h4 cd n1

Dihedral Coeffs

1 0.2  3 0 0.0  # charmm DMS h1 c3 s4 o
2 0.2  3 0 0.0  # charmm DMS h1 c3 s4 c3
3 3.99732847258  2 180 0.0  # charmm PYR cd cc cc n1
4 3.99732847258  2 180 0.0  # charmm PYR cd cc cc h4
5 3.99732847258  2 180 0.0  # charmm PYR ha cc cc n1
6 3.99732847258  2 180 0.0  # charmm PYR h4 cc cc ha
7 0.0  2 180 0.0  # charmm PYR cc cc n1 cd
8 0.0  2 180 0.0  # charmm PYR h4 cc n1 cd
9 3.99732847258  2 180 0.0  # charmm PYR cc cc cd cd
10 3.99732847258  2 180 0.0  # charmm PYR ha cc cd cd
11 3.99732847258  2 180 0.0  # charmm PYR cc cc cd ha
12 3.99732847258  2 180 0.0  # charmm PYR ha cc cd ha
13 3.99732847258  2 180 0.0  # charmm PYR cc cd cd n1
14 3.99732847258  2 180 0.0  # charmm PYR ha cd cd n1
15 3.99732847258  2 180 0.0  # charmm PYR cc cd cd h4
16 3.99732847258  2 180 0.0  # charmm PYR h4 cd cd ha
17 0.0  2 180 0.0  # charmm PYR cd cd n1 cc
18 0.0  2 180 0.0  # charmm PYR h4 cd n1 cc

Improper Coeffs

1 1.09926135821 -1  2  # cvff PYR cc h4 cc n1
2 1.09926135821 -1  2  # cvff PYR cc cd cc ha
3 1.09926135821 -1  2  # cvff PYR cc cd cd ha
```

```
4 1.09926135821 -1  2  # cvff PYR cd h4 cd n1
```

4.8 LAMMPS Initialization File for DMSO/$LiPF_6$

```
#OPLS DMSO/LiPF6

# Intialization
units           real
dimension       3
boundary        p p p
atom_style      full

variable        NRUNP equal 2E6
variable        NRUNE equal 1E6
variable        NRUNV equal 10E6
variable        NRUND equal 1E6
variable        VTEMP equal 298
variable        VPRES equal 1.0
pair_style      lj/charmm/coul/long 10.0 12.0
pair_modify     tail yes
pair_modify     mix arithmetic
bond_style      harmonic
angle_style     harmonic
dihedral_style  charmm
kspace_style    pppm 1.0E-4

read_data       electrolyte.data

group           dmso type 1 2 3 4
group           li type 5
group           pf6 type 6 7

# Setup atoms
velocity        all create ${VTEMP} 118647 mom yes rot yes dist gaussian

# Settings
timestep        1.0
neighbor        2.0 bin
neigh_modify    delay 0 every 1 check yes

# Operations
fix             1 all npt temp ${VTEMP} ${VTEMP} 100 iso ${VPRES} ${VPRES} 1000

# Output
thermo          5
thermo_style    custom time temp press pe ke etotal density vol
log             npt.lammps

# Actions
run             ${NRUNP}

# Operations
unfix           1
fix             2 all nvt temp ${VTEMP} ${VTEMP} 100

run             ${NRUNE}

# Output
thermo          5
```

```
thermo_style    custom time pxx pxy pxz pyy pyz pzz density vol
log             nvt.lammps

# Actions
run             ${NRUNV}

reset_timestep  0
# Output
thermo          5
thermo_style    custom time temp etotal density vol
log             nvtd.lammps
dump            myDump1 li custom 5 li.data id type mass vx vy vz
dump            myDump2 pf6 custom 5 pf6.data id type mass vx vy vz
compute         myRDF all rdf 120 5 2 5 4 5 6 5 7
fix             RDF all ave/time 1 1E6 1E6 c_myRDF[*] file rdf.data mode vector

# Actions
run             ${NRUND}
```

4.9 LAMMPS Initialization File for DMSO/LiPyr

```
#OPLS DMSO/LiPYR

# Intialization
units           real
dimension       3
boundary        p p p
atom_style      full

variable        NRUNP equal 2E6
variable        NRUNE equal 1E6
variable        NRUNV equal 10E6
variable        NRUND equal 1E6
variable        VTEMP equal 298
variable        VPRES equal 1.0
pair_style      lj/charmm/coul/long 10.0 12.0
pair_modify     tail yes
pair_modify     mix arithmetic
bond_style      harmonic
angle_style     harmonic
dihedral_style  charmm
improper_style  cvff
kspace_style    pppm 1.0E-4

read_data       electrolyte.data

group           dmso type 1 2 3 4
group           li type 5
group           pyr type 6 7 8 9 10

# Setup atoms
velocity        all create ${VTEMP} 432393 mom yes rot yes dist gaussian

# Settings
timestep        1.0
neighbor        2.0 bin
neigh_modify    delay 0 every 1 check yes

# Operations
```

```
fix             1 all npt temp ${VTEMP} ${VTEMP} 100 iso ${VPRES} ${VPRES} 1000

# Output
thermo          5
thermo_style    custom time press pe ke etotal density vol
log             npt.lammps

# Actions
run             ${NRUNP}

# Operations
unfix           1
fix             2 all nvt temp ${VTEMP} ${VTEMP} 100

run             ${NRUNE}

# Output
thermo          5
thermo_style    custom time pxx pxy pxz pyy pyz pzz density vol
log             nvt.lammps

# Actions
run             ${NRUNV}

reset_timestep  0
# Output
thermo          5
thermo_style    custom time temp etotal density vol
log             nvtd.lammps
dump            myDump1 li custom 5 li.data id type mass vx vy vz
dump            myDump2 pyr custom 5 pyr.data id type mass vx vy vz
compute         myRDF all rdf 120 5 2 5 4 5 8 5 9 5 10
fix             RDF all ave/time 1 1E6 1E6 c_myRDF[*] file rdf.data mode vector

# Actions
run             ${NRUND}
```

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