MISPR: An open-source package for high-throughput multiscale molecular simulations

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1. **File storage**

Every time a workflow is created and executed, the infrastructure automatically creates a single folder for the workflow with an assigned unique name that can either be provided by the user or automatically determined from the structural representation of the molecule or system of molecules (e.g., molecular formula). Within this main folder, multiple subfolders are created for calculation steps included in the workflow (e.g., geometry optimization and frequency calculation in DFT, ensemble type in MD) with a name corresponding to the type of calculation. A subfolder is also created for the final analysis performed to derive a property (such as binding energy, diffusion, or viscosity) using data parsed from the individual steps. Any file, if present, associated with a calculation is stored within its corresponding subfolder. The number and names of subfolders created are workflow-specific. All folders resulting from a workflow are confined within a parent directory configured when loading and setting the workflow input parameters.
Fig. S1 Code snippet of the submission of a bond dissociation energy calculation

```python
from fireworks import LaunchPad
from mispr.gaussian.workflows.base.bde import get_bde

lpad = LaunchPad.auto_load()

wf = get_bde(mol_operation_type="get_from_file",
             mol="dme.xyz",
             bonds=[[1, 6]],
             open_rings=False,
             process_mol_func=False,
             skips=None,
             mol_name="dme",
             solvent_gaussian_inputs="(SMD, Solvent=TetraHydroFuran)",
             save_to_db=False,
             save_to_file=True,
             visualize=True,
             tag="bde-example")

lpad.add_wf(wf)
```
Table S1 Sample ESP and RESP charges for a monoglyme molecule computed at the B3LYP/6-31+G* level of theory and compared to OPLS charges

| Number | Atom | Computed ESP charges | Derived RESP charges | OPLS charges |
|--------|------|-----------------------|----------------------|--------------|
| 1      | O    | -0.450597             | -0.396634            | -0.4         |
| 2      | O    | -0.448858             | -0.396634            | -0.4         |
| 3      | C    | 0.168498              | 0.106870             | 0.14         |
| 4      | C    | 0.173399              | 0.106870             | 0.14         |
| 5      | C    | 0.10666               | 0.057713             | 0.11         |
| 6      | C    | 0.096242              | 0.057713             | 0.11         |
| 7      | H    | 0.0358                | 0.047255             | 0.03         |
| 8      | H    | 0.036371              | 0.047255             | 0.03         |
| 9      | H    | 0.033803              | 0.047255             | 0.03         |
| 10     | H    | 0.034374              | 0.047255             | 0.03         |
| 11     | H    | 0.05954               | 0.045847             | 0.03         |
| 12     | H    | 0.021866              | 0.045847             | 0.03         |
| 13     | H    | 0.021589              | 0.045847             | 0.03         |
| 14     | H    | 0.025167              | 0.045847             | 0.03         |
| 15     | H    | 0.060705              | 0.045847             | 0.03         |
| 16     | H    | 0.025442              | 0.045847             | 0.03         |
Fig. S2 Distribution of error associated with (a) $^{13}$C and (b) $^1$H chemical shift predictions in a chloroform solvent
Table S2 BDE results with experimental data retrieved from the iBond database and computational data obtained using MISPR; broken bonds are highlighted in the 2D structure of the molecule.

| Bond number | InChI code | InChI code | Molecule name | 2D representation | Experimental BDE (eV) | Computed BDE (eV) | Absolute error (eV) |
|-------------|-------------|-------------|---------------|--------------------|----------------------|-------------------|---------------------|
| 1           | InChI=1S/CH4/h1H4 | methane     | ![methane 2D structure](image) | 4.5150             | 4.4980               | 0.0169            |
| 2           | InChI=1S/CHN/c1-2h1H | formonitrile | ![formonitrile 2D structure](image) | 5.3750             | 5.6117               | 0.2367            |
| 3           | InChI=1S/C2H6/c1-2h1-2H3 | ethane     | ![ethane 2D structure](image) | 3.8786             | 3.9347               | 0.0561            |
| 4           | InChI=1S/CH3F/c1-2h1H3 | fluoromethane | ![fluoromethane 2D structure](image) | 4.7214             | 4.7687               | 0.0473            |
| 5           | InChI=1S/CH3F/c1-2h1H3 | fluoromethane | ![fluoromethane 2D structure](image) | 4.7988             | 4.2804               | 0.5183            |
| 6           | InChI=1S/C2H3N/c1-3-2h1H3 | isocyanomethane | ![isocyanomethane 2D structure](image) | 4.1581             | 4.0451               | 0.1129            |
| 7           | InChI=1S/CH2N2/c2-1-3h2H2 | cyanamide | ![cyanamide 2D structure](image) | 4.2570             | 4.0311               | 0.2258            |
| 8           | InChI=1S/C2H6O/c1-3-2h1-2H3 | methoxymethane | ![methoxymethane 2D structure](image) | 3.6163             | 3.5138               | 0.1024            |
| 9           | InChI=1S/CH3F/c1-2-3-4h2-3H2,1H3 | 1-fluoropropane | ![1-fluoropropane 2D structure](image) | 3.9388             | 4.3316               | 0.3928            |
| 10          | InChI=1S/CH3F/c1-2-3-4h2-3H2,1H3 | 1-fluoropropane | ![1-fluoropropane 2D structure](image) | 3.9388             | 4.3316               | 0.3928            |
|   | InChI             | Structure                                                                 |   |   |   |
|---|-------------------|---------------------------------------------------------------------------|---|---|---|
| 11 | InChI=1S/CH4S/c1-2h2H,1H3 | methanethiol                                                             | 3.9732 | 4.0309 | 0.0577 |
| 12 | InChI=1S/CH4S/c1-2h2H,1H3 | methanethiol                                                             | 3.7582 | 3.6603 | 0.0978 |
| 13 | InChI=1S/CH4O2/c1-3-2h2H,1H3 | hydroperoxymethane                                                       | 1.9436 | 1.7591 | 0.1844 |
| 14 | InChI=1S/C3H7F/c1-3(2)/4h3H,1-2H3 | 2-fluoropropene                                                          | 4.7343 | 4.9154 | 0.1811 |
| 15 | InChI=1S/CH3F/c1-2-3h2H2,1H3 | fluoroethane                                                             | 4.6311 | 4.8545 | 0.2234 |
| 16 | InChI=1S/CH3Cl/c1-2hH3 | chloromethane                                                            | 4.3000 | 4.2064 | 0.0935 |
| 17 | InChI=1S/CH3CN/c1-2-1-3-5h1H2 | propanedinitrile                                                         | 4.3817 | 4.7628 | 0.3811 |
| 18 | InChI=1S/C5H12O/c1-2-3-4-5-6h6H2,-5H2,1H3 | pentan-1-ol                                                             | 3.6550 | 3.6437 | 0.0112 |
| 19 | InChI=1S/CH3Cl/c1-2hH3 | chloromethane                                                            | 3.5991 | 3.6438 | 0.0447 |
| 20 | InChI=1S/C12H9N/c13-9-8-11-6-3-5-10-4-1-2-7-12(10)11/h1-7H,8H2 | 2-naphthalen-1-ylacetonitrile                                              | 3.4959 | 3.4197 | 0.0761 |
| 21 | InChI=1S/CH2O3/c2-1-4-3/h1,3H | peroxyformic acid                                                        | 4.2355 | 3.7367 | 0.4987 |
| 22 | InChI=1S/C4H10O/c1-2-3-4-5h5H,2-4H2,1H3 | butan-1-ol                                                               | 3.6722 | 3.5984 | 0.0737 |
|   | InChI=1S/C2H2ClF3/c3-1-2(4,5)6/h1H2   | 2-chloro-1,1,1-trifluorohane          | 4.3774 | 4.1860 | 0.1913 |
|---|-------------------------------------|--------------------------------------|--------|--------|--------|
| 24 | InChI=1S/C5H12c1-4-5(2)3/h5H,4H2,1-3H3 | 2-methylbutane                        | 3.7840 | 3.8374 | 0.0534 |
| 25 | InChI=1S/C3H4O/c1-2-3-4h2H,1H3        | Methylketene                         | 4.0119 | 4.0019 | 0.0099 |
| 26 | InChI=1S/C3H8/c1-3-2h3,1-2H3          |                                      | 4.2183 | 4.3126 | 0.0943 |
| 27 | InChI=1S/C4H10/c1-4-2(3)h4H,1-3H3     |                                      | 4.1151 | 4.0563 | 0.0587 |
| 28 | InChI=1S/C6H14/c1-3-5-6-4/h3-6H2,1-2H3|                                      | 4.2570 | 4.3373 | 0.0803 |
| 29 | InChI=1S/C5H12c1-4-5(2)3/h5H,4H2,1-3H3|                                      | 4.1194 | 4.0778 | 0.0415 |
| 30 | InChI=1S/C7H16/c1-4-6-7(3)5-2/h7H,4-6H2,1-3H3/| | 4.0807 | 4.0971 | 0.0164 |
Fig. S3 Binding energy between lithium polysulfides ($\text{Li}_2\text{S}_x$, $x = 2, 4, 8$) and a functionalized graphene model at the PBE1PBE/6-31+G* level of theory.
Table S3 Methods supported by the redox potential workflow in MISPR; redox potential calculations can be done in any phase and at any charge state (i.e., any number of electron and hydrogen transfers)

| Method | Notes | Example scheme(s) | Equations | Abbreviations |
|--------|-------|-------------------|-----------|---------------|
| HOMO/LUMO | Geometry optimization is done for the molecule at the reference state to calculate the HOMO/LUMO energies. |  | IP = HOMO  
EA = LUMO | IP:\ ionization potential (eV)  
EA: electron affinity (eV) |
| Direct electron transfer | Geometry optimization and frequency calculation are done at each charge state in one phase specified by the user (vacuum or solution). | $\Delta G_{\text{ox} \rightarrow \text{net}} = G(M^{2+}) - G(M)$  
$\Delta G_{\text{red} \rightarrow \text{net}} = G(M^{2-}) - G(M)$ | $\Delta G_{\text{ox} \rightarrow \text{net}} = \frac{\Delta G_{\text{ox}, \text{net}}}{2F}$  
$\Delta G_{\text{red} \rightarrow \text{net}} = \frac{\Delta G_{\text{red}, \text{net}}}{2F}$  
$EA = -\frac{\Delta G_{\text{red}, \text{net}}}{F}$  
$EA_1 = -\frac{\Delta G_{\text{red}, \text{1}}}{F}$  
$EA_2 = -\frac{\Delta G_{\text{red}, \text{2}}}{F}$ | $\Delta G_{\text{ox} \rightarrow \text{net}}$: Net Gibbs free energy oxidation  
$\Delta G_{\text{red} \rightarrow \text{net}}$: Net Gibbs free energy of reduction  
$\Delta G_{\text{red}, \text{1}}$: Gibbs free energy of reduction for the first electron transfer  
$\Delta G_{\text{red}, \text{2}}$: Gibbs free energy of reduction for the second electron transfer  
$EA$: electron affinity from the first electron transfer  
$EA_2$: electron affinity from the second electron transfer |
| Vertical IP/EA | Geometry optimization is done for molecules at the reference state only at each phase specified by the user. Frequency calculation is done at each charge state and phase. | $M(g)\rightarrow M^{-}(g)$ | $G = H - T\Delta S = E_{\text{SCF}} + E_{\text{ZPE}} + H_{\text{corr}} - T\Delta S_{\text{corr}}$  
$\Delta G_{\text{ox} \rightarrow \text{g}}(g) = G(M^{2+}) - G(M)$  
$\Delta G_{\text{red} \rightarrow \text{g}}(g) = G(M^{2-}) - G(M)$  
$\Delta G_{\text{ox} \rightarrow \text{s}}(g) = G(M^{2+}) - G(M)$  
$\Delta G_{\text{red} \rightarrow \text{s}}(g) = G(M^{2-}) - G(M)$ | $E_{\text{SCF}}$: energy  
$E_{\text{ZPE}}$: zero-point vibrational energy correction  
$S_{\text{corr}}$: correction to entropy  
$H_{\text{corr}}$: correction to enthalpy  
$\Delta G_{\text{ox} \rightarrow \text{g}}(g)$: Gibbs free energy of reduction in the gas phase  
$\Delta G_{\text{red} \rightarrow \text{g}}(g)$: Gibbs free energy of reduction in the gas phase  
$\Delta G_{\text{ox} \rightarrow \text{s}}(g)$: Gibbs free energy of reduction in the solution phase  
$\Delta G_{\text{red} \rightarrow \text{s}}(g)$: Gibbs free energy of reduction in the solution phase  
$F$: Faraday constant  
n: Number of electrons |
| Adiabatic IP/EA | Geometry optimization and frequency calculation are done at each charge state and phase. |  |  |  |
| Sequential proton-coupled electron transfer (PCET) | Direct as well as adiabatic calculations are supported. Number of hydrogen transfer steps is assumed to be equal to the number of electron transfer steps. | $pK_a = \frac{\Delta G}{2.303RT}$  
$K_u = 10^{-pK_a}$ | $pK_a$: acid dissociation constant at the logarithmic scale  
$K_u$: acid dissociation constant  
T: temperature  
R: gas constant  
$E^*$: reduction potential  
$E_{\text{app}}$: experimentally measured reduction potential of the reference compound  
$E_{\text{avg}}$: average potential |
### Table S4 Details of the library used for the redox potential calculations

| Molecule number | InChI code                                                                 | Molecule name               | 2D representation | Type                              | Note                                      |
|-----------------|---------------------------------------------------------------------------|----------------------------|--------------------|-----------------------------------|------------------------------------------|
| 1               | InChI=1S/C₄H₁₀Oc1·d(2,3)5/h5H₁-3H₃                                      | tert-butanol                 | ![ tert-butanol ]   | Linear oligo (ether carbonate)    | formed by ring opening of EC             |
| 2               | InChI=1S/C₅H₁₀O₂c1·d(3-7-5)2/h6H₃-4H₂1-2H₃                          | n-Propyl acetate             | ![ n-Propyl acetate ] | Solvent                           | Ester                                    |
| 3               | InChI=1S/C₈H₁₈O₃Sc1·d(1-2-4-6-9-10)8-6-4-2H₃-8H₂1-2H₃                 | butyl sulfone                | ![ butyl sulfone ]  | Electrolyte additive              | SEI forming additive                     |
| 4               | InChI=1S/C₃H₆O₂Sc4·d(6(7)1-2-6-7)/h1-3H₂                            | 1,3-propane sulfone          | ![ 1,3-propane sulfone ] | Electrolyte additive              | Suppresses decomposition of solvents with graphite electrode |
| 5               | InChI=1S/C₄H₈O₂Sc5·d(6(7)/1-2-4-7)/h1-4H₂                          | tetra methylene sulfolane    | ![ tetra methylene sulfolane ] | Electrolyte additive              |                                         |
| 6               | InChI=1S/C₃H₆O₂Sc1·d(6(2,4)/h3H₂-1-2H₃                           | ethyl methyl sulfone          | ![ ethyl methyl sulfone ] | Electrolyte additive              |                                         |
| 7               | InChI=1S/C₃H₆O₂Sc4·d(6(2,4)/h3H₂-1-2H₃                           | tri-methylene sulfone         | ![ tri-methylene sulfone ] | Electrolyte additive              | Regulates Li deposition                 |
| 8               | InChI=1S/C₆H₁₄O₂Sc1·d(4-6(3(9,7,8)5-2)h6H₄-5H₂1-3H₃             | ethyl sec-butyl sulfone       | ![ ethyl sec-butyl sulfone ] | Electrolyte additive              | Low boiling point and high conductivity |
| 9               | InChI=1S/C₆H₁₄O₂Sc1·d(4-9(7,8)5-6(2)/h6H₄-5H₂1-3H₃             | ethyl iso-butyl sulfone       | ![ ethyl iso-butyl sulfone ] | Electrolyte additive              | Low melting point (< 0 °C)               |
| 10              | InChI=1S/C₅H₁₂O₂Sc1·d(6(2,4)/h3H₅-4H₂1-3H₃                        | ethyl iso-propyl sulfone      | ![ ethyl iso-propyl sulfone ] | Electrolyte additive              | Hydrolysis-resistant                     |
| 11              | InChI=1S/C₇H₇FO₂Sc1·d(1-11(9,10)/3·2-4-6(7)8/h2-5H,1H₃         | 1-flouro-2- (methyl-sulfonyl) benzene | ![ 1-flouro-2- (methyl-sulfonyl) benzene ] | Electrolyte additive              |                                         |
| InChI   | CAS  | Name                      | Role               |
|---------|------|---------------------------|--------------------|
| 12      | C5H12O3S/c1-3(9,6,7)5-4-8-2h3-5H2,1-2H3 | ethyl 2-methoxymethylethylsulfone | Electrolyte additive |
| 13      | C7H16O4S/c1-3-12,8(9)7-6-11-5-4-10-2h3-7H2,1-2H3 | ethyl methoxyethoxymethylethylsulfone | Electrolyte additive, Large oxidation potential |
| 14      | C4H8O2/c1-3-6-4(2)5/h3h3H2,1-2H3 | ethyl acetate | Solvent, Low viscosity and melting point compared to carbonates |
| 15      | C3H6O2/c1-3(4)/5-2h1-2H3 | methyl acetate | Solvent, Low viscosity and melting point compared to carbonates |
| 16      | C2H4O2/c1-4-2-3H2H1H3 | methyl formate | Solvent |
| 17      | C5H10O2/c1-3-5(6)7-4-2h3-4H2,1-2H3 | ethyl propionate | Solvent |
| 18      | C6H10O2/c1-3-5-6(7)8-4-2h3-5H2,1-2H3 | ethyl butyrate | Solvent |
| 19      | C4H7FO2/c1-2-7-4(6)3-5h2-3H2,1H3 | ethyl fluoroacetate | Solvent, Fluorinated |
| 20      | C3H6O3/c1-3(6)2(4)5/h3h3H2,1H3 | dimethyl carbonate | Solvent-Additive, Fluorinated |
| 21      | C5H9FO2/c1-3-8-5(7)4(2)6h4H,3H2,1-2H3 | ethyl 2-fluoroacetopropionate | Additive, Fluorinated |
| 22      | C5H9FO2/c1-2-3(7)8-4-3-6h2-4H2,1H3 | 2-fluoroethyl propionate | Additive, Fluorinated |
| 23      | C5H9FO2/c1-2-8-5(7)3-4-6h2-4H2,1H3 | ethyl 3-fluoroacetopropionate | Additive, Fluorinated |
| 24      | C5H10O3/c1-3-7-5(6)8-4-2h3-4H2,1-2H3 | diethyl carbonate | Solvent |
| 25      | C3H6O3/c1-5-3(4)/6-2h1-2H3 | dimethyl carbonate | Solvent |
| InChI          | Structure           | Description                                      |
|---------------|---------------------|--------------------------------------------------|
| 26 InChI=1S/C3H4O3/c4-3-5-1-2-6-3/h1-2H2 | ![Structure](image1.png) | ethylene carbonate                               |
| 27 InChI=1S/C4H6O3/c1-3-2-6-4(5/-3/h3H2,1H3 | ![Structure](image2.png) | propylene carbonate                               |
| 28 InChI=1S/C4H8O3/c1-3-7-4(5)/6-2/h3H2,1-2H3 | ![Structure](image3.png) | ethyl methyl carbonate                            |
| 29 InChI=1S/C4H10O2/c1-5-3-4-6-2/h3-4H2,1-2H3 | ![Structure](image4.png) | 1,2-dimethoxyethane                               |
| 30 InChI=1S/C3H6O2/c1-2-5-3-4-1/h1-3H2 | ![Structure](image5.png) | Dioxolane                                        |
| 31 InChI=1S/C4H7FO2/c1-4(6)/7-3-2-5/h2-3H2,1H3 | ![Structure](image6.png) | Fluoroethyl acetate                               |
| 32 InChI=1S/C4H10O2/c1-4-5-2-3-6-4/h4H2,2-3H2,1H3 | ![Structure](image7.png) | 2-methyl-1,3-dioxolane                            |
| 33 InChI=1S/C5H8O4/c6-5-8-3-1-7-2-4-9-5/h1-4H2 | ![Structure](image8.png) | 1,3,6-trioxocan-2-one                             |
| 34 InChI=1S/C5H10O3/c1-5-3-2-4-6-5/h5H2-4H2,1H3 | ![Structure](image9.png) | methyl tetrahydrofuran                            |
| 35 InChI=1S/C2H3N/c1-2-3/h1H3 | ![Structure](image10.png) | Acetonitrile                                      |
| 36 InChI=1S/C4H6O2/c5-4-2-1-3-6-4/h1-3H2 | ![Structure](image11.png) | Gamma-Butyrolactone                               |
| 37 InChI=1S/C4H10O3/c1-3-5-4-2/h3-4H2,1-2H3 | ![Structure](image12.png) | Diethyl ether                                     |
| 38 InChI=1S/C2H6O3S/c1-4(2)/3/h1-2H3 | ![Structure](image13.png) | Dimethyl sulfoxide                                |
| 39 InChI=1S/C4H7NO2/c1-5-2-3-7-4(5)/6h2-3H2,1H3 | ![Structure](image14.png) | 3-methyl oxazolidin-2-one                         |
| InChI         | Name                          | Type             |
|--------------|-------------------------------|------------------|
| InChI=1S/C4H8O/c1-2-4-5-3-1/h1-4H2 | tetrahydrofuran  | Solvent         |
| InChI=1S/C5H10O2S/c1-5-2-3-8(6,7)-4-5/h5H,2-4H2,1H3 | 3-methyl sulfolane | Solvent-additive |
| InChI=1S/C4H8O2/c1-4-2-5-3-6-4/h4H2,2-3H2,1H3 | 4-methyl dioxolane | Solvent         |
| InChI=1S/C5H8O/c1-2-4-3-7-5(6)8-4/h4H2,2-3H2,1H3 | 1,2-butylene carbonate | Solvent         |
| InChI=1S/C5H9CO2/c1-2-3-5(7)-8-4-6/h2-4H2,1H3 | chloromethyl butyrate | Solvent         |
| InChI=1S/C6H14O2/c1-3-7-5-6-8-4-2/h3-4H2,1-2H3 | 1,2-diethoxethane | Solvent         |
| InChI=1S/C4H10S/c1-3-5-4-2/h3-4H2,1-2H3 | diethyl sulfoxide | Additive         |
| InChI=1S/C4H6F2O3/c1-4-7-9-2-3(5)/6/h3H2,1H3 | difluoro ethyl methyl carbonate | Solvent         |
| InChI=1S/C3H8O2/c1-4-3-5-2/h3H2,1-2H3 | dimethoxymethane | Solvent         |
| InChI=1S/C2H6S/c1-3-2/h1-2H3 | dimethyl sulfide | Solvent         |
| InChI=1S/C3H8O2/c6-5-3-1-2-4-7-5/h1-4H2 | δ-valero lactone | Lactone         |
| InChI=1S/C4H6F2O2/c1-2-8-4(7)-3(5)/6/h3H2,1H3 | ethyl difluoro acetate | Solvent-Additive |
| InChI=1S/C5H9F2O3/c1-2-9-5(8)10-3-4(6)/7/h4H2,2-3H2,1H3 | ethyl difluoro ethyl carbonate | Solvent         |
| No. | InChI          | Chemical Name                     | Property                                      |
|-----|----------------|-----------------------------------|-----------------------------------------------|
| 53  | InChI=1S/C6H12F2O2/c1-2-9-3-4-10-5-6(7)8h6H2-5H2,1H3 | ethoxy difluoro ethoxy ethane | Solvent Fluorinated                            |
| 54  | InChI=1S/C5H9FO3/c1-2-8-5(7)9-4-3-6h2-4H2,1H3 | ethyl fluoroethyl carbonate          | Solvent Offers higher conductivity than diethyl carbonate |
| 55  | InChI=1S/C6H13FO2/c1-2-8-5-6-9-4-3-7h2-6H2,1H3 | ethoxy fluoro ethoxy ethane         | Solvent Fluorinated                            |
| 56  | InChI=1S/C2H6O2/c3-1-2-4h3-4H1-2H2 | ethylene glycol                    | Filler material Component of solid-state polymer electrolytes |
| 57  | InChI=1S/C3H8O2/c1-5-3-2-4h4H2-3H2,1H3 | 2-methoxyethanol                   | Solvent                                      |
| 58  | InChI=1S/C5H12O2/c1-3-7-5-4-6-2h3-5H2,1-2H3 | 1-ethoxy-2-methoxyethane           | Solvent High relative permittivity and lower viscosity compared to dimethyl carbonate |
| 59  | InChI=1S/C4H10O2S/c1-3-7(5,6)4-2h3-4H2,1-2H3 | ethyl methyl sulfone               | Solvent Low melting point and high conductivity |
| 60  | InChI=1S/C2H4O/c1-2-3-1h1-2H2 | ethylene oxide                     | Polymer host Polymer electrolyte material         |
| 61  | InChI=1S/C6H12O3/c1-3-5-9-6(7)8-4-2h3-5H2,1-2H3 | ethyl propyl carbonate             | Solvent                                      |
| 62  | InChI=1S/C5H12O3/c1-3-5-6-4-2h3-5H2,1-2H3 | ethyl propyl ether                 | Solvent                                      |
| 63  | InChI=1S/C2H4O3S/c3-6-4-1-2-5-6h1-2H2 | ethylene sulfite                  | Additive Film forming electrolyte additive    |
| 64  | InChI=1S/C7H14OS2S/c1-2-10(8,9)7-5-3-4-6-7h7H2-6H2,1H3 | ethyl cyclopentyl sulfone          | Solvent High oxidation potential              |
| 65  | InChI=1S/C5H7F3O3/c1-2-10(4)11-3-5(6,7)8h62-3H2,1H3 | ethyl trifluoro ethyl carbonate    | Solvent Fluorinated Good low temperature performance |
| InChI          | Description                                                                 |
|----------------|-----------------------------------------------------------------------------|
| C6H6F9O4P     | tris(2,2,2-trifluoroethyl) phosphate                                        |
| Co-solvent     | Flame-retarding in EC-PC-EMC electrolytes                                   |
| 1S/C4H8O2S/c1 | ethyl vinyl sulfone                                                         |
| Solvent       | High conductivity in LiTFSI electrolyte                                      |
| 1S/C4H9F3O2S/c1| trifluoro propyl methyl sulfone                                             |
| Solvent       | Fluorinated; Forms a protective SEI layer on the graphite anode upon reduction|
| 1S/C4H5FO2/c5 | fluoro propylene carbonate                                                  |
| Solvent       | Highly polar                                                                |
| 1S/C5H10O2/c1 | methyl butyrate                                                             |
| Cosolvent     | Film-forming additive used in gel-based electrolytes                         |
| 1S/C4H5NO2/c1 | methyl cyanoacetate                                                         |
| Additive      | nucleophile                                                                 |
| 1S/C3H5FO3/c1 | mono fluoro dimethyl carbonate                                             |
| Solvent       | Fluorinated, Higher conductivities than dimethyl carbonates at low concentrations|
79. InChI=1S/C4H7FO3/c1-7-4(6)8-3-2-5h2-3H2,1H3
Mono fluoro ethyl methyl carbonate
Solvent
Fluorinated

80. InChI=1S/C5H10O3/c1-4(2)-8-5(6)7-3/h4H,1-3H3
methyl isopropyl carbonate
Solvent
Alkyl carbonate

81. InChI=1S/C5H10O3/c1-3-4-8-5(6)-7-2/h3-4H2,1-2H3
methyl propyl carbonate
Solvent

82. InChI=1S/C4H8O3S/c1-4-3-2-8-7(4,5)/6/h4H,2-1H3
methyl triethylene sulfone
Solvent

83. InChI=1S/C2H6O2S/c1-5(2,3)/4/h1-2H3
dimethyl sulfone
Solvent
Enhanced safety with ethylene carbonate due to the high flash point of the mixture

84. InChI=1S/C5H5F5O3/c1-12-3(11)13-2-4(6,7)/5(8,9)/10/h2H2,1H3
tenpa fluoro propyl methyl carbonate
Solvent
Fluorinated; High molecular volume and molecular weight

85. InChI=1S/C3H6O3S/c1-3-2-5-7(4)/6-3/h3H,2-1H3
propylene sulfate
Additive
Film-forming

86. InChI=1S/C5H9F4O3/c1-11-4(10)/12-2-5(8,9)/3(6)/7/h3H,2-1H3
tenpa fluoro propyl methyl carbonate
Solvent
Fluorinated

87. InChI=1S/C4H5F3O3/c1-9-3(8)/10-2-4(5,6)/7/h2H2,1H3
trifluoro ethyl methyl carbonate
Solvent
Fluorinated

88. InChI=1S/C5H7F3O3/c1-10-4(9)/11-3-2-5(6,7)/8/h2-3H2,1H3
trifluoro propyl methyl carbonate
Solvent
Fluorinated

89. InChI=1S/C12H26O2S/c1-7-11(9)/3(6)15(13,14)12(8-2)/10(5,6)h9-12H,7-8H2,1-6H3
ethyl iso-butyl sulfone
Solvent
| InChI | Structure | Identity | Notes |
|-------|----------|----------|-------|
| 90    | ![Structure](https://example.com/structure90.png) | InChI=1S/C10H22O2S/c1-7-9(3,4)13(11,12)10(5,6)8-2/h7-8H2,1-6H3 | ethyl-isopropyl sulfone | Solvent |
| 91    | ![Structure](https://example.com/structure91.png) | InChI=1S/C8H12F6O2S/c9-7(10,11)3-1-5-17(15,16)6-2-4-8(12,13)14/h1-6H2 | 3,3,3-trifluoropropyl methyl sulfone | Solvent |
| 92    | ![Structure](https://example.com/structure92.png) | InChI=1S/C4H8O3/c1-6-3-4(5)7-2/h3H2,1-2H3 | methyl methoxy acetate | Solvent |
| 93    | ![Structure](https://example.com/structure93.png) | InChI=1S/C6H12O3/c1-5-8-3-9-6(2)7/h5H,4H2,1-3H3 | methoxy-2-propyl acetate | Solvent |
| 94    | ![Structure](https://example.com/structure94.png) | InChI=1S/C3H5FO2/c1-6-3(5)2-4/h2H2,1H3 | methyl fluoro acetate | Solvent |
| 95    | ![Structure](https://example.com/structure95.png) | InChI=1S/C5H12O2/c1-3-6-5-7-4-2/h3-5H2,1-2H3 | ethoxy methoxy ethane | Solvent |
| 96    | ![Structure](https://example.com/structure96.png) | InChI=1S/C2H6O3S/c1-4-6(3)5-2/h1-2H3 | dimethyl sulfite | Solvent |
| 97    | ![Structure](https://example.com/structure97.png) | InChI=1S/C2H6O3S/c1-5-6(2,3)4/h1-2H3 | methyl methane sulfonate | Solvent |
| 98    | ![Structure](https://example.com/structure98.png) | InChI=1S/C2H6O4S/c1-5-7(3,4)6-2/h1-2H3 | dimethyl sulfate | Solvent |
| 99    | ![Structure](https://example.com/structure99.png) | InChI=1S/C4H8O2S/c1-4-2-7(5,6)3-4/h4H2,1H3 | 2-methyltrimethylene sulfone | Solvent |
| 100   | ![Structure](https://example.com/structure100.png) | InChI=1S/C5H8O2/c1-4-2-3-5(6)7-4/h4H2,1H3 | γ-valero lactone | Solvent |

**Improvement in safety compared to ethylene carbonate**
Fig. S4 Example of a (a) force field dictionary and (b) the labeled structure of the corresponding molecule.

Fig. S5 (a) Solvents used for MD simulations with 1 M lithium bis(trifluoromethylsulfonyl)imide, (b) coordination number, and (c) diffusion coefficients computed using MISPR.
Fig. S6 Code snippet of the submission of a hybrid DFT-MD workflow for a lithium bis(trifluoromethylsulfonyl)imide in monoglyme liquid solution using the default MD recipe in MISPR, GAFF parameters for the anion and solvent, and user-defined parameters for the cation
Fig. S7 Example of (a) binding energy document from the DFT database and (b) MD document
Table S5 Details of the library used for the NMR calculations along with the experimental measurements made in chloroform solvent at 298 K and referenced to tetramethylsilane

| Molecule number | InChI code | Molecule name | 2D representation | $^1$C NMR spectra frequency (MHz) | $^1$H NMR spectra frequency (MHz) | $^1$C NMR chemical shift (ppm) | $^1$H NMR chemical shift (ppm) | Ref |
|-----------------|------------|---------------|-------------------|---------------------------------|---------------------------------|-------------------------------|-------------------------------|-----|
| 1               | InChI=1S/H2O/h1H2 | water | | 75.5, 126, 151 | | 1.2: 1.56 | | 2 |
| 2               | InChI=1S/C2H4O2/c 1-2(3)(4)h1H3,(H,3,4) | acetic acid | | 300, 500, 600 | 75.5, 126, 151 | 3: 175.99 | 4,5,6: 2.10 | 2 |
| 3               | InChI=1S/C3H6O/c1 -3(2)4/h1-2H3 | acetone | | 300, 500, 600 | 75.5, 126, 151 | 1: 207.07 | 2,3: 30.92 | 4,5,6,7,8,9: 2.17 | 2 |
| 4               | InChI=1S/C2H3N/c1 -2-3/h1-2H2 | acetonitrile | | 300, 500, 600 | 75.5, 126, 151 | 1: 1.89 | 2: 116.43 | 3,4,5: 2.10 | 2 |
| 5               | InChI=1S/C6H6/c1- 2-4-6-5-3-1/h1-6H | benzene | | 300, 500, 600 | 75.5, 126, 151 | 0,1,2,3,4,5: 128.37 | 6,7,8,9,10,11: 7.36 | 2 |
| 6               | InChI=1S/C4H10O/c 1-4(2,3)5/h5H,1-3H3 | tert -butyl alcohol | | 25.16 | 300 | 2.3,4: 31.23 | 1: 69.05 | 5,6,7,8,9,10,11,12,13: 1.262 | 14: 2.01 | 3 |
| 7               | InChI=1S/CO2/c2-1-3 | carbon dioxide | | 300, 500, 600 | 75.5, 126, 151 | 2: 124.99 | | 2 |
| 8               | InChI=1S/CS2/c2-1-3 | carbon disulfide | | 300, 500, 600 | 75.5, 126, 151 | 2: 192.83 | | 2 |
| 9               | InChI=1S/CCl4/c2- 1(3,4)5 | carbon tetrachloride | | 300, 500, 600 | 75.5, 126, 151 | 4: 96.34 | | 2 |
19 InChI=1S/C4H10O2/c1-5-3-4-6-2h3-4H2,1-2H3 1,2-dimethoxyethane 300, 500, 600 75.5, 126, 151 2.3: 71.84 4.5: 59.08 6,7,8,9: 3.55 10,11,12,13,14,15: 3.40

20 InChI=1S/C2H6/c1-2h1-2H3 ethane 300, 500, 600 75.5, 126, 151 0.1: 6.89 2.3,4,5,6,7: 0.87

21 InChI=1S/C2H6O/c1-2-3h1,2H2,1H3 ethanol 300, 500, 600 75.5, 126, 151 1: 58.28 2: 18.41 3.4: 3.66 5,6,7: 1.19 8: 1.33

22 InChI=1S/C4H8O2/c1-3-6-4-2h3H2,1-2H3 ethyl acetate 300, 500, 600 75.5, 126, 151 2: 60.49 3: 14.19 4: 171.36 5: 21.04 6,7: 4.12 8,9,10: 1.26 11,12,13: 2.05

23 InChI=1S/C2H4/c1-2h1-2H2 ethylene 300, 500, 600 75.5, 126, 151 0.1: 123.13 2,3,4,5: 5.4

24 InChI=1S/C2H6O2/c3-1-2h1-2H2 ethylene glycol 300, 500, 600 75.5, 126, 151 2.3: 63.79 4.5,6,7: 3.76

25 InChI=1S/C12H18/c1-7- 8(2)10(4)12(6)11(5)9(7)3/h1-6H3 hexamethylbenzene 300, 500, 600 75.5, 126, 151 0,1,2,3,4: 132.21 6,7,8,9,10,11: 16.98 12,13,14,15,16,17, 18,19,20,21,22,23, 24,25,26,27,28,29: 2.24

26 InChI=1S/C6H14/c1-3-5-6-4-2h3-6H2,1-2H3 n-hexane 300, 500, 600 75.5, 126, 151 0,1: 31.64 2,3: 22.70 4,5: 14.14 14,15,16,17,18,19: 0.89 6,7,8,9,10,11,12,13: 1.27

27 InChI=1S/C6H18OSi2/c1-3-5-6-4-2h3-6H2,1-2H3 hexamethyldisiloxane 300, 500, 600 75.5, 126, 151 3.5,6,8: 1.97 9,10,11,15,16,17,18, 19,20,24,25,26, 0.07
37 InChI=1S/C3H6/c1-3-2/h3H,1H2,2H3 300, 500, 600 75.5, 126, 151 0: 19.50, 1: 133.91, 2: 115.74 3,4,5: 1.73 6: 5.83, 7: 4.94, 8: 5.03

38 InChI=1S/C5H5N/c1-2-4-6-5-3/h1-5H 300, 500, 600 75.5, 126, 151 1: 135.96 2,3: 123.75 4,5: 149.90 6: 7.68, 7: 7.29, 9: 8.62

39 InChI=1S/C4H5N/c1-2-4-5-3/h1-5H 300, 500, 600 75.5, 126, 151 1,2: 117.77, 3,4: 107.98 5: 8.40, 6: 6.7, 7: 6.83, 8: 6.26

40 InChI=1S/C4H9N/c1-2-4-5-3-1/h1-4H2 300, 500, 600 75.5, 126, 151 1,2: 25.56 3,4: 46.93 5,6,7,8: 1.68, 9,10,11,12: 2.87

41 InChI=1S/C4H9O2/c1-2-4-5-3-1/h1-4H2 300, 500, 600 75.5, 126, 151 1,2: 25.62 3,4: 67.97 5,6,7,8: 1.85, 9,10,11,12: 3.76

42 InChI=1S/C7H8/c1-7-5-3-2-4-6-7/6H,1H3 25.16 89.56 0: 137.83 1,2: 129.09 3: 21.41 4,5: 128.28 6: 125.38 7,8,12,13,14: 7.38, 7.0, 9,10,11: 2.34

43 InChI=1S/C6H15N/c1-4-7(5-2)6-3/h4-6H2,1-3H3 15.09 300 1,2,3: 46.46, 4,5,6: 11.78 7,8,12,13,14: 4.5,6: 3.325 13,14,15: 0.97

44 InChI=1S/C2H3NS/c1-3-2-4/h1H3 50.18 300 2: 30.48, 3: 128.9 4,5,6: 3.325

45 InChI=1S/C4H2O3/c5-3-1-2-4-6(7-3)/H-1-2H 25.16 300 1: 136.76, 2: 125.38 3,4: 164.58 7,8: 7.048
46 InChI=1S/C5H6N2/c 1-5-4-6-2-3-7-5h2-4H,1H3
  2- methylpyrazine
   25.16  89.56
   2: 154.11
   3: 21.53
   4: 144.85
   5: 141.90
   6: 143.90

47 InChI=1S/C3H7N/c1-2-3-4H2H1,1,3-4H2
  allylamine
   25.16  89.56
   1: 44.82
   2: 140.01
   3: 113.48

48 InChI=1S/C2H4O/c1-2-3/h2H,1H3
  acetaldehyde
   50.18  300
   1: 107.81
   2: 137.52

49 InChI=1S/CH2O2/c2-1-3/h1H,(H,2,3)
  formic acid
   15.09  89.56
   1: 50.40
   2: 82.18

50 InChI=1S/C3H6N2/c1-3-2h3H,2H2,1H3
  methyl hydrazine
   25.16  89.56
   2: 43.49

51 InChI=1S/C3H3N/c1-2-3-4H2H1,1H2
  acrylonitrile
   15.09  89.56
   1: 107.81
   2: 137.52

52 InChI=1S/C3H7N/c1-2-3-4-2h1-2H3
  2-butynyl
   50.18  300
   0.1: 3.33
   2.3: 74.56

53 InChI=1S/C3H4O/c1-2-3-4h1,4H,3H2
  propargyl alcohol
   25.16  89.56
   1: 50.40
   2: 82.18

54 InChI=1S/C3H7N/c1-3-2-4-3h3-4H2H1,1H3
  2methyl aziridine
   25.16  89.56
   1: 25.23
   2: 28.6
   3: 19.84

3
55  InChI=1S/C2H5NO/c 1-3-2- 4H2,1H3, (H,3,4)  N-methyl formamide  15.09  399.65  2: 28.21  3: 166.49  4,5,6: 2.815  7: 7.4  8: 8.159

56  InChI=1S/C3H9N/c1-3-2- 4H3,1H2,1- 2H3  isopropylamine  15.09  89.56  1: 42.83  2-3: 26.21  4: 3.102  5,6,7,8,9,10: 1.071  11,12: 1.221

57  InChI=1S/C3H8O/c1-2-3-4H2,1- 3H2,1H3  propanol  15.09  89.56  1: 25.89  2: 64.25  3: 10.28  4: 3.102  5,6,7: 3.582  8,9,10: 0.94  11: 2.26

58  InChI=1S/CH4NO2/c 1-2-3-4H1H3, (H,3,4)/q +1  nitromethane  15.09  399.65  3: 62.59  4,5,6: 4.341

59  InChI=1S/C2H7NO/c 3-1-2-4H1H1- 3H2  ethanolamine  15.09  89.56  2: 43.96  3: 63.18  4: 3.102  5,6,7,8,9: 1.071  11,12: 1.221

60  InChI=1S/C3H2N2/c 4-2-1-3-5H1H2  malononitrie  25.16  300  2: 8.77  3,4: 109.35  5: 3.662

61  InChI=1S/C3H4N2/c 1-2-5-3-4H1-1H1- 3H, (H,4,5)  imidazole  15.09  89.56  2,4: 121.88  3: 135.35  4,5: 7.129  7: 7.729

62  InChI=1S/C5H8/c1-3-5-4-2H3,1H1- 2,5H2  1,4-pentadiene  25.16  300  0: 38.01  1,2: 136.46  3,4: 115.47  5,6: 2.723  7: 7.729

63  InChI=1S/C5H8/c1-2-4-5-3-1H1-2H3, 5H2  cyclopentene  25.16  89.56  0: 22.98  1,2: 32.59  3,4: 130.77  5,6: 1.82  7: 7.4  8: 8.159  11,12: 2.30
| **CAS** | **InChI** | **Name** | **H** | **M** | **D** |
|---------|-----------|----------|-------|------|-------|
| 64      | InChI=1S/C4H7N/c1-4(2)3-5/h4H1-2H3 | isobutyronitrile | 5.16  | 399.65 | 2: 19.87, 3: 19.98, 4: 123.83, 6: 7.8, 8, 10, 11: 1.331 |
| 65      | InChI=1S/C4H6O/c1-2-3-4-5/h1-5H3-4H2 | 3-butyln-1-OL | 3.16  | 89.65  | 1: 22.68, 2: 60.79, 3: 81.40, 4: 70.11, 5: 6.24, 9: 3.48, 10: 2.077 |
| 66      | InChI=1S/C4H6O/c1-2-3-4-5/h1-5H3-2+  | crotonaldehyde  | 15.09 | 89.65  | 1: 154.32, 2: 18.61, 3: 134.61, 4: 194.04, 5: 6.88, 6: 6.146, 7: 9.497 |
| 67      | InChI=1S/C4H6O/c1-3-4-5/h1-4-4H3-2+  | 3-Butyn-2-ol    | 25.16 | 89.65  | 1: 57.86, 2: 24.16, 3: 86.03, 4: 72.12, 5: 6.88, 6: 6.146, 7: 9.497 |
| 68      | InChI=1S/C4H6O/c1-2-4-5-3-1/h1-2H3-4H2-5-1/h2-2H3 | 2,5-dihydrofuran | 25.16 | 89.65  | 1.2: 75.42, 3.4: 126.34, 5: 2.61, 6: 6.24, 7: 9.497, 8: 9.508, 9: 6.211 |
| 69      | InChI=1S/C4H6O/c1-2-4-5-3-1/h1-3H2,4H2 | 2,5-dihydrofuran | 25.16 | 89.65  | 1: 29.28, 2: 198.82, 3: 137.49, 4: 128.96, 5: 6.67, 6: 6.146, 7: 9.497, 8: 9.508, 9: 6.211 |
| 70      | InChI=1S/C4H6O/c1-3-4-5-3-1/h1-2H3-4H2 | methyl vinyl ketone | 15.09 | 89.56  | 1: 26.32, 2: 198.82, 3: 137.49, 4: 128.96, 5: 6.67, 6: 6.146, 7: 9.497, 8: 9.508, 9: 6.211 |
| 71      | InChI=1S/C4H6O/c1-3-5-4-2/h1H4H2,2H3 | ethoxyethane    | 15.09 | 300    | 1: 74.61, 2: 14.22, 3: 90.85, 4: 26.51, 5: 6.67, 6: 6.146, 7: 9.497, 8: 9.508, 9: 6.211 |
| 72      | InChI=1S/C5H10/c1-2-4-5-3-1/h1-5H2 | cyclopentane    | 15.09 | 300    | 0: 1, 2, 3, 4: 26.51, 5: 6.67, 6: 6.146, 7: 9.497, 8: 9.508, 9: 6.211, 10: 1.530 |
InChI=1S/C2H3NS/c 1-4-2-3/h1H3 N-methyl thiocyanate 25.16 300 2: 16.39 4,5,6: 2.596

InChI=1S/C3H7NO/c 1-2-3(4)/h3H,1H3,(H2, 4,5) N,N-dimethyl formamide 25.16 89.56 2: 36.43 3: 21.67 4: 15.0 5: 31.5 6: 1.89 7,8: 4.01 9,10: 3.97 11: 8.6

InChI=1S/C3H7NO/c 1-2-3(4)/h3H,1H3,(H2, 4,5) N,N-dimethyl formamide 25.16 89.56 2: 28.95 3: 9.76 4: 177.68 5: 6.2 6: 2.43 7,8: 4.01 9,10: 3.97 11: 8.6

InChI=1S/C3H7NO/c 1-2-3(4)/h3H,1H3,(H2, 4,5) N,N-dimethyl formamide 25.16 89.56 2: 155.51 3: 21.67 4: 15.0 5: 31.5 6: 1.89 7,8: 4.01 9,10: 3.97 11: 8.6

InChI=1S/C3H7NO/c 1-2-3(4)/h3H,1H3,(H2, 4,5) N,N-dimethyl formamide 25.16 89.56 2: 155.51 3: 21.67 4: 15.0 5: 31.5 6: 1.89 7,8: 4.01 9,10: 3.97 11: 8.6

InChI=1S/C4H11N/c 1-2-3-4(2)5/h4H2,1H3,(H,4, 5) sec-butyramine 25.16 89.56 1: 48.55 2: 32.95 3: 23.50 4: 10.68 5: 2.79 6: 1.36 7: 6.6 8: 1.41

InChI=1S/C4H11N/c 1-2-3-4(2)5/h4H2,1H3,(H,4, 5) sec-butyramine 25.16 89.56 1: 48.55 2: 32.95 3: 23.50 4: 10.68 5: 2.79 6: 1.36 7: 6.6 8: 1.41

InChI=1S/C4H11N/c 1-2-3-4(2)5/h4H2,1H3,(H,4, 5) sec-butyramine 25.16 89.56 1: 48.55 2: 32.95 3: 23.50 4: 10.68 5: 2.79 6: 1.36 7: 6.6 8: 1.41

InChI=1S/C4H11N/c 1-2-3-4(2)5/h4H2,1H3,(H,4, 5) sec-butyramine 25.16 89.56 1: 48.55 2: 32.95 3: 23.50 4: 10.68 5: 2.79 6: 1.36 7: 6.6 8: 1.41

InChI=1S/C2H3NS/c 1-4-2-3/h1H3 N-methyl thiocyanate 25.16 300 2: 16.39 4,5,6: 2.596

InChI=1S/C2H6N2O/c 1-2-3/h1H3 (N,N-dimethyl dimethyldiamino) 25.16 399.65 1: 58.8 2: 12.97 3: 45.11 4: 114.15 5: 7.95 6: 3.317 7,8,9,10,11,12: 1.36 13: 1.053 14,15: 1.25

InChI=1S/C2H6N2O/c 1-2-3/h1H3 (N,N-dimethyl dimethyldiamino) 25.16 399.65 1: 58.8 2: 12.97 3: 45.11 4: 114.15 5: 7.95 6: 3.317 7,8,9,10,11,12: 1.36 13: 1.053 14,15: 1.25

InChI=1S/C2H6N2O/c 1-2-3/h1H3 (N,N-dimethyl dimethyldiamino) 25.16 399.65 1: 58.8 2: 12.97 3: 45.11 4: 114.15 5: 7.95 6: 3.317 7,8,9,10,11,12: 1.36 13: 1.053 14,15: 1.25

InChI=1S/C2H6N2O/c 1-2-3/h1H3 (N,N-dimethyl dimethyldiamino) 25.16 399.65 1: 58.8 2: 12.97 3: 45.11 4: 114.15 5: 7.95 6: 3.317 7,8,9,10,11,12: 1.36 13: 1.053 14,15: 1.25

InChI=1S/C2H6N2O/c 1-2-3/h1H3 (N,N-dimethyl dimethyldiamino) 25.16 399.65 1: 58.8 2: 12.97 3: 45.11 4: 114.15 5: 7.95 6: 3.317 7,8,9,10,11,12: 1.36 13: 1.053 14,15: 1.25

InChI=1S/C2H6N2O/c 1-2-3/h1H3 (N,N-dimethyl dimethyldiamino) 25.16 399.65 1: 58.8 2: 12.97 3: 45.11 4: 114.15 5: 7.95 6: 3.317 7,8,9,10,11,12: 1.36 13: 1.053 14,15: 1.25

InChI=1S/C2H6N2O/c 1-2-3/h1H3 (N,N-dimethyl dimethyldiamino) 25.16 399.65 1: 58.8 2: 12.97 3: 45.11 4: 114.15 5: 7.95 6: 3.317 7,8,9,10,11,12: 1.36 13: 1.053 14,15: 1.25

InChI=1S/C2H6N2O/c 1-2-3/h1H3 (N,N-dimethyl dimethyldiamino) 25.16 399.65 1: 58.8 2: 12.97 3: 45.11 4: 114.15 5: 7.95 6: 3.317 7,8,9,10,11,12: 1.36 13: 1.053 14,15: 1.25

InChI=1S/C2H6N2O/c 1-2-3/h1H3 (N,N-dimethyl dimethyldiamino) 25.16 399.65 1: 58.8 2: 12.97 3: 45.11 4: 114.15 5: 7.95 6: 3.317 7,8,9,10,11,12: 1.36 13: 1.053 14,15: 1.25
Fig. S8 Structure of Li$_2$S$_x$ ($x = 2, 4, 8$) species and pristine graphene model used in the BE calculations

Table S6 Benchmarking results of the adiabatic IP/EA calculations using the SMD solvation model; potentials are reported relative to the Li$^+$/Li potential scale

|                      | Experimental IP (V) | B3LYP/6-311++G** | B3LYP/def2-TZVPD |
|----------------------|---------------------|-------------------|------------------|
|                      | IP (eV)             | EA (eV)           | IP (eV)          | EA (eV)          |
| 6 – ethyl methyl sulfone |                     |                   |                  |
| THF ($\varepsilon = 7.4257$) |                     |                   |                  |
| Acetone ($\varepsilon = 20.493$) | 5.5 (LiTFSI)$^4$ | 5.964             | -0.776           | 5.947            | 0.527            |
| Water ($\varepsilon = 78.355$) |                     | 6.072             | -0.690           | 6.030            | 0.770            |
| 27 – propylene carbonate |                     |                   |                  |
| THF ($\varepsilon = 7.4257$) |                     |                   |                  |
| Acetone ($\varepsilon = 20.493$) | 5.8 (LiClO$_4$)$^5$ | 6.904             | -0.858           | 6.828            | -0.734           |
| Water ($\varepsilon = 78.355$) |                     | 6.697             | -0.260           | 6.627            | -0.493           |
| 53 – ethoxy difluoro ethoxy ethane |                     |                   |                  |
| THF ($\varepsilon = 7.4257$) |                     |                   |                  |
| Acetone ($\varepsilon = 20.493$) |                     | 5.025             | -1.031           | 5.002            | 0.507            |
| Water ($\varepsilon = 78.355$) |                     | 4.995             | -0.952           | 4.910            | 0.701            |
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