Supporting Information

Fluorine-rich Interface for Garnet-based High Performance All-solid-state Lithium Batteries

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Experimental details

Preparation of Al-doped LLZO (Al-LLZO)

Al-doped lithium garnet electrolyte, $Li_{6.28}Al_{0.24}La_3Zr_2O_{12}$ (Al-LLZO) was synthesized via solid-state reaction method. Typically, LiOH (Sigma Aldrich, 98%), Al_2O_3 (Spectrochem, 99%), preheated La_2O_3 (Sigma Aldrich, 99.9%), and ZrO_2 (Sigma Aldrich, 99%) were mixed in stoichiometric ratio with an excess 10 wt% LiOH and were calcined in alumina crucibles at 950 ℃ for 12 h in a muffle furnace. The obtained powder was ground further, and pellets were sintered at 1180 ℃ for 12 h. To avoid the lithium loss during high temperatures, sintering pellets were covered by the mother powder. The retrieved pellets were polished with different-grade emery sheets and were stored inside the glove box for further use.

Preparation of composite polymer electrolyte (CPE)

The composite polymer electrolyte was prepared by a simple solution casting method. Poly (ethylene)oxide (PEO) (avg M_w=300,000), and lithium bis(trifluromethanesulfonyl) imide (LiTFSI) was purchased from Sigma Aldrich. Initially, PEO and LiTFSI, with a weight ratio of 5:1 was dissolved in acetonitrile.

Table S1. Composition of the prepared composite electrolytes.

Electrolyte Name	PEO (mg)	LiTFSI (mg)	Al-LLZO (mg)	FS (µl)
CPE (20)	50	10	20	-
CPE (40)	50	10	40	-
CPE (60)	50	10	60	-
CPE (40) FS	50	10	40	1

Later, the required amount of Al-LLZO was added and the solution was kept for stirring for 12 h. After thorough mixing, the slurry was cast on the Teflon sheet, and the dried membranes were hot pressed to obtain the final free-standing CPE membranes with an average thickness of ~100 µm. The slurry formulation of each CPE composition is listed

in Table S1. The fluorine-based membrane was obtained by adding an organic additive 4-fluorostyrene (FS) (Sigma Aldrich, 99%) into the above polymer slurry in the proper volume fraction (10 µl of FS in 1 gram of the composite). As control experiments, membranes consisting of fluoroethylene carbonate (FEC) instead of FS and $LiClO_4$ instead of LiTFSI were also prepared. All synthesis was carried out in an argon-filled glove box (O_2<0.1 ppm, H_2O< 0.1 ppm).

Material Characterization

The phase analysis was carried out by Bruker Powder X-ray diffractometer (Cu Kα) in the range 10-80°. Horiba Raman Spectrometer with an excitation wavelength of 532 nm was used for further phase analysis. Fourier Transformed Infrared Spectrum of the CPE membrane was captured using Thermoscientific Nicolet iS50 in attenuated total reflectance mode. Thermogravimetric analysis was carried out by TA SDT-Q600 TGA analyzer. The Glass transition temperature and the melting point of the CPE membrane were obtained by differential scanning calorimetry (DSC) measurement (Hitachi DSC7020 calorimeter.) The surface morphology of the as-prepared membranes and the cross-sectional view of the cycled cell were evaluated using Scanning Electron microscopy (Nova NANOSEM 450**).** FEI TECNAI G2 F30 S-Twin Transmission Electron Microscope (TEM) was used to image the filler particle morphology. High-resolution X-ray photoelectron spectroscopy (XPS, cientia Omicron ESCA Plus system, with a Mg-Kα source) was used for distinguishing the different layers formed on the microparticles and membrane before and after cycling.

Computational details

All the density functional theory-based calculations were performed using the Gaussian 16 program package.[1] Geometry optimization of PEO, FS, FEC, and their Li- ion complexes was carried out using the M06-2X/6-31+G(d,p) level of theory.[2] The normal mode analysis was employed to characterize the nature of the stationary points on the potential energy surface and all the minimum energy structures reported in this work were confirmed by the absence of imaginary vibrational modes. The computed free energy values at 298.15 K include zero-point energy and thermal corrections to enthalpy and entropy. The PEO chain is modeled using an oligomer with four monomeric units. Different possible configurations were considered for the PEO, FS, FEC, and their Li-ion complexes, and the lowest energy configurations and their energies are used for the discussions in the manuscript (**Table S5-S7,** and **Fig. S14-S19**).

The binding energies, ΔG_{BE}, were computed using the formula below,

$$\Delta G_{\mathrm{BE}} = G(\mathrm{Li-A\ or\ Li-AB}) - (G(\mathrm{Li^+}) + G(\mathrm{A\ or\ AB})) \quad (1)$$

where $G(\mathrm{Li-A\ or\ Li-AB})$ is the free energy of the Li ion complex formed between Li ion and a molecule A or a non-covalent adduct formed between molecules A and B (eg. FS and PEO) and $G(\mathrm{Li^+})$, $G(\mathrm{A\ or\ AB})$ are the free energies of Li^+ ion, and the molecule or non-covalent adduct between molecules A and B, respectively.

Electrochemical characterization

The ionic conductivity of the CPE membrane was measured in Swagelok cells in a frequency range of 1MHz to 1 Hz with an AC perturbation of 50 mV. Stainless steel discs were used as blocking electrodes. The ionic conductivity (σ) was calculated using the following equation

$$\sigma = \frac{t}{RA} \quad (2)$$

Where *t* is the thickness of the membrane, *R* is the resistance, and *A* is the total contact area. The temperature-dependent conductivity measurements were carried out in a temperature range of 30 -60 °C. For stabilization, the cell was held at each temperature for 1 h prior to conductivity measurements. The activation energy (E_a) was obtained from the Arrhenius plot using the equation.

$$\sigma = \sigma_0 \exp(\frac{-E_a}{kT}) \quad (3)$$

Where σ is the ionic conductivity of the membrane, σ_0 is the pre-exponential factor, *k* is the Boltzmann constant and T is the absolute temperature.

To study the potential stability range of FS-based CPE membrane, Li|CPE(40)FS|SS cells were fabricated and CV measurements were carried out between -0.1 to 6 V *vs.* Li/Li^+. The lithium-ion transport number was calculated according to Bruce and Vincent method by

$$t_{Li} = \frac{I_{ss}(\Delta V - I_0 R_0)}{I_0(\Delta V - I_{ss} R_{ss})} \quad (4)$$

Where $I_{0,}$ and I_{ss} are the initial and steady-state current, R_0 and R_{ss} are the resistance before and after polarisation and ΔV is the applied potential respectively.

To study the interface resistance between lithium metal anode and CPE membranes Li|CPE|Li symmetric cells were fabricated. The EIS analysis was carried out in the

frequency range of 1MHz to 100 mHz with a voltage perturbation of 50 mV. To understand the behaviour of interface resistance over time, the cell was kept at 55 ℃ under open circuit conditions, and the EIS was measured every 24 h for 15 days. In addition, critical current density measurements were carried out by increasing the current in a step of 0.1 mA cm^{-2}. All electrochemical characterizations were carried out in a Biologic workstation, and all measurements were carried out at 55 ℃ unless stated otherwise.

Full cell studies

For full cell assembly, the LFP cathode was prepared by mixing commercial LFP, super P, and PVDF in a weight ratio of 70:20:10 in NMP and was coated on aluminium foil with a loading of about 2-3 mg cm^{-2}. All-solid-state batteries were assembled by stacking lithium metal foil, CPE(40)FS membrane, and LFP cathode in a CR2032 coin cell. It is noteworthy that liquid electrolyte was not used in these systems. The fabricated all-solid-state batteries were cycled between 2.5 to 4 V vs. Li/Li^+ at 55 and 70℃.

The ability of the diffusion of sodium ions also called its diffusivity (D_{Li+}) can be estimated from Fick's second law of diffusion as given by the equation (5)

$$D_{Li^+} = \frac{4}{\pi\tau}\left[\frac{m_B V_M}{M_B S}\right]^2 \left[\frac{\Delta E_s}{\Delta E_t}\right]^2 \qquad (5)$$

where τ is the pulse time in s, m_B and M_B are the mass and molar mass of LFP, V_M is the molar volume, and S is the active surface area of the electrode. ΔE_s and ΔE_t are obtained from the GITT curves.

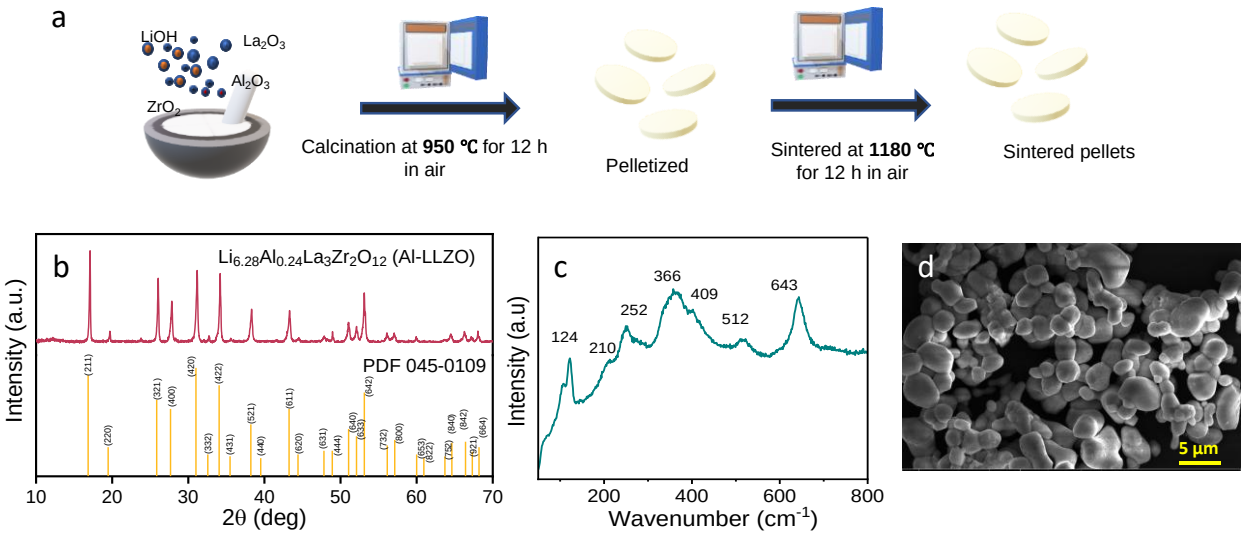

Fig. S1. (a) Synthesis procedure of Al-LLZO ($Li_{6.28}Al_{0.24}La_3Zr_2O_{12}$), (b) XRD pattern and (c) Raman spectrum of the prepared Al-LLZO, (d) SEM image of the crushed Al-LLZO particles.

The $Li_{6.28}Al_{0.24}La_3Zr_2O_{12}$ (Al-LLZO) was synthesized using the solid-state reaction method. The XRD pattern of synthesized Al-LLZO matched well with the JCPDS without the presence of any impurities, indicating the formation of cubic Al-LLZO with a space group of ($Ia\bar{3}d$). The Raman spectrum of Al-LLZO showed distinguished broad peaks between 200 to 500 cm^{-1} corresponding to LiO_4 and LiO_6 modes. In addition, the peaks in the 100-150 cm^{-1} region correspond to La vibrations, and the peak around 640 cm^{-1} corresponds to Zr-O stretching.

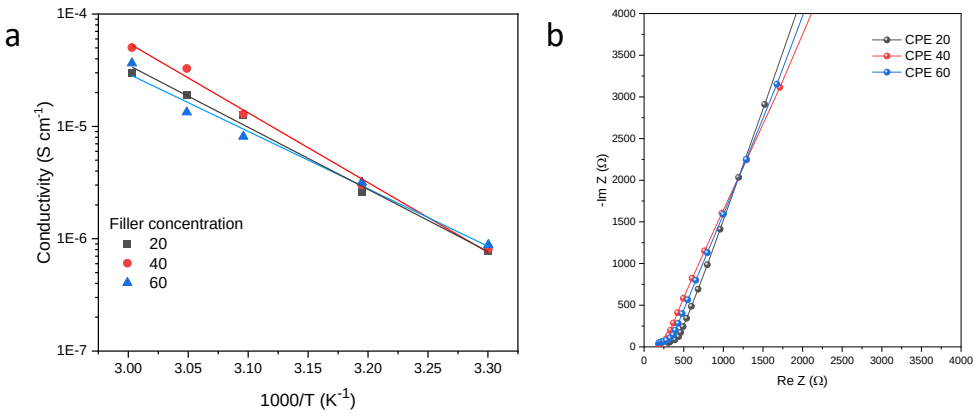

Fig. S2. (a) Arrhenius plot and (b) Nyquist profile of different compositions of CPEs.

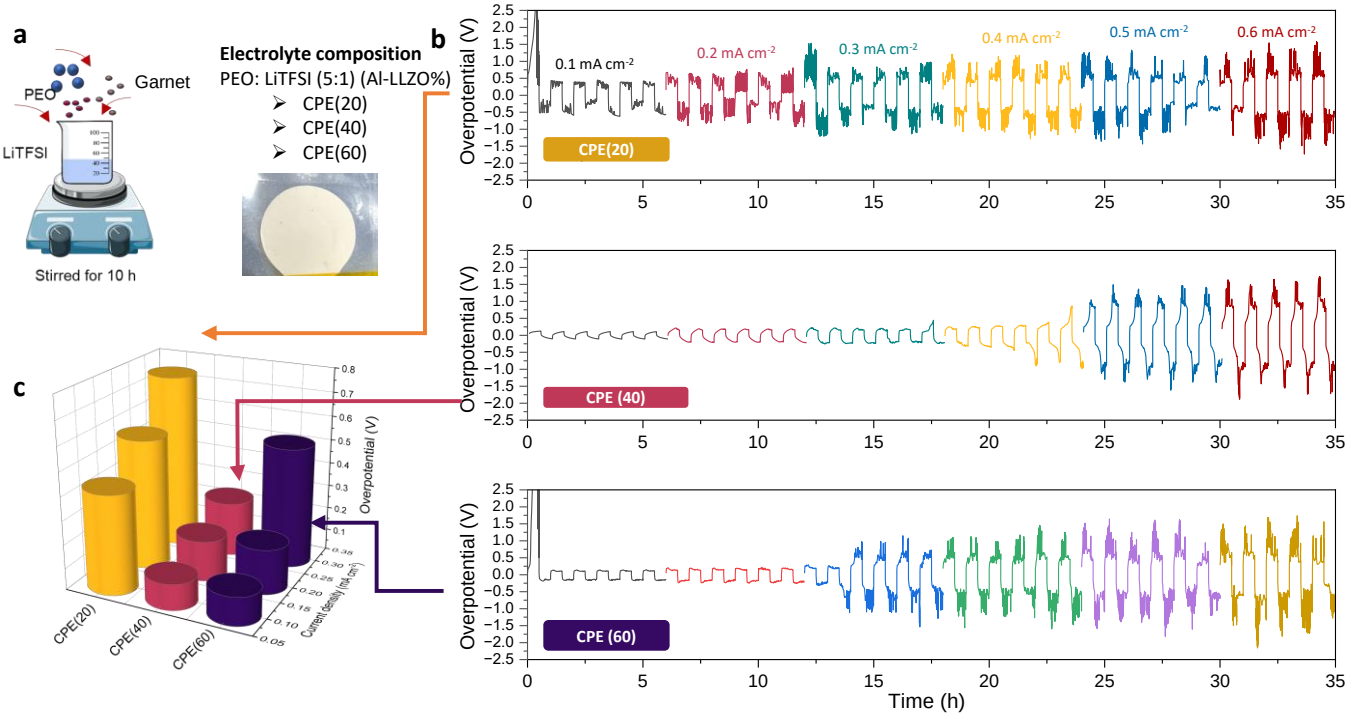

Fig. S3. (a) The synthesis procedure and the digital photograph of the CPE membranes, (b) Lithium stripping-plating profile of different compositions of CPEs up to 0.6 mA cm^{-2} and (c) its overpotential

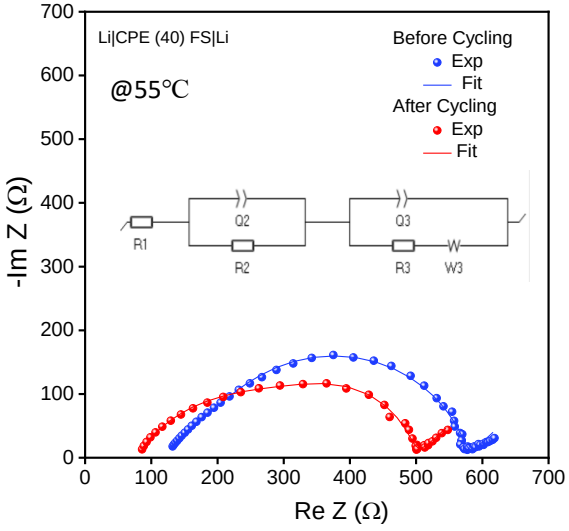

Fig. S4. Nyquist plot of Li|Li symmetric cell before and after long-term platting stripping studies at 0.1 mA cm^{-2}

Table S2: Li-ion Binding Energy (BE) with PEO, FS, FEC, and complexes of PEO with FS (PEO-FS) and FEC (PEO-FEC).

Complex	BE (in eV)	
	ΔE_{BE}	ΔG_{BE}
Li-PEO (PEO double chain)	-4.655	-4.317
Li-PEO_1 (PEO single chain)	-3.577	-3.034
Li-FS	-1.505	-1.113
Li-FEC	-1.960	-1.636
Li-FS-PEO	-3.955	-3.382
Li-FEC-PEO	-4.271	-3.826

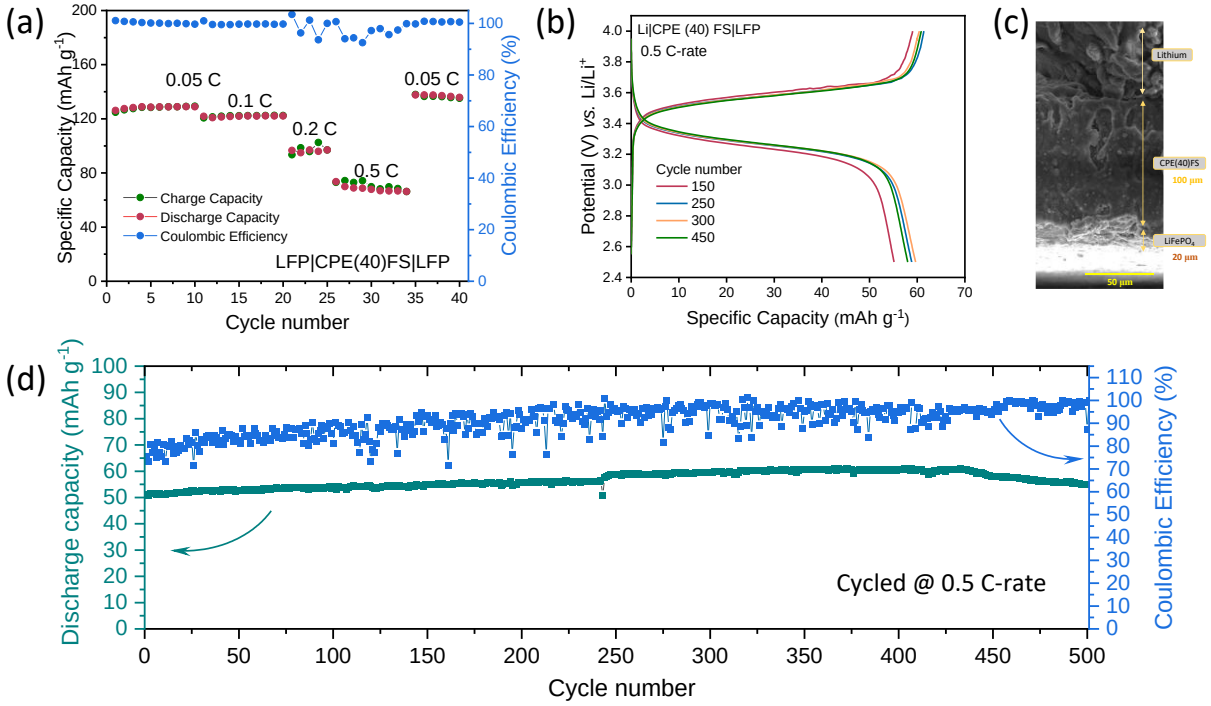

Fig. S5. (a) Rate capability of the full cell at 55 °C. (b) cycling profile of LFP|Li full cell cycled at 0.5 C-rate at 55 °C. (c) cross-section SEM image of the cycled cell. (d) discharge capacity and Coulombic efficiency as a function of cycle number for the LFP|Li full cell cycled at 0.5 C-rate at 55 °C.

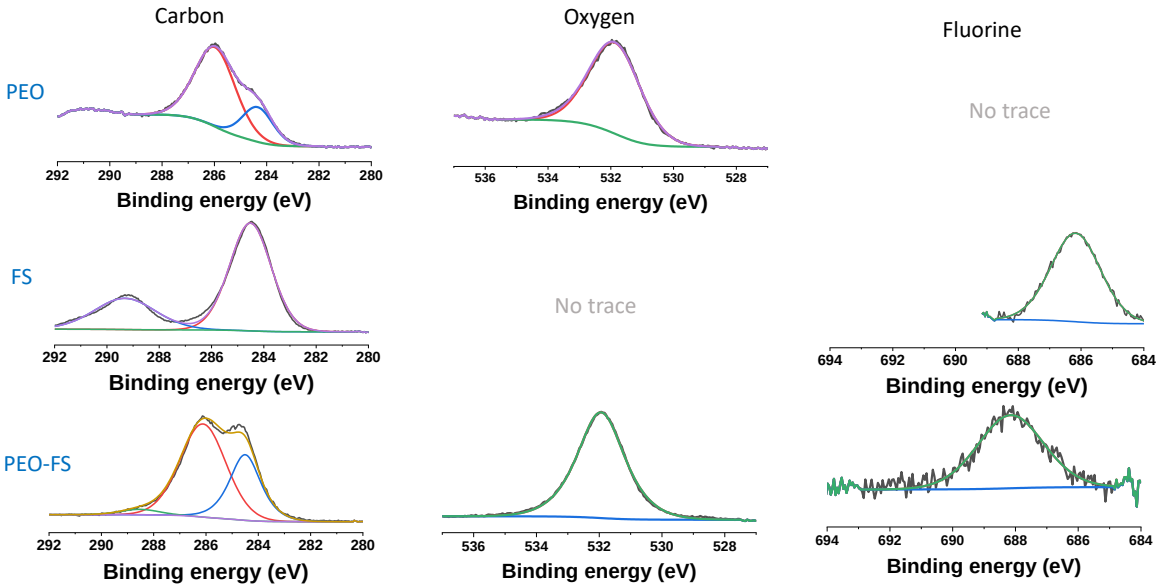

Fig. S6. XPS spectrum of C 1s, O 1s, and F 1s in PEO, FS and PEO-FS

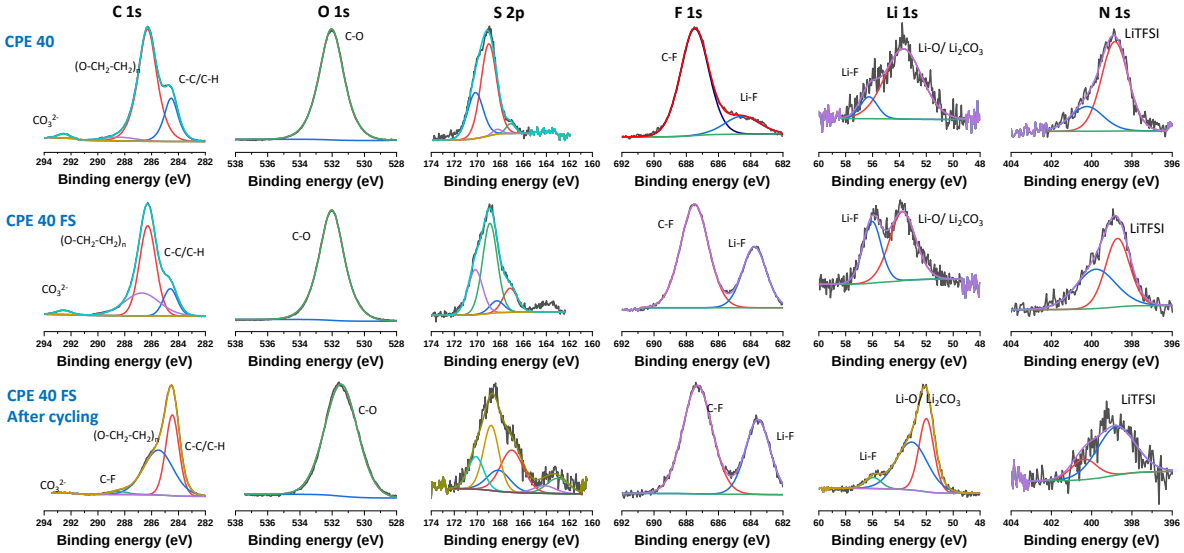

Fig. S7. XPS spectrum of C 1s, O 1s, S 2p, F 1s, Li 1s, and N 1s in CPE (40), CPE (40) FS, and cycled CPE (40) FS.

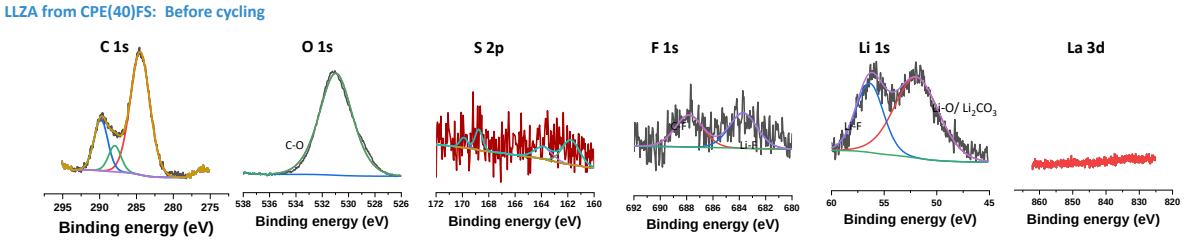

Fig. S8. XPS spectrum of C 1s, O 1s, S 2p, F 1s, Li 1s, and N 1s in Al-LLZO powder obtained after washing the cycled CPE (40) FS electrolyte membrane with LiTFSI as salt.

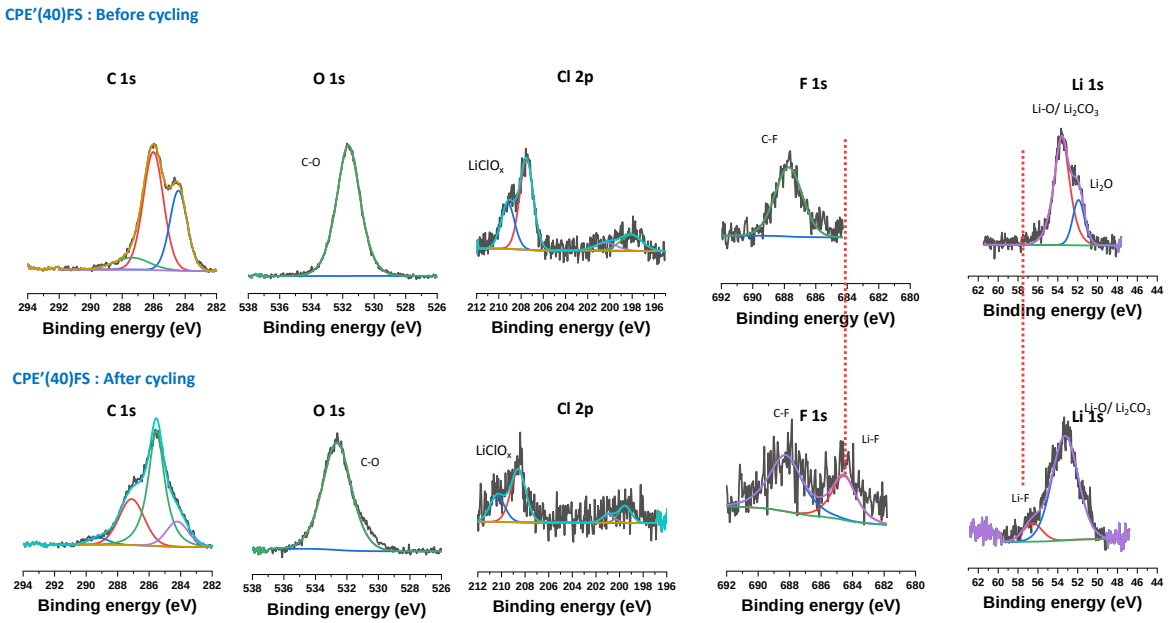

Fig. S9. XPS spectrum of C 1s, O 1s, Cl 2p, F 1s, and Li 1s in Al-LLZO powder obtained after washing the cycled CPE' (40) FS membrane with $LiClO_4$ salt before cycling (top), after cycling (bottom).

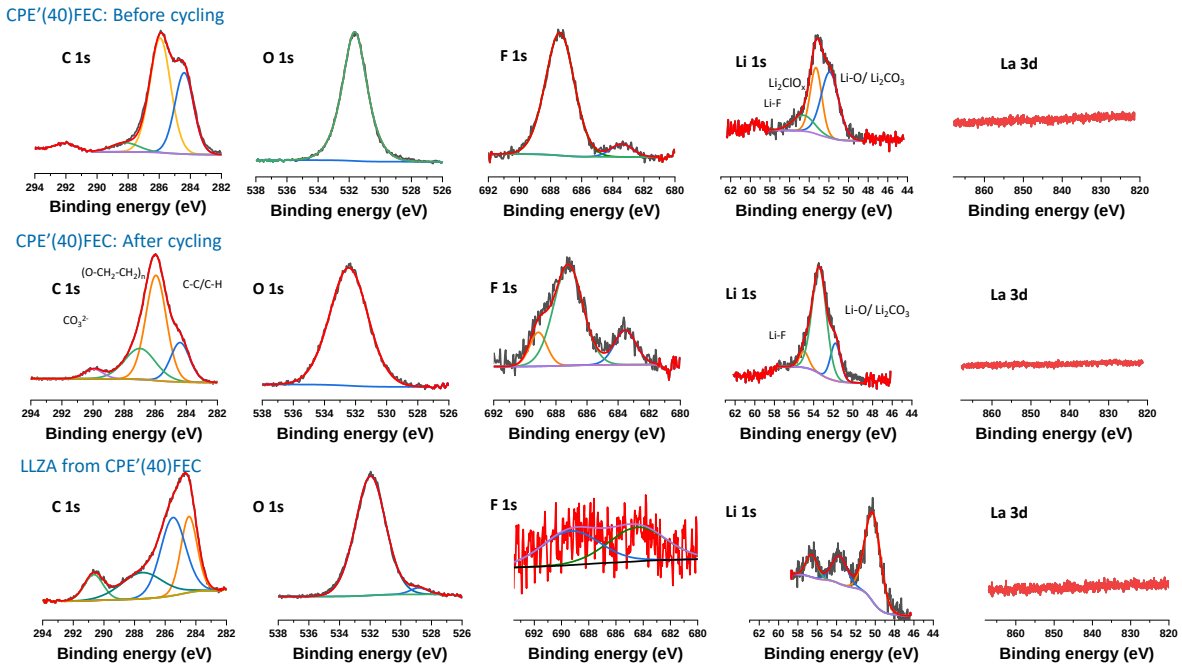

Fig. S10. XPS spectrum of C 1s, O 1s, S 2p, F 1s, Li 1s, and La 3d in CPE'(40) FEC before cycling, after cycling and Al-LLZO powder obtained from the cycled CPE' (40) FEC.

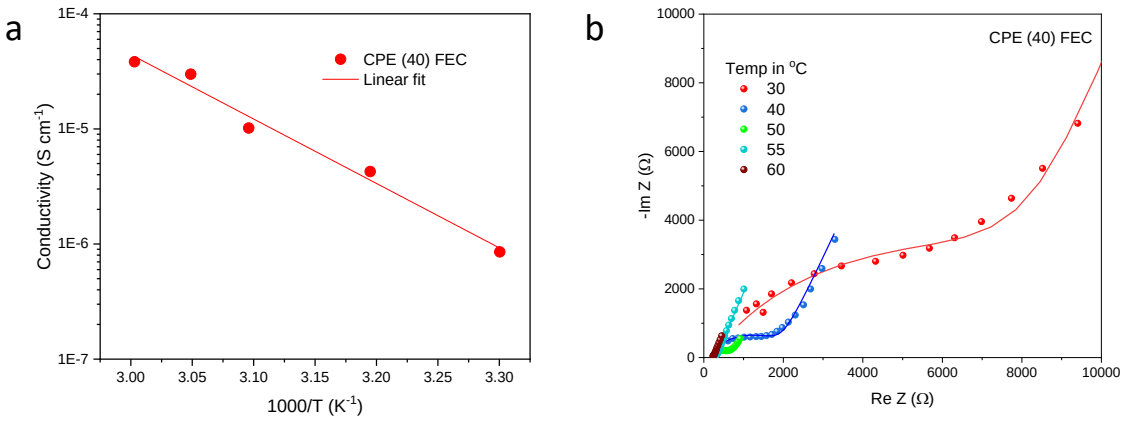

Fig. S11. (a)Arrhenius plot and (b) Nyquist profile of different compositions of CEP (40) FEC

Fig. S12. The digital photograph of CPE (40) FS (left) and CPE (40) FEC (right) membranes

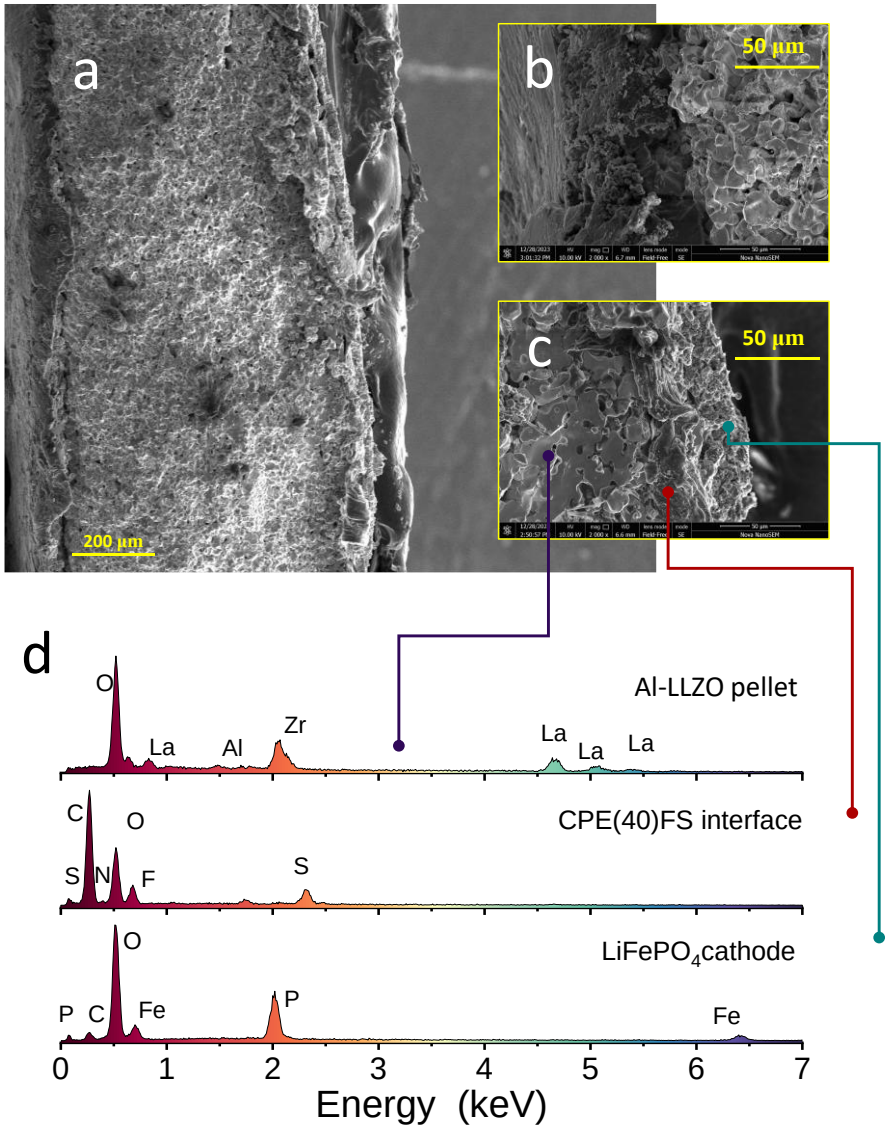

Fig. S13 . Post cycling SEM cross section of the full cell with CPE(40)FS as cathode interface modifier with EDS mapping

Table S3. Comparison table of various F-based additives from recent literature and our work.

Additive	Conductivity @ Temp	Transference number	Electro chemical Window (V)	Symmetric cell Overpotential/current density duration@ Temp	Cycling performance Capacity/rate Cathode@Temp	Liquid electrolyte content	Ref
Poly(2,2,3,3-tetrafluoro butyl carbonate)	5.3×10^{-4} S cm^{-1} @60 °C	0.33	4.7	39 mV/0.1 mA cm^{-2} 300 h @ RT	150 mAh g^{-1}/ 0.1C LFP@RT	Not mentioned	3
FEC with LATP	1.9×10^{-4} S cm^{-1} @30 °C	NA	NA	10 mV/0.2 mA cm^{-2} 2000 h @25 °C	130 mA g^{-1} / 0.1C LFP@25 °C	Quasi	4
2D fluorinated graphene-reinforced PVDF-HFP-LiTFSI	1.3×10^{-4} S cm^{-1} @30 °C	0.472	4.72	100 mV/0.1 mA cm^{-2} 1000 h @30 °C	118 mAh g^{-1}/1C NMC@30 °C	No liquid	5
FEC	6.5×10^{-5} S cm^{-1} @50 °C	0.62	5.2	120 mV/0.2 mA cm^{-2} 500 h @50 °C	132 mAh g^{-1}/0.2C LFP@50 °C	No liquid	6
AlF_3	2.7×10^{-4} S cm^{-1} @60 °C	0.67	5	25 mV/0.1mA cm^{-2} 1200 h@ 60 °C	167 mAh g^{-1}/50 mA g^{-1} LFP@60 °C	No liquid	7
$Li_{0.33}La_{0.557}TiO_3$-Nanofiber	1.1×10^{-4} S cm^{-1} @60 °C	0.62	4.8	37 mV/0.2 mA cm^{-2} 560 h @ RT	136 mAh g^{-1}/0.1C LFP@RT	With Liquid	8
MgPFPAA	1.4×10^{-4} S cm^{-1} @60 °C	0.342	4.8	100 mV/0.2 mA cm^{-2} 2400 h@ 60 °C	120 mAh g^{-1}/5C NMC@60 °C	No liquid	9
Trifluoroethyl methacrylate (TFEMA)	5.0×10^{-5} S cm^{-1} @RT	0.44	5.7	5 mV/0.2 mA cm^{-2} 300 h @ 60 °C	300 mAh g^{-1}/0.1C NMC@RT	No liquid	10
AlF_3	7.7×10^{-4} S cm^{-1} @25 °C	0.67	NA	151 mV/0.1 mA cm^{-2} 1700 h @ 60 °C	150 mAh g^{-1}/0.5C LFP@RT	Semi solid	11
2,2,3,3,4,4,5,5-octafluoro-1,6-hexanediol diacrylate (OFHDODA)	1.1×10^{-3} S cm^{-1} @25°C		5.08	43 mV/0.1 mA cm^{-2} 2500 h @30 °C	185 mAh g^{-1}/0.1C NMC@30°C	---	12
1-butyl-3-methylimidazolium tetrafluoroborate ([BMIM]BF_4)	5.26×10^{-3} S cm^{-1} @25°C	0.229	5.6	60 mV/0.1 mA cm^{-2} 800 h @30 °C	156 mAh g^{-1}/0.2C LFP@55 °C	Ionic liquid	13
LiF	3.4×10^{-4} S cm^{-1} @ 20 °C.	NA	NA	250 mV/0.2 mA cm^{-2} 800 h @RT	595 mAh g^{-1} /0.1C sulphur @RT	No liquid	14
F-PEO	1.1×10^{-4} S cm^{-1} @40 °C	0.28-0.39	NA	95 mV/0.1 mA cm^{-2} 1000 h @40 °C.	155 mAh g^{-1} /0.1C LFP@40 °C	No liquid	15
Fluorostyrene	1.0 x 10^{-4} S cm^{-1} @55 °C	0.67	5.2	104 mV/0.1 mA cm^{-2} 2000 h @ 55 °C.	140 mAh g^{-1}/ 0.1C LFP@ 70°C.	No liquid	Our work

FS, as an additive, contributes more towards the anode electrolyte interface and also aids in improving the ion transport across the garnet-loaded polymer electrolyte. An increase in the capacity when cycled at higher temperatures is presumably because of the increased contact between the cathode and electrolyte. We very commonly identify reports from teams renowned for LLZO electrolyte research, which add a few drops of liquid electrolyte/catholyte/ionic liquid as a wetting agent. In this present study, we, however, wanted to ensure that our cell configuration does not incorporate liquid electrolytes. A comparison of the performance with other PEO-based configurations with no cathode modification is presented in **Table S4.** The cathode electrolyte interface improvement will be taken up as further studies. For instance, employing a dry-slurry mixing process[16], enhancing the pressure in PEO-based SPE[17], and incorporating PEO in the cathode[18,19] are a few commonly adopted strategies.

Table S4. Comparison table of the highest reported C rate, temperature and corresponding capacity achieved for LIBs with no cathode modification and PEO-based electrolytes.

Cathode	Electrolyte	Rate and temp	Capacity	Ref
LFP	PEO+LiTFSI + ceramic fillers (40% filler) + FS	1C at 70°C	74 mAh g^{-1} 100th cycle	Our work
LFP	PEO+LiTFSI+MOF	1C at 60°C	60 mAh g^{-1}	20
LFP	PEO+LiTFSI + ceramic fillers (50% filler)	0.1C at 60°C	120 mAh g^{-1}	21
NMC622	PEO+LiTFSI + benzophenone	1C 60 °C	<20 mAh g^{-1}	17
LFP	PEO–$LiClO_4$–EmimFSI with ceramic fillers	0.05 C and 40 °C	100 mAh g^{-1}	22

Table S5. Total electronic energy (in au) free energies (in au) of Li-complexes of **FS**, **FEC**, **PEO**, **FS-PEO** adduct, and **FEC-PEO** adduct and Li^+, **FS**, **FEC**, and **PEO**.

Name	Configuration	E(au)	G(au)
Li-FS	Li-FS-C1	-416.0573361	-415.967075
	Li-FS-C2	-416.0634503	-415.969503
	Li-FS-C3	-416.067997	-415.973075
Li-FEC	Li-FEC-C1	-448.8518916	-448.813924
	Li-FEC-C2	-448.8518789	-448.813822
Li-PEO (2 chains)	Li-PEO-C1	-1390.43867	-1389.957021
	Li-PEO-C2	-1390.428874	-1389.942022

Li-PEO_1 (1 chain)	Li-PEO_1-C1	-698.827224	-698.603340
	Li-PEO_1-C2	-698.8954332	-698.663854
Li-FS-PEO	Li-FS-PEO-C1	-1107.594807	-1107.256983
	Li-FS-PEO-C2	-1107.649633	-1107.302839
	Li-FS-PEO-C3	-1107.604435	-1107.265839
	Li-FS-PEO-C4	-1107.632347	-1107.289481
	Li-FS-PEO-C5	-1107.597206	-1107.257616
	Li-FS-PEO-C6	-1107.576291	-1107.235184
	Li-FS-PEO-C7	-1107.551221	-1107.217218
Li-FEC-PEO	Li-FEC-PEO-C1	-1140.325304	-1140.044309
	Li-FEC-PEO-C2	-1140.384632	-1140.101805
	Li-FEC-PEO-C3	-1140.353421	-1140.071327
	Li-FEC-PEO-C4	-1140.384592	-1140.102144
	Li-FEC-PEO-C5	-1140.383394	-1140.098599
	Li-FEC-PEO-C6	-1140.436014	-1140.141032
	Li-FEC-PEO-C7	-1140.442103	-1140.148408
PEO_1 (single chain)	-	-691.4829384	-691.258541
Li ion	-	-7.281048711	-7.293797
FS	-	-408.7316467	-408.638358
FEC	-	-441.4987947	-441.459993
PEO (2 chains)	PEO-C1	1382.985074	-1382.497323
	PEO-C2	-1382.986552	-1382.504566

Table S6. Binding energies of Li-complexes of **FS**, **FEC**, **PEO** (single and double chain), **FS-PEO** adduct, and **FEC-PEO** adduct.

Name	**Configuration**	**ΔE (au)**	**ΔE (eV)**	**ΔG (au)**	**ΔG (eV)**
Li-FS	Li-FS-C1	-0.04464	-1.215	-0.03492	-0.950
	Li-FS-C2	-0.05075	-1.381	-0.03735	-1.016
	Li-FS-C3	-0.0553	-1.505	-0.04092	-1.113
Li-FEC	Li-FEC-C1	-0.07205	-1.960	-0.06013	-1.636
	Li-FEC-C2	-0.07204	-1.960	-0.06003	-1.633
Li-PEO	Li-PEO-C1	-0.1711	-4.655	-0.1587	-4.317

(PEO: 2 chains)	Li-PEO-C2	-0.1613	-4.388	-0.1437	-3.909
Li-FS-PEO	Li-FS-PEO-C1	-0.09053	-2.463	-0.07844	-2.134
	Li-FS-PEO-C2	-0.14535	-3.955	-0.12429	-3.382
	Li-FS-PEO-C3	-0.10016	-2.725	-0.08729	-2.375
	Li-FS-PEO-C4	-0.12807	-3.485	-0.11094	-3.019
	Li-FS-PEO-C5	-0.09293	-2.529	-0.07907	-2.152
	Li-FS-PEO-C6	-0.07201	-1.959	-0.05664	-1.541
	Li-FS-PEO-C7	-0.04694	-1.277	-0.03867	-1.052
Li-FEC-PEO	Li-FEC-PEO-C1	-0.04017	-1.093	-0.0365	-0.993
	Li-FEC-PEO-C2	-0.0995	-2.707	-0.09399	-2.558
	Li-FEC-PEO-C3	-0.06829	-1.858	-0.06352	-1.728
	Li-FEC-PEO-C4	-0.09946	-2.706	-0.09433	-2.567
	Li-FEC-PEO-C5	-0.09826	-2.674	-0.09079	-2.470
	Li-FEC-PEO-C6	-0.15088	-4.105	-0.13322	-3.625
	Li-FEC-PEO-C7	-0.15697	-4.271	-0.1406	-3.826
Li-PEO_1	Li-PEO_1-C1	-0.06324	-1.721	-0.05100	-1.388
(PEO: single chain)	Li-PEO_1-C2	-0.13145	-3.577	-0.11152	-3.034

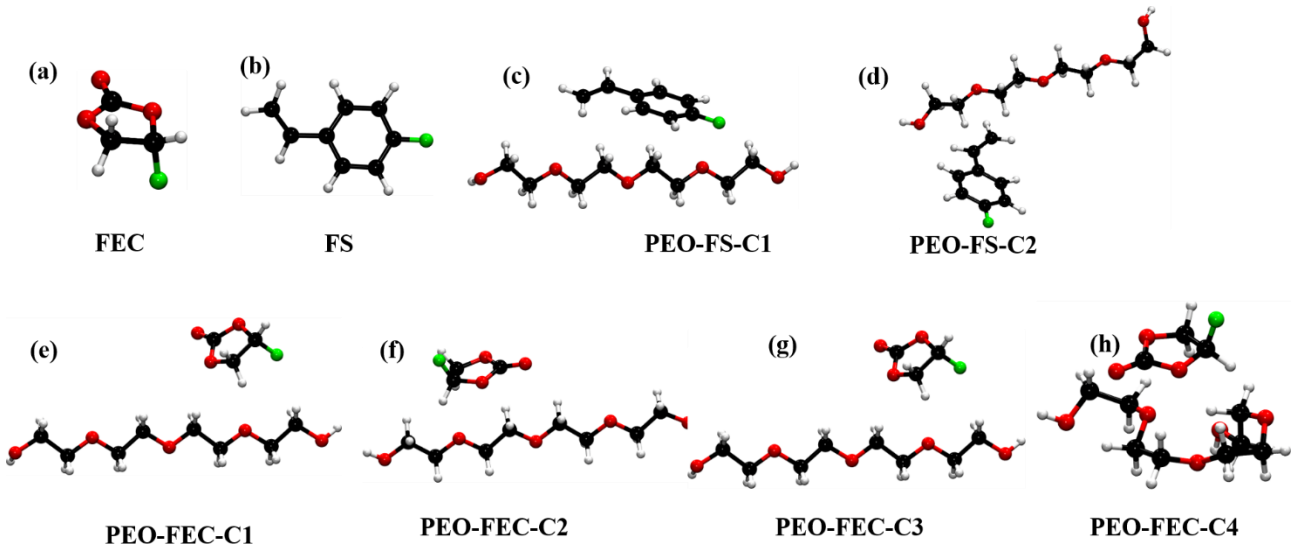

Fig. S14. Optimized structures of (a) **FEC** (b) **FS** (c-d) different configurations of **PEO-FS** adduct (PEO-FS-C1 & PEO-FS-C2) (e-h) different configurations of **PEO-FEC** adduct (PEO-FEC-C1, PEO-FEC-C2, PEO-FEC-C3, PEO-FEC-C4).

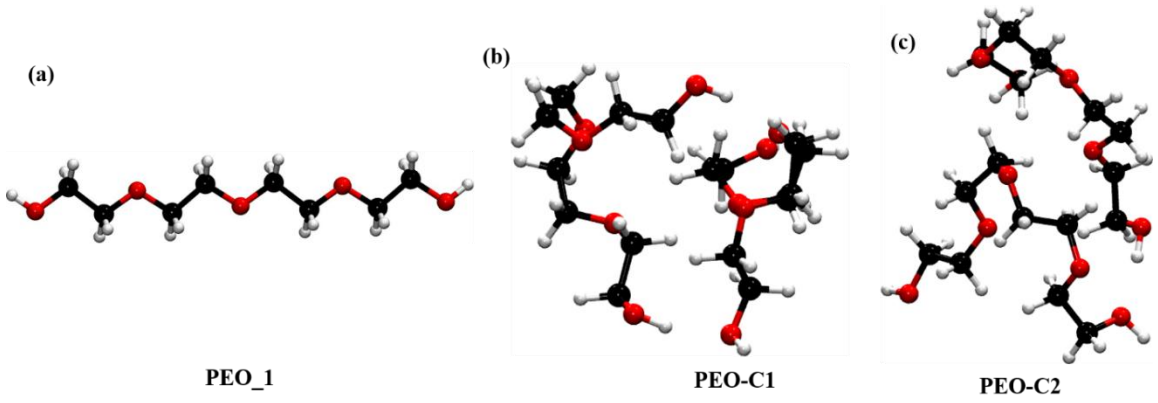

Fig S15. Optimized structures of (a) **PEO_1** (single chain of PEO) (b- c) different configurations of PEO double chain (PEO-C1 & PEO-C2).

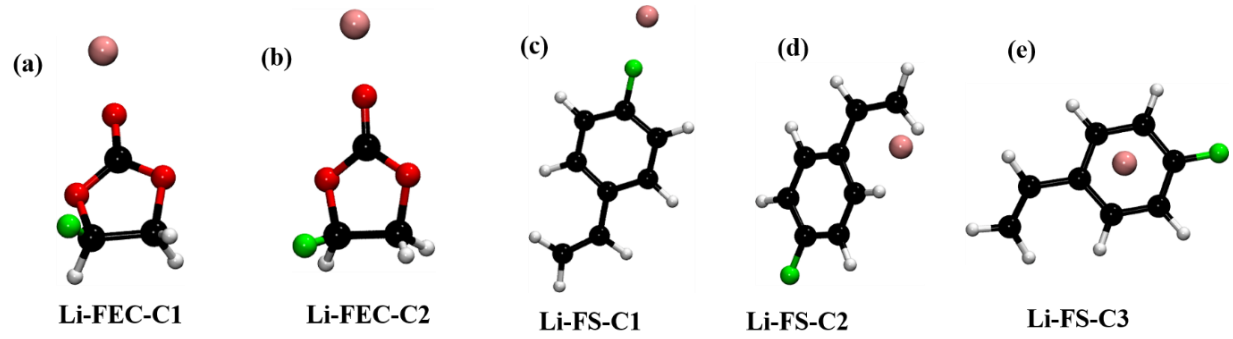

Fig S16. Optimized structures of (a,b) different configurations of **Li- FEC** and (c-e) different configurations of **Li-FS**.

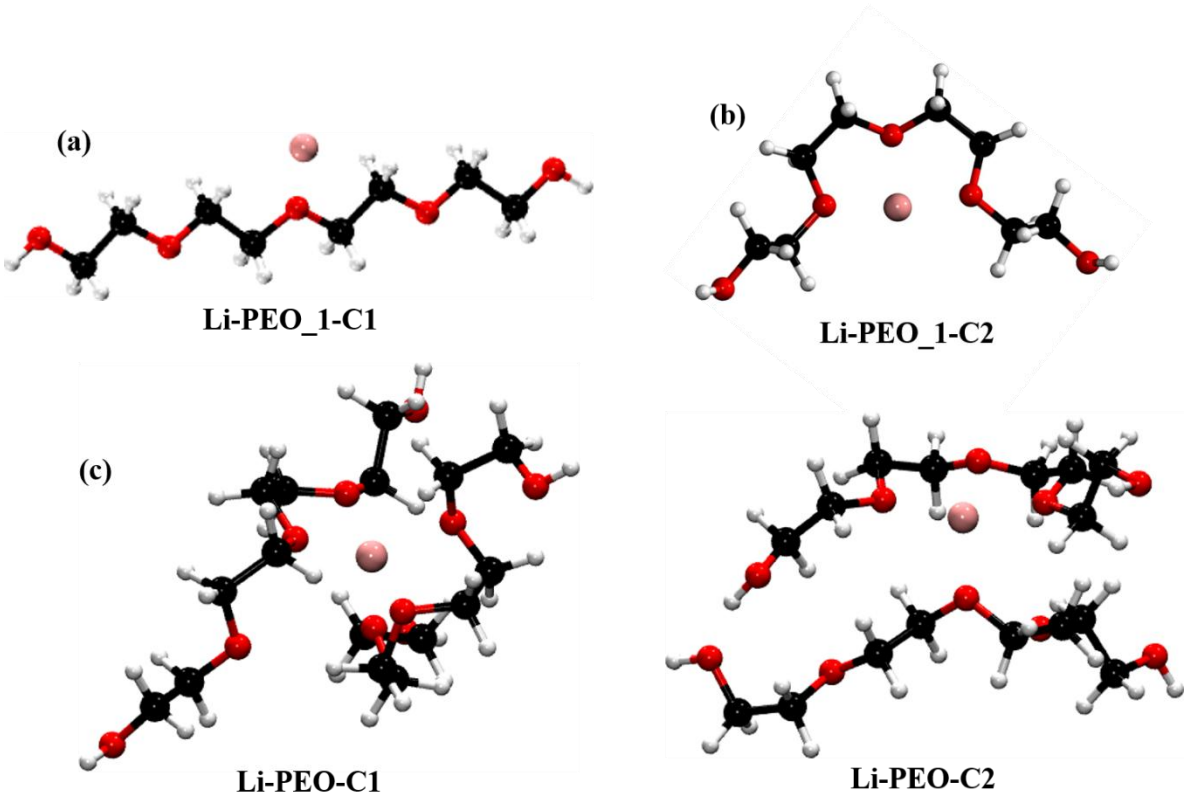

Fig S17. Optimized structures of (a,b) different configurations of **Li-PEO** single chain and (c,d) different configurations of **Li-PEO** double chain.

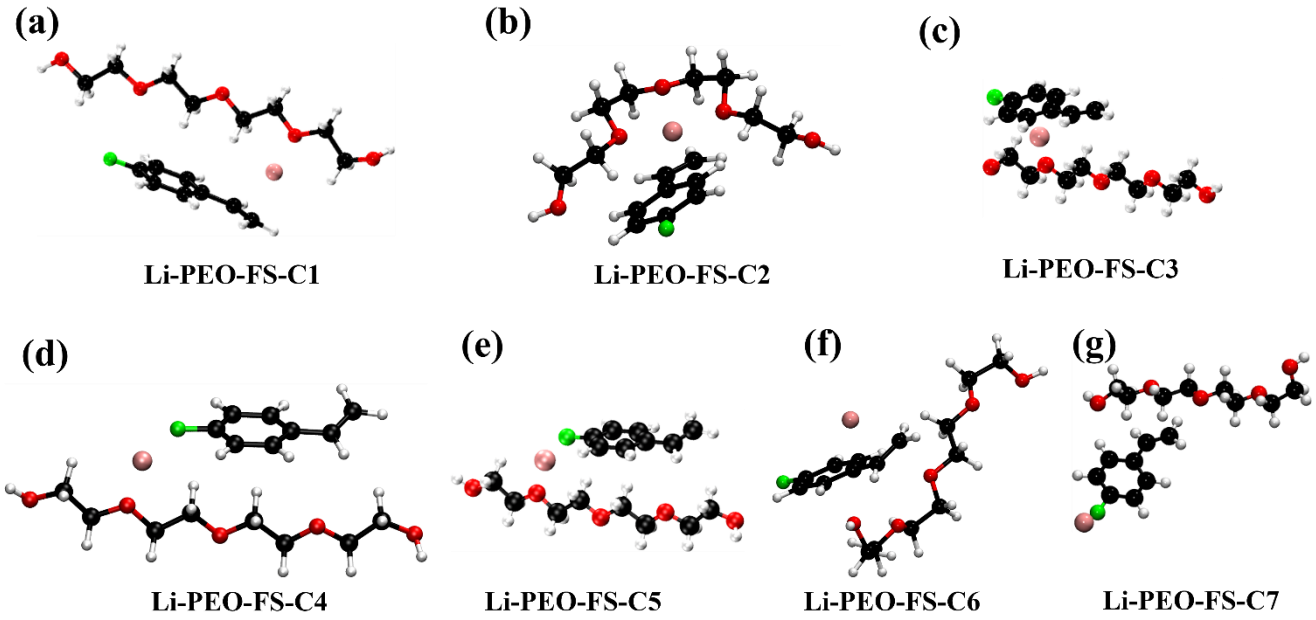

Fig. S18. Optimized structures of (a-g) different configurations **Li-PEO-FS**.

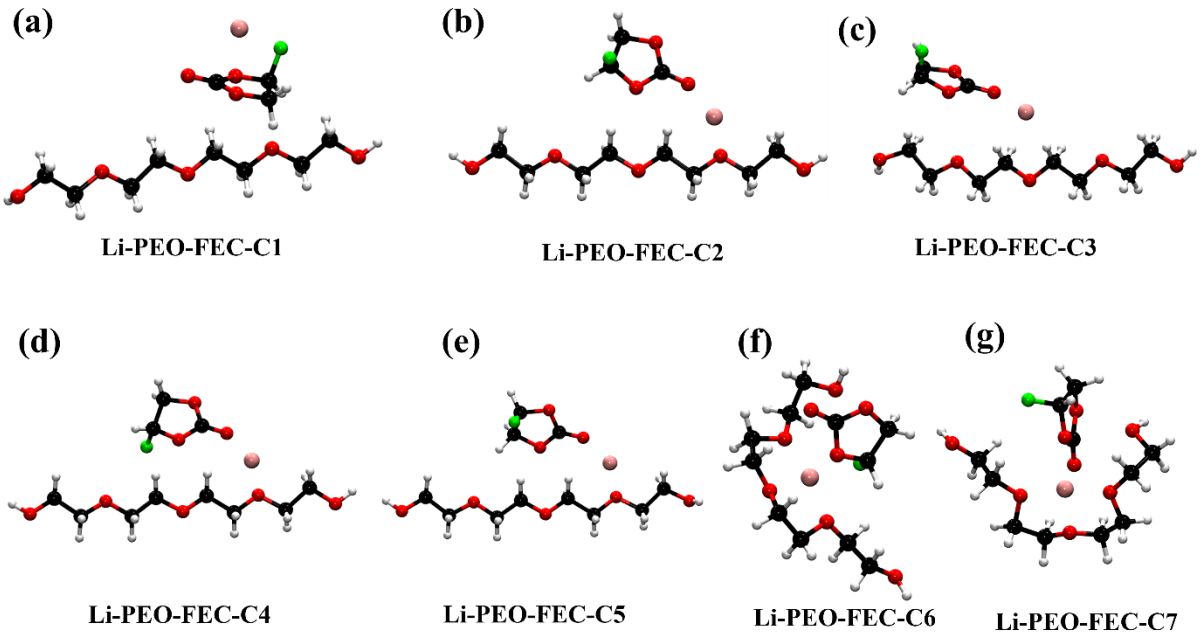

Fig. S19. Optimized structures of (a-g) different configurations **Li-PEO-FEC**.

Table S7. Cartesian coordinates of optimized structures

FEC			
O	-9.29112	6.703857	6.006242
C	-9.95031	7.754565	6.591049
O	-9.10582	8.799373	6.723259
C	-7.85783	8.490789	6.11129
C	-7.92668	6.975402	5.949121
H	-7.50898	6.563176	5.031543
F	-7.30486	6.36377	7.008499
H	-7.04559	8.790886	6.772481
H	-7.78971	9.00481	5.149237
O	-11.0919	7.737572	6.910089

FS			
C	-9.30007	8.884196	6.444298
C	-8.08648	8.760212	5.779039
C	-7.65311	7.491038	5.420209
C	-8.38909	6.351598	5.697879
C	-9.60248	6.498623	6.365462
C	-10.0749	7.757471	6.757634
C	-11.3606	7.849315	7.47473
C	-11.8476	8.921528	8.104734
H	-10.1938	5.615751	6.592474
H	-8.01423	5.380836	5.393957
H	-9.65295	9.87503	6.711743
H	-7.47997	9.623332	5.528594
F	-6.47756	7.366705	4.772408
H	-11.9464	6.931161	7.484628
H	-11.3092	9.863272	8.155586
H	-12.8107	8.882685	8.601012

PEO-FS-C1			
C	-0.21719	0.6336	1.25673
C	1.101682	1.362282	1.107561
O	2.090506	0.557428	1.71166
H	1.045346	2.344955	1.598979
H	1.327859	1.523092	0.042798

C	3.381015	1.111458	1.629216
C	4.337106	0.167765	2.342077
H	3.416425	2.103666	2.103808
H	3.680215	1.231108	0.573423
O	5.662486	0.661276	2.319237
H	4.264886	-0.83273	1.895633
H	4.052625	0.088168	3.393886
H	6.008542	0.601874	1.42228
O	-1.23196	1.443378	0.710863
C	-2.0593	-2.22933	2.725201
C	-3.2021	-2.39389	1.93046
C	-4.40049	-1.75682	2.238654
C	-4.44881	-0.96596	3.375157
C	-2.15881	-1.42975	3.873665
C	-3.35137	-0.79533	4.207724
H	-3.14471	-3.01505	1.040445
H	-5.27881	-1.84832	1.610083
H	-1.29828	-1.31787	4.52648
H	-3.44285	-0.17998	5.095857
F	-5.60466	-0.34845	3.690843
C	-0.80202	-2.89483	2.333078
C	0.428473	-2.52318	2.696647
H	1.299564	-3.06939	2.351607
H	0.615883	-1.65321	3.320356
H	-0.91661	-3.74607	1.663084
C	-2.49143	0.817386	0.808014
C	-3.55535	1.788333	0.341849
H	-2.69748	0.528393	1.84826
H	-2.51893	-0.09556	0.193662
O	-4.79472	1.136408	0.505287
H	-3.39356	2.065141	-0.71084
H	-3.51482	2.70506	0.948929
C	-5.89667	1.949528	0.176035
C	-7.1511	1.148262	0.461275
H	-5.8702	2.237665	-0.88578
H	-5.89932	2.868229	0.781293
O	-8.2493	1.970319	0.107687
H	-7.16834	0.878537	1.524793

H	-7.13142	0.225385	-0.13434
H	-9.06996	1.530048	0.348474
H	-0.17149	-0.33935	0.744407
H	-0.41281	0.437273	2.322892

PEO-FS-C2			
C	5.120988	8.738225	-2.30931
C	5.908031	7.450969	-2.45052
O	5.479572	6.824278	-3.63522
H	5.727292	6.80707	-1.57554
H	6.984154	7.675828	-2.49316
C	6.142762	5.607092	-3.88041
C	5.722252	5.082714	-5.23289
H	5.887187	4.870913	-3.10119
H	7.233657	5.755109	-3.8755
O	6.342822	5.874396	-6.22832
H	6.033067	4.031677	-5.31804
H	4.627911	5.133813	-5.30252
H	5.910403	5.727545	-7.07484
O	5.539701	9.364184	-1.11873
H	4.043955	8.514407	-2.27498
H	5.308949	9.384743	-3.17923
C	3.615253	10.457	4.361204
C	3.779292	9.071405	4.495611
C	4.629485	8.540752	5.45985
C	5.310498	9.415596	6.29445
C	4.313517	11.30509	5.232769
C	5.169633	10.79096	6.203273
H	3.220656	8.397777	3.852904
H	4.762293	7.471562	5.581643
H	4.199881	12.38181	5.125468
H	5.722359	11.43413	6.878848
F	6.132975	8.905492	7.234129
C	2.743995	11.05468	3.331414
C	2.37646	10.48125	2.182256
H	1.746215	11.00733	1.473191
H	2.707387	9.484079	1.902127
H	2.422697	12.07488	3.5409

C	4.878012	10.58429	-0.88186
C	5.423438	11.16028	0.408845
H	3.792106	10.42868	-0.7841
H	5.049332	11.28917	-1.70937
O	4.748843	12.37508	0.642443
H	6.50854	11.32021	0.321346
H	5.242673	10.45695	1.236356
C	5.07089	12.94224	1.890198
C	4.062713	14.04037	2.170896
H	6.096186	13.34173	1.888366
H	5.000854	12.18817	2.686302
O	4.161748	14.34593	3.555527
H	3.063326	13.66339	1.916108
H	4.270987	14.92088	1.551195
H	3.700764	15.17075	3.737448

PEO-FEC-C1			
C	0.213473	0.90401	1.567311
C	1.477746	1.606664	1.115186
O	2.564571	0.961673	1.736605
H	1.437275	2.668321	1.401392
H	1.563617	1.550064	0.01953
C	3.810051	1.507276	1.373269
C	4.888656	0.760284	2.142161
H	3.857007	2.57942	1.616873
H	3.972546	1.400164	0.286793
O	6.17577	1.2642	1.839927
H	4.810259	-0.31456	1.93472
H	4.73937	0.907545	3.214172
H	6.420316	0.997402	0.947374
O	-0.87582	1.570516	0.969673
C	-3.68914	-3.20596	2.304519
O	-4.9087	-3.39864	2.901489
C	-5.50819	-2.16784	3.1565
O	-3.36556	-1.89901	2.3494
C	-4.35055	-1.17854	3.091025
O	-3.02646	-4.0729	1.838379
C	-2.11469	0.988834	1.296281

C	-3.19034	1.784966	0.584554
H	-2.28253	1.024408	2.385906
H	-2.15403	-0.06378	0.981673
O	-4.43695	1.216147	0.926276
H	-3.02988	1.736854	-0.50184
H	-3.14726	2.839321	0.893976
C	-5.52594	1.840159	0.278792
C	-6.77999	1.075019	0.651416
H	-5.38941	1.820602	-0.81178
H	-5.61826	2.888969	0.59657
O	-7.86184	1.752689	0.041123
H	-6.88278	1.057342	1.745982
H	-6.69309	0.040227	0.298212
H	-8.66873	1.242491	0.160737
H	0.240491	-0.15209	1.262304
H	0.139319	0.942641	2.664538
H	-4.60894	-0.26884	2.545497
H	-3.95316	-0.95302	4.084369
H	-6.05655	-2.21565	4.096509
F	-6.41506	-1.90161	2.157496

PEO-FEC-C2			
C	0.09167	0.610472	1.476857
C	1.352883	1.384904	1.151479
O	2.445156	0.646577	1.644873
H	1.311333	2.380322	1.618977
H	1.434239	1.52208	0.0622
C	3.68527	1.257807	1.385904
C	4.7704	0.392478	2.007476
H	3.725187	2.269232	1.818069
H	3.847818	1.349317	0.297669
O	6.054379	0.948312	1.793619
H	4.695464	-0.62923	1.613987
H	4.625421	0.347333	3.089055
H	6.29199	0.849676	0.865499
O	-0.99673	1.367323	0.982801
C	-2.73082	-1.91888	2.867208
O	-3.59711	-2.14933	1.836152

C	-4.89337	-1.7908	2.205029
O	-3.36914	-1.28246	3.868096
C	-4.69154	-0.9389	3.45396
O	-1.57958	-2.21325	2.851705
C	-2.23282	0.741832	1.209538
C	-3.31162	1.636207	0.633169
H	-2.40313	0.610269	2.291943
H	-2.26635	-0.24736	0.729258
O	-4.56448	1.029149	0.896105
H	-3.16419	1.755421	-0.44911
H	-3.2619	2.6297	1.101112
C	-5.64671	1.812323	0.435517
C	-6.92508	1.034504	0.679394
H	-5.54234	2.025508	-0.63759
H	-5.68982	2.769941	0.974108
O	-7.98911	1.877479	0.291199
H	-6.98987	0.768876	1.745665
H	-6.90657	0.108231	0.088141
H	-8.8235	1.402625	0.357458
H	0.12101	-0.38193	1.005748
H	0.003358	0.465375	2.56293
H	-4.72978	0.126381	3.214664
H	-5.39478	-1.20377	4.243115
F	-5.59635	-2.93019	2.514708
H	-5.38228	-1.29778	1.367207

PEO-FEC-C3			
C	2.831255	-0.44762	0.357304
C	2.835323	-1.38032	-0.84842
O	1.655688	-0.99413	-1.55213
C	0.845253	-0.31277	-0.72147
O	1.494092	-0.05316	0.45236
O	-0.26539	0.039212	-0.96508
F	3.594628	0.664689	0.090127
O	0.127471	-2.72496	0.178925
C	-1.08007	-2.61355	0.918502
C	-0.82932	-1.68577	2.082687
O	0.160912	-2.26425	2.910782

C	0.938757	-1.33948	3.637819
C	2.157633	-2.05909	4.181973
O	3.143616	-2.34697	3.205442
C	2.789078	-3.26161	2.178317
C	2.346972	-4.62912	2.674522
O	2.308121	-5.44539	1.511468
C	0.098872	-3.69188	-0.85293
C	-0.7237	-3.27728	-2.05898
H	-0.5258	-2.22133	-2.27889
H	1.837766	-2.97366	4.700747
H	2.65863	-1.4149	4.909776
H	3.703868	-3.39812	1.589946
H	1.990671	-2.86506	1.540037
H	1.354237	-4.56032	3.134573
H	3.068055	-5.01369	3.409859
H	1.890248	-6.2855	1.723852
H	-0.49192	-0.7125	1.705482
H	-1.76361	-1.53764	2.644035
H	-1.88435	-2.21305	0.291766
H	-1.37891	-3.60947	1.278094
H	-0.27628	-4.64966	-0.46317
H	1.140264	-3.83814	-1.1574
O	-2.09856	-3.49567	-1.76681
H	-0.41481	-3.88663	-2.9206
H	0.360129	-0.91409	4.473874
H	1.257107	-0.51291	2.984489
H	3.160732	-0.86747	1.309332
H	3.703251	-1.21659	-1.48627
H	2.747966	-2.42752	-0.54889
H	-2.63792	-3.06221	-2.43608

PEO-FEC-C4			
O	3.159507	0.196154	-0.2886
C	2.695064	-0.98199	-0.7465
O	1.344533	-1.02121	-0.65456
C	0.882872	0.016477	0.157619
C	2.077542	0.972259	0.22315
O	3.368377	-1.84623	-1.22093

O	-0.6068	-3.51912	-1.14521
C	0.684775	-4.08604	-1.1572
C	1.067373	-4.44893	0.259874
O	1.071862	-3.27174	1.032317
C	1.78421	-3.36824	2.243045
C	3.254482	-3.04054	2.058057
O	3.361022	-1.64884	1.798524
C	-0.88784	-2.71018	-2.26098
C	-2.13021	-1.89747	-1.95715
O	-1.91351	-0.98905	-0.89196
C	-2.30133	-1.47728	0.387634
C	-3.76761	-1.1595	0.638645
O	-4.08882	-1.66752	1.921522
H	-2.96538	-2.57255	-1.72459
H	-2.40122	-1.30897	-2.84059
H	-1.68116	-0.97247	1.132146
H	-2.10961	-2.55145	0.469884
H	-4.39014	-1.62463	-0.13999
H	-3.91374	-0.07191	0.586976
H	-5.0041	-1.45831	2.130936
H	1.416043	-3.36582	-1.54449
H	0.70485	-4.9886	-1.78902
H	2.063285	-4.91873	0.23454
H	0.352717	-5.17333	0.681551
H	1.675839	-4.37026	2.686446
H	1.34383	-2.63568	2.926885
H	3.661271	-3.61864	1.216853
H	3.808918	-3.30704	2.969307
H	4.218404	-1.46526	1.397579
H	-1.05818	-3.32259	-3.16309
H	-0.04712	-2.02884	-2.45212
F	0.607712	-06075	1.410039
H	-0.04661	0.398459	-0.26501
H	1.946472	1.854293	-0.40714
H	2.293085	1.251202	1.254903

PEO_1			
C	-2.26639	2.248935	-1.17085

C	-1.48126	2.804826	0.000091
O	-0.11529	2.753983	-0.34065
H	-1.68316	2.204913	0.900174
H	-1.7969	3.839754	0.200342
C	0.721464	3.248283	0.678509
C	2.150574	3.136647	0.18678
H	0.599002	2.66456	1.603144
H	0.485739	4.299286	0.903238
O	2.988806	3.630166	1.205282
H	2.273	3.720684	-0.73775
H	2.385792	2.085531	-0.03831
O	-3.63389	2.309173	-0.80677
H	-1.94323	1.217769	-1.36383
H	-2.05741	2.852721	-2.06345
H	-4.17311	1.966075	-1.52568
C	4.353904	3.577681	0.862801
C	5.139385	4.132439	2.034073
H	4.554586	4.177555	-0.0376
H	4.667036	2.542198	0.661417
O	6.503915	4.079814	1.689887
H	4.93935	3.532514	2.934491
H	4.82613	5.16775	2.235772
C	7.344299	4.572841	2.707356
C	8.773282	4.46107	2.215367
H	7.223839	3.989036	3.632272
H	7.110985	5.624224	2.933107
O	9.598868	4.96127	3.251932
H	8.882871	5.044917	1.292284
H	8.995667	3.409693	1.991495
H	10.52064	4.908923	2.981947

PEO-C1			
O	3.399848	1.081098	0.592959
C	4.10886	1.297568	-0.60607
C	4.117818	0.124037	-1.58495
O	2.852736	-0.42051	-1.87407
C	1.95694	0.451537	-2.54981
C	0.949393	1.067839	-1.59059

O	0.285295	2.100541	-2.29768
C	3.858059	0.03015	1.416267
C	3.122502	-1.27804	1.171028
O	1.748988	-1.05617	1.407535
C	0.87937	-1.85225	0.620022
C	0.786387	-3.27821	1.15759
O	-0.00017	-4.09405	0.31342
H	4.715166	-0.70285	-1.18592
H	4.612796	0.466329	-2.50876
H	1.441833	-0.13769	-3.31489
H	2.506417	1.257081	-3.0587
H	1.481518	1.45488	-0.71376
H	0.233447	0.308361	-1.24354
H	-0.52317	2.312315	-1.80664
H	3.670639	0.34741	2.44785
H	4.942605	-0.1221	1.29727
H	3.524653	-2.03879	1.858941
H	3.265606	-1.6263	0.141605
H	1.224404	-1.87148	-0.42416
H	-0.09624	-1.35192	0.651561
H	0.397507	-3.25971	2.184926
H	1.7885	-3.72141	1.191479
H	-0.93116	-4.03911	0.578863
H	5.158205	1.561857	-0.39104
H	3.634091	2.170072	-1.06645
O	-2.20489	2.049108	-1.03949
C	-2.98623	1.432697	-2.04119
C	-3.36547	-0.0061	-1.73969
H	-2.36322	1.454837	-2.94026
H	-3.90055	2.017603	-2.2255
O	-2.18229	-0.71966	-1.48205
H	-3.88919	-0.42083	-2.61745
H	-4.06203	-0.05296	-0.89007
C	-2.36423	-2.07276	-1.13368
C	-2.85253	-2.23649	0.30655
H	-1.38666	-2.55601	-1.22625
H	-3.05963	-2.56486	-1.83639
O	-2.76576	-3.59591	0.724173

H	-3.88036	-1.87326	0.435128
H	-2.20242	-1.65987	0.971294
H	-3.37744	-4.13691	0.211607
C	-2.82095	2.341865	0.201922
H	-2.33225	3.243662	0.579474
C	-2.69575	1.224757	1.239322
H	-3.88776	2.572391	0.05734
H	-3.36486	0.393306	1.002827
H	-3.00697	1.646101	2.205767
O	-1.41378	0.640664	1.322661
C	-0.31204	1.517998	1.494322
C	-0.28399	2.218143	2.836719
H	-0.28215	2.269674	0.692543
H	0.576074	0.885281	1.405067
O	-1.25071	3.267053	2.839841
H	0.724613	2.625448	2.988934
H	-0.49558	1.488264	3.629954
H	-1.19935	3.74733	3.672373

PEO-C2			
C	-3.7125	-1.03323	-1.59084
C	-4.6777	0.040642	-1.133
O	-3.98298	1.203618	-0.71914
C	-4.10352	1.548971	0.646241
C	-3.24213	0.694695	1.574508
O	-3.34748	1.174912	2.908276
O	-3.02748	-1.51733	-0.46178
C	-1.92172	-2.33413	-0.77947
C	-1.21828	-2.71714	0.501024
O	-0.78015	-1.53626	1.145578
C	-0.08299	-1.7563	2.357722
C	1.416947	-1.72234	2.146548
H	1.922128	-1.8021	3.12171
O	4.472371	-1.89525	0.96757
C	4.884149	-1.07897	-0.12355
C	3.646967	-0.45872	-0.72818
O	2.918713	-1.47463	-1.38197
C	1.521794	-1.24118	-1.45254

C	1.181327	-0.14414	-2.45942
O	-0.19283	0.20035	-2.4382
C	-0.66393	0.846486	-1.26043
C	0.088958	2.112068	-0.89882
O	1.24768	1.783512	-0.14216
C	2.230196	2.792742	-0.11938
C	1.801798	4.020445	0.673095
O	2.938462	4.862274	0.737821
H	-5.29817	-0.35256	-0.31635
H	-5.33549	0.314461	-1.96717
H	-5.15345	1.502621	0.971171
H	-3.78433	2.596601	0.715213
H	-2.20275	0.675621	1.222946
H	-3.58188	-0.34206	1.58558
H	-2.90371	2.027473	2.970895
H	-1.24101	-1.79182	-1.45142
H	-2.25384	-3.25199	-1.29206
H	-0.36531	-3.37022	0.274089
H	-1.91959	-3.2559	1.156797
H	-0.37797	-2.71995	2.796566
H	-0.37535	-0.95866	3.05058
H	1.682401	-0.74928	1.70614
O	1.772203	-2.78617	1.290058
H	-4.26964	-1.8461	-2.086
H	-3.00358	-0.60884	-2.31878
H	-0.65518	0.168517	-0.39593
H	-1.70619	1.102299	-1.46934
H	-0.57459	2.760831	-0.30802
H	0.375372	2.655864	-1.81361
H	2.504685	3.093401	-1.14338
H	3.116083	2.364592	0.360064
H	1.473797	3.701494	1.672186
H	0.96422	4.527688	0.175082
H	2.709989	5.683899	1.183323
H	1.386974	-0.49092	-3.47595
H	1.804759	0.741384	-2.2726
H	1.130263	-0.99121	-0.45883
H	1.074108	-2.19106	-1.7592

H	3.037655	0.000278	0.064006
H	3.947445	0.335493	-1.42868
H	5.55871	-0.2868	0.226395
H	5.394785	-1.67791	-0.88711
H	5.195468	-2.46595	1.246638
H	2.67884	-2.63895	0.97548

Li-FEC-C1			
O	-8.9914	6.74085	5.695587
C	-9.63203	7.894641	5.843981
O	-8.83355	8.885364	6.162351
C	-7.46987	8.408401	6.168604
C	-7.65459	6.891953	6.165457
Li	-12.5831	8.050199	5.533615
H	-6.9916	6.311221	5.527105
F	-7.61051	6.405715	7.427758
H	-6.98102	8.761173	7.075274
H	-6.97317	8.782701	5.27265
O	-10.8341	8.012592	5.685928

Li-FEC-C2			
O	-9.36534	6.71644	6.030295
C	-9.96397	7.762949	6.5872
O	-9.16885	8.798158	6.715375
C	-7.88938	8.486379	6.121304
C	-7.96432	6.968955	5.961902
H	-7.57742	6.546348	5.036666
F	-7.38833	6.35097	7.019173
H	-7.10204	8.789456	6.809622
H	-7.81676	9.015064	5.170085
O	-11.1333	7.75617	6.928905
Li	-12.8157	7.581851	7.401263

Li-FS-C1			
C	-9.40602	8.986795	6.466964
C	-8.15796	8.964749	5.851066
C	-7.64352	7.724805	5.541409
C	-8.25916	6.519795	5.78821

C	-9.50663	6.576721	6.407589
C	-10.0915	7.799345	6.766736
F	-6.37288	7.689566	4.907836
C	-11.4059	7.798947	7.437273
C	-11.9007	8.801494	8.165595
Li	-5.00504	7.626701	3.813442
H	-10.0292	5.650289	6.624402
H	-7.796	5.577421	5.518811
H	-9.85586	9.945526	6.700803
H	-7.61969	9.876289	5.617304
H	-11.9849	6.884165	7.330792
H	-11.3531	9.723228	8.340362
H	-12.8768	8.719565	8.629708

Li-FS-C2			
C	-8.16772	8.803899	5.730992
C	-7.91326	7.553614	5.172821
C	-8.67352	6.431267	5.479056
C	-9.73187	6.572022	6.370298
C	-10.0274	7.8178	6.95578
C	-9.22556	8.930961	6.624253
C	-11.2048	7.932247	7.848934
C	-11.8515	9.072069	8.150769
F	-6.90039	7.430495	4.322121
H	-10.327	5.70123	6.632988
H	-8.42576	5.476205	5.029483
H	-9.38502	9.887903	7.114692
H	-7.52346	9.640534	5.484072
H	-11.5951	6.992397	8.235895
H	-11.4968	10.05454	7.834215
H	-12.7209	9.064564	8.798035
Li	-11.6751	8.678906	5.765345

Li-FS-C3			
C	-9.24814	6.562791	6.374459
C	-9.88737	7.785426	6.671776
C	-9.14667	8.974133	6.489153
C	-7.81242	8.945414	6.070712

C	-7.20678	7.710004	5.826193
C	-7.91456	6.513864	5.949702
C	-11.2865	7.780815	7.14177
C	-11.88	8.790041	7.782442
Li	-9.16706	7.861223	4.455385
F	-5.93851	7.677574	5.431865
H	-9.79769	5.633498	6.493882
H	-7.41773	5.572583	5.738011
H	-9.61673	9.935546	6.669662
H	-7.23725	9.85661	5.941185
H	-11.8349	6.856366	6.9757
H	-11.3692	9.718229	8.022365
H	-12.9085	8.702728	8.113702

Li-PEO_1-C1			
C	-2.29199	2.315481	-1.21487
O	-3.64386	2.409669	-0.82336
C	-1.49975	2.842794	-0.03481
O	-0.12002	2.799329	-0.37631
C	0.713538	3.245751	0.638678
C	2.143224	3.038645	0.172104
O	3.003457	3.712621	1.107381
C	4.403994	3.491342	0.865466
C	5.169993	4.138066	2.005458
O	6.512916	4.127576	1.65791
C	7.366224	4.618055	2.684281
C	8.795431	4.53567	2.185463
O	9.582524	5.058062	3.232982
H	-1.69301	2.223154	0.851313
H	-1.80513	3.876271	0.18236
H	0.532841	2.701115	1.580318
H	0.536646	4.330531	0.82998
H	2.282922	3.464382	-0.82696
H	2.394179	1.974192	0.153991
H	-1.99238	1.280045	-1.42076
H	-2.07551	2.926239	-2.10076
H	-4.21556	2.066036	-1.5177
H	4.687343	3.945879	-0.08953

H	4.59805	2.415498	0.829864
H	4.991079	3.593684	2.947581
H	4.818459	5.187845	2.143321
H	7.253375	4.014385	3.594979
H	7.116971	5.662738	2.918826
H	8.893555	5.122847	1.263358
H	9.043699	3.489982	1.963691
H	10.51582	5.015838	3.000177
Li	2.405766	5.042635	2.187004

Li-PEO_1-C2			
Li	0.476153	-2.69185	2.052873
O	-0.97732	-3.59882	1.230471
C	-2.17241	-2.84507	1.420246
C	-2.13008	-2.3623	2.854299
O	-0.84878	-1.74867	3.051077
C	-0.74459	-0.98676	4.264094
C	-1.22121	0.443483	4.061088
O	-1.06903	1.051719	5.320124
C	-0.6366	-3.91162	-0.11803
C	0.797286	-4.39506	-0.07775
O	1.548981	-3.41366	0.649424
C	2.972761	-3.56811	0.540953
C	3.5154	-2.84533	-0.68261
O	4.899817	-3.09234	-0.65738
H	-2.23565	-3.19892	3.555125
H	-2.93345	-1.64041	3.031863
H	0.307922	-0.98292	4.55741
H	-1.32063	-1.47256	5.059266
H	-2.26811	0.454213	3.725637
H	-0.60717	0.926441	3.289014
H	-1.33389	1.977271	5.286499
H	-0.72148	-3.00703	-0.73458
H	-1.29951	-4.6873	-0.51643
H	1.186871	-4.50158	-1.09506
H	0.874051	-5.35828	0.440482
H	3.229628	-4.63235	0.501639
H	3.416822	-3.142	1.443765

H	3.282598	-1.7746	-0.60679
H	3.046923	-3.23609	-1.5972
H	5.338141	-2.65555	-1.39563
H	-3.05645	-3.46715	1.243237
H	-2.18036	-1.99381	0.726769

Li-PEO-C1			
Li	-0.44761	-0.22731	-0.05855
O	0.935205	-0.36008	-1.42993
C	1.917331	-1.3831	-1.58315
C	3.327065	-0.83031	-1.52877
O	3.543194	-0.32005	-0.23335
C	4.652954	0.552769	-0.11743
C	5.989525	-0.16799	-0.22661
O	6.967161	0.817535	0.028396
C	0.610828	0.339137	-2.62411
C	-0.26816	1.505632	-2.2271
O	-1.28335	0.970854	-1.38808
C	-2.38064	1.840154	-1.11501
C	-3.46839	1.684799	-2.16601
O	-4.49278	2.5731	-1.78423
H	3.46907	-0.03484	-2.27728
H	4.02877	-1.6427	-1.76668
H	4.582743	1.017024	0.869356
H	4.598103	1.346601	-0.8761
H	6.114777	-0.60235	-1.22876
H	6.021704	-0.98155	0.511131
H	7.849319	0.43803	-0.03991
H	0.073214	-0.3363	-3.3042
H	1.513167	0.706874	-3.12671
H	-0.69624	1.975634	-3.12033
H	0.310232	2.256191	-1.67059
H	-2.04733	2.884681	-1.06704
H	-2.77622	1.551411	-0.13755
H	-3.81176	0.640589	-2.17331
H	-3.07088	1.924998	-3.16266
H	-5.20401	2.566084	-2.43329
H	1.752088	-1.91619	-2.52883

H	1.759155	-2.07562	-0.75185
O	0.291959	-1.73893	1.173656
C	1.196567	-1.04493	2.030566
C	0.5704	0.231139	2.567995
H	2.056673	-0.79624	1.401981
H	1.519846	-1.69444	2.852938
O	0.008034	0.903098	1.447377
H	1.342199	0.855201	3.036892
H	-0.20789	0.02356	3.315878
C	-0.27557	2.283133	1.631683
C	-1.49929	2.516329	2.506656
H	-0.47558	2.692867	0.63854
H	0.601477	2.795842	2.044766
O	-1.82004	3.876678	2.33015
H	-1.27939	2.285405	3.558327
H	-2.31225	1.855226	2.168626
H	-2.51851	4.142772	2.937498
C	-0.79445	-2.42031	1.804919
H	-0.88977	-3.39591	1.32138
C	-2.07824	-1.61758	1.633413
H	-0.58729	-2.58461	2.86914
H	-2.06719	-0.71474	2.250321
H	-2.94387	-2.22804	1.90557
O	-2.19179	-1.12766	0.295296
C	-2.32112	-2.10349	-0.74161
C	-3.50546	-3.03511	-0.58012
H	-1.40237	-2.70327	-0.82205
H	-2.4329	-1.51215	-1.65479
O	-3.15893	-4.03355	0.366793
H	-3.72415	-3.48373	-1.55733
H	-4.38296	-2.45859	-0.25553
H	-3.84859	-4.70539	0.407431

Li-PEO-C2			
Li	0.503922	-1.44383	0.167341
O	1.203811	-1.40155	1.993543
C	2.399718	-0.64361	1.881068
C	3.248183	-1.39752	0.876273

O	2.429531	-1.63101	-0.27299
C	3.150443	-1.95448	-1.46201
C	3.920211	-3.27	-1.36441
O	4.592502	-3.49546	-2.58218
C	0.173205	-0.82762	2.78491
C	-1.0582	-1.67119	2.518161
O	-1.18042	-1.78213	1.102732
C	-2.39706	-2.39789	0.665858
C	-3.61478	-1.49787	0.88448
O	-4.45828	-1.6923	-0.2255
H	3.573657	-2.35329	1.300824
H	4.130965	-0.80644	0.597661
H	3.847296	-1.14066	-1.70716
H	2.404906	-2.02259	-2.26011
H	3.237192	-4.08741	-1.10044
H	4.68802	-3.21014	-0.58701
H	4.059506	-4.04163	-3.16897
H	0.011609	0.214603	2.473396
H	0.438429	-0.84794	3.8484
H	-1.94313	-1.18645	2.947891
H	-0.94883	-2.67342	2.95188
H	-2.50147	-3.37357	1.155553
H	-2.28747	-2.55975	-0.40931
H	-3.28303	-0.45048	0.944209
H	-4.13147	-1.7483	1.821446
H	-5.18835	-1.05378	-0.15936
H	2.915846	-0.57457	2.846239
H	2.154968	0.367272	1.521401
O	0.106381	0.21696	-0.71317
C	0.942072	0.88625	-1.66061
C	2.112915	1.576319	-0.98835
H	0.341299	1.615558	-2.21407
H	1.314375	0.142899	-2.37214
O	1.613813	2.390355	0.046382
H	2.656889	2.157151	-1.74747
H	2.807308	0.829085	-0.57556
C	2.616248	3.078993	0.776783
C	3.043564	4.374021	0.100371

H	3.500473	2.438883	0.921159
H	2.194585	3.308891	1.758627
O	4.067483	4.900474	0.916519
H	2.180091	5.048113	0.034455
H	3.405876	4.174779	-0.91817
H	4.333506	5.770176	0.600516
C	-1.066	0.962193	-0.34966
H	-1.3462	0.650311	0.657791
C	-2.20612	0.652199	-1.30717
H	-0.83092	2.029278	-0.32981
H	-1.97243	1.019046	-2.32021
H	-2.36833	-0.436	-1.36976
O	-3.34896	1.287861	-0.79405
C	-4.45605	1.231412	-1.67501
C	-5.69613	1.645501	-0.92042
H	-4.57967	0.208996	-2.06002
H	-4.2976	1.913855	-2.5229
O	-6.00837	0.621069	0.018806
H	-6.51772	1.777753	-1.63421
H	-5.50942	2.594196	-0.40393
H	-6.81592	0.842634	0.494815

Li-PEO-FEC-C1			
C	0.053321	0.552693	1.369909
C	1.314979	1.34931	1.104001
O	2.390688	0.563444	1.549386
H	1.272677	2.306092	1.645268
H	1.400117	1.567198	0.028693
C	3.641001	1.206602	1.413138
C	4.707183	0.275256	1.969462
H	3.654293	2.154505	1.970256
H	3.839711	1.431063	0.352106
O	5.98128	0.88268	1.930556
H	4.687696	-0.67796	1.42565
H	4.490382	0.067303	3.01999
H	6.318825	0.875471	1.028594
O	-1.04624	1.317651	0.910257

C	-2.84608	-1.93209	2.969547
O	-3.72495	-2.1092	1.86466
C	-4.98838	-1.61142	2.192135
O	-3.47121	-1.22767	3.897453
C	-4.76233	-0.79174	3.450054
O	-1.77309	-2.42312	2.977296
C	-2.27291	0.690764	1.128553
C	-3.35971	1.600614	0.591162
H	-2.43471	0.531411	2.212272
H	-2.31154	-0.2879	0.621074
O	-4.61949	1.008534	0.886653
H	-3.24451	1.728093	-0.49243
H	-3.28277	2.586046	1.068368
C	-5.69612	1.840276	0.473035
C	-7.00121	1.125166	0.768035
H	-5.62569	2.050734	-0.60162
H	-5.67164	2.793972	1.016039
O	-8.02181	2.021959	0.414722
H	-7.04228	0.865723	1.839942
H	-7.05354	0.19588	0.178359
H	-8.88883	1.618338	0.527372
H	0.099697	-0.41064	0.84104
H	-0.04119	0.351955	2.447288
H	-4.71787	0.269848	3.199131
H	-5.49623	-1.00068	4.228431
F	-5.72901	-2.79299	2.455269
H	-5.44976	-1.1021	1.349681
Li	-4.29479	-3.99166	1.67247

Li-PEO-FEC-C2			
C	-0.58008	0.836123	1.362986
C	0.792997	1.410535	1.074792
O	1.749735	0.554906	1.71773
H	0.879761	2.425143	1.478093
H	0.986936	1.429444	-0.00248
C	3.096807	1.032408	1.60342
C	4.029925	-0.05058	2.114228

H	3.216932	1.941657	2.202511
H	3.31384	1.260309	0.554995
O	5.295889	0.544833	2.192589
H	4.01518	-0.91039	1.430342
H	3.687033	-0.38727	3.111451
H	5.981224	-0.11849	2.329221
O	-1.52726	1.647809	0.741948
C	-1.34672	-2.1956	3.371169
O	-2.29006	-1.43234	2.805934
C	-3.50708	-2.16268	2.756168
O	-1.8463	-3.28027	3.919919
C	-3.28347	-3.25389	3.800773
O	-0.17048	-1.89917	3.37682
C	-2.85145	1.196739	0.962083
C	-3.80444	2.142236	0.261298
H	-3.07157	1.183396	2.040384
H	-2.97736	0.178396	0.565104
O	-5.09915	1.662833	0.527864
H	-3.5998	2.152254	-0.81912
H	-3.6724	3.163773	0.646872
C	-6.10721	2.454685	-0.07313
C	-7.45044	1.83825	0.262967
H	-5.97609	2.483448	-1.16392
H	-6.0672	3.484844	0.307976
O	-8.42014	2.666769	-0.34285
H	-7.56954	1.801567	1.354349
H	-7.48657	0.812705	-0.12823
H	-9.30135	2.313001	-0.18659
H	-0.64169	-0.20005	0.982091
H	-0.75206	0.806917	2.455748
H	-3.70507	-3.00415	4.775393
H	-3.62363	-4.22906	3.456095
F	-3.60669	-2.70462	1.515909
H	-4.3378	-1.47725	2.917388
Li	1.17523	-0.8407	2.782483
Li-PEO-FEC-C3			
C	-1.17544	0.909164	1.086963
C	0.301182	1.159198	1.31615

O	0.710424	0.099807	2.150395
H	0.450437	2.133179	1.800742
H	0.841534	1.151512	0.360265
C	2.066818	0.173773	2.549629
C	2.31243	-1.03714	3.436535
H	2.257586	1.094291	3.117403
H	2.726755	0.16073	1.669416
O	3.573096	-1.0136	4.05468
H	2.149131	-1.95595	2.854295
H	1.573406	-1.00544	4.245582
H	4.265478	-1.21579	3.415094
O	-1.7436	1.874925	0.253662
C	-1.6507	-2.04801	3.503744
O	-1.40119	-1.27098	4.558515
C	-0.813	-2.05816	5.584518
O	-1.09078	-3.23204	3.604813
C	-0.33814	-3.30084	4.832386
O	-2.32993	-1.69487	2.560256
C	-3.1087	1.631781	0.050272
C	-3.71117	2.68865	-0.85563
H	-3.657	1.663606	1.015777
H	-3.2595	0.644872	-0.43633
O	-5.06497	2.348002	-0.98233
H	-3.1963	2.679247	-1.82657
H	-3.58175	3.681009	-0.4013
C	-5.78329	3.24796	-1.81367
C	-7.22385	2.780261	-1.87455
H	-5.35362	3.260161	-2.82446
H	-5.73996	4.265566	-1.4025
O	-7.88856	3.704345	-2.70801
H	-7.64475	2.766166	-0.86032
H	-7.25818	1.761241	-2.28248
H	-8.81637	3.463901	-2.79649
H	-1.26658	-0.09994	0.634424
H	-1.66285	0.918703	2.084286
H	0.724601	-3.27422	4.589208
H	-0.60527	-4.21841	5.354815
F	-1.7914	-2.38105	6.466108

H	-0.05248	-1.46693	6.092242
Li	-3.15739	-0.49702	1.537202

Li-PEO-FEC-C4			
C	-1.26516	-0.88328	-0.07317
C	-2.581	-1.62636	-0.19435
O	-3.62415	-0.64034	-0.16588
H	-2.71171	-2.32177	0.641542
H	-2.62764	-2.17899	-1.13828
C	-4.93834	-1.21366	-0.15006
C	-5.9464	-0.0984	-0.3609
H	-5.11586	-1.69977	0.815428
H	-5.01967	-1.95785	-0.94872
O	-7.20167	-0.66949	-0.11304
H	-5.86156	0.293938	-1.38373
H	-5.73623	0.723046	0.350648
H	-7.91022	-0.08517	-0.40431
O	-0.2324	-1.81525	-0.15376
C	-0.80714	2.76716	0.449642
O	0.212446	1.908516	0.326785
C	1.397558	2.526343	0.807318
O	-0.40237	3.981776	0.746318
C	1.039655	4.010285	0.765544
O	-1.9661	2.446018	0.2909
C	1.04533	-1.21428	-0.04544
C	2.09796	-2.29676	-0.16115
H	1.143501	-0.70094	0.922659
H	1.184979	-0.47655	-0.85023
O	3.341016	-1.64604	-0.06821
H	1.995232	-2.82054	-1.12278
H	1.973707	-3.03201	0.647093
C	4.432864	-2.54297	-0.15673
C	5.711438	-1.73966	-0.02578
H	4.423321	-3.06844	-1.12206
H	4.382874	-3.29194	0.645995
O	6.767529	-2.67052	-0.13502
H	5.718315	-1.22508	0.944386
H	5.748704	-0.98502	-0.82316

H	7.613769	-2.22387	-0.0327
H	-1.18112	-0.1382	-0.88681
H	-1.22627	-0.34043	0.889494
H	1.366837	4.537653	1.660148
H	1.386098	4.507341	-0.14161
H	2.239192	2.196199	0.200242
F	1.58001	2.116957	2.088199
Li	-3.20793	1.141772	0.083047

Li-PEO-FEC-C5			
C	-0.43862	0.759439	1.362625
C	0.951272	1.250725	1.013201
O	1.872257	0.395245	1.707795
H	1.092491	2.285494	1.34302
H	1.131731	1.183116	-0.06456
C	3.241946	0.792353	1.553088
C	4.114078	-0.28124	2.190045
H	3.406198	1.751649	2.055692
H	3.46464	0.902504	0.485431
O	5.440331	0.158207	2.294317
H	4.027204	-1.22314	1.631168
H	3.765984	-0.45881	3.21968
H	5.953927	-0.10865	1.52422
O	-1.38291	1.54391	0.701364
C	-1.43789	-1.98005	3.169416
O	-2.0731	-3.10763	2.856439
C	-3.44069	-2.81305	2.612553
O	-2.27237	-0.98272	3.401035
C	-3.62944	-1.46428	3.3025
O	-0.22974	-1.88646	3.231909
C	-2.69787	1.15014	1.041412
C	-3.69805	1.981183	0.267953
H	-2.86402	1.289531	2.120349
H	-2.84632	0.085202	0.797022
O	-4.96386	1.526863	0.684935
H	-3.56102	1.836611	-0.8131
H	-3.56443	3.048343	0.495841

C	-6.0272	2.202709	0.036673
C	-7.33243	1.638262	0.561268
H	-5.97099	2.054642	-1.05061
H	-5.98063	3.280834	0.243573
O	-8.35513	2.337146	-0.11498
H	-7.38292	1.790526	1.648022
H	-7.36947	0.559735	0.355505
H	-9.2181	2.02744	0.177567
H	-0.53907	-0.29885	1.056705
H	-0.58627	0.817323	2.456253
H	-4.20729	-0.76609	2.69402
H	-4.03676	-1.55285	4.3106
H	-4.04903	-3.64291	2.96655
F	-3.59552	-2.68014	1.270163
Li	1.271877	-0.9393	2.857351

Li-PEO-FEC-C6			
O	2.723927	0.320949	-0.14511
C	2.320128	-0.81184	-0.72093
O	0.959575	-0.97877	-0.50345
C	0.513193	-0.07432	0.458512
C	1.699326	0.861726	0.689386
O	2.966362	-1.55924	-1.37674
Li	-0.05094	-2.63023	0.504431
O	-0.27408	-3.85119	-0.97452
C	1.033492	-4.25481	-1.37719
C	1.746231	-4.678	-0.10836
O	1.514147	-3.65624	0.863821
C	2.3486	-3.73069	2.021481
C	3.62325	-2.94578	1.818507
O	3.253537	-1.58066	1.696537
C	-1.03966	-3.18533	-1.96824
C	-2.25759	-2.63936	-1.25465
O	-1.7847	-1.87938	-0.13863
C	-2.82172	-1.39089	0.715952
C	-3.68313	-0.32742	0.044695
O	-4.35232	0.317938	1.102272

H	-2.89237	-3.45661	-0.88834
H	-2.83687	-2.00773	-1.93683
H	-2.32396	-0.93789	1.577351
H	-3.43956	-2.22568	1.068898
H	-4.39057	-0.77846	-0.66291
H	-3.03283	0.364958	-0.51319
H	-5.0876	0.843473	0.76933
H	1.552894	-3.40733	-1.84025
H	0.97826	-5.08983	-2.08497
H	2.818288	-4.78321	-0.30957
H	1.351376	-5.62696	0.274638
H	2.563693	-4.77952	2.256119
H	1.77978	-3.29395	2.846942
H	4.142715	-3.28564	0.912588
H	4.280889	-3.1024	2.682373
H	4.040236	-1.06051	1.489733
H	-1.33915	-3.87932	-2.76227
H	-0.44685	-2.36928	-2.40314
F	0.233967	-0.82594	1.59571
H	-0.427	0.378778	0.146517
H	1.496963	1.885367	0.375131
H	2.019803	0.820146	1.732096

Li-PEO-FEC-C7			
O	1.642982	0.547075	-0.07692
C	1.044575	-0.63025	-0.07263
O	0.513284	-0.90663	1.15757
C	0.652309	0.215116	1.998693
C	1.673403	1.076196	1.257933
O	0.911384	-1.39604	-0.98521
Li	-0.09984	-2.77664	0.234757
O	-0.335	-4.24285	-1.00033
C	0.982788	-4.5985	-1.3994
C	1.75157	-4.84252	-0.11568
O	1.542899	-3.70149	0.718778
C	2.472898	-3.5499	1.785887
C	3.715976	-2.80417	1.34846
O	3.343398	-1.46595	1.036838

C	-1.17203	-3.71113	-2.02335
C	-2.3783	-3.13469	-1.30959
O	-1.87789	-2.27326	-0.28668
C	-2.84592	-1.40847	0.30786
C	-2.92998	-0.09366	-0.4512
O	-3.88846	0.674668	0.235899
H	-2.97913	-3.92843	-0.84923
H	-2.99977	-2.57634	-2.01844
H	-2.52524	-1.21618	1.334773
H	-3.82563	-1.89866	0.337495
H	-3.22187	-0.27455	-1.49547
H	-1.93981	0.385215	-0.45013
H	-4.03597	1.513236	-0.21385
H	1.430899	-3.76754	-1.95993
H	0.97199	-5.5016	-2.02087
H	2.816111	-4.97024	-0.34293
H	1.38343	-5.73632	0.402431
H	2.739964	-4.53254	2.193405
H	1.960053	-2.98026	2.566477
H	4.162085	-3.29178	0.47298
H	4.447859	-2.82255	2.165403
H	4.050167	-1.05434	0.525275
H	-1.47362	-4.4969	-2.72548
H	-0.63112	-2.92091	-2.56057
H	0.931111	-0.11107	2.999696
F	-0.55639	0.84134	2.061694
H	1.375978	2.12347	1.228743
H	2.678581	0.948996	1.66062

Li-PEO-FS-C1			
C	-3.57547	-1.00454	3.924417
C	-4.42789	-1.27497	2.855536
C	-4.01506	-1.97806	1.733011
C	-2.70032	-2.42763	1.687633
C	-1.80807	-2.17858	2.74245
C	-2.26695	-1.45909	3.860718
C	-0.45249	-2.73857	2.658751
C	0.543735	-2.64297	3.56595

F	-5.68972	-0.85215	2.924828
O	-4.86762	1.313665	0.675387
C	-6.00776	2.07906	0.328373
C	-7.23843	1.285644	0.720035
O	-8.34511	2.052709	0.293767
C	-3.65872	1.984475	0.41858
C	-2.57214	0.998173	0.787714
O	-1.29998	1.618087	0.66832
C	-0.29389	0.783402	1.130649
C	1.050295	1.463493	0.958957
O	2.017464	0.545204	1.490174
C	3.361837	1.047466	1.486641
C	4.282843	-0.07114	1.955116
O	5.573259	0.422358	2.190575
H	1.084663	2.404296	1.518107
H	1.26262	1.655403	-0.09749
H	3.434752	1.900672	2.169417
H	3.615411	1.374953	0.471771
H	4.275476	-0.89735	1.230971
H	3.916023	-0.45521	2.917647
H	6.113665	0.369869	1.39465
H	-2.36378	-2.99352	0.822576
H	-4.71486	-2.15685	0.924839
H	-1.6091	-1.26998	4.703931
H	-3.95217	-0.4591	4.782227
H	1.462826	-3.20878	3.429914
H	0.418563	-2.13246	4.518517
H	-0.26594	-3.34109	1.767209
H	-2.72618	0.664181	1.823874
H	-2.62271	0.119159	0.129778
H	-3.579	2.272218	-0.63982
H	-3.57008	2.89325	1.031885
H	-6.0241	2.278017	-0.75239
H	-6.00132	3.041917	0.858249
H	-7.24145	1.128451	1.805956
H	-7.20701	0.304162	0.226885
H	-9.16464	1.621248	0.555253
H	-0.29722	-0.17811	0.57475

H	-0.45838	0.554042	2.206459
Li	1.262376	-0.93868	2.270693

Li-PEO-FS-C2			
C	2.710691	-0.24265	-0.4979
C	1.601102	-0.35306	-1.35076
C	0.323915	-0.17995	-0.79724
C	0.157832	0.094129	0.56207
C	1.289562	0.193949	1.365282
C	2.570923	0.031596	0.859039
C	1.816108	-0.63256	-2.78427
C	0.904403	-0.53638	-3.75634
Li	-0.16385	-2.3586	0.424505
O	-0.2417	-3.81586	-0.84255
C	1.089782	-4.11061	-1.24578
C	1.866007	-4.26729	0.044646
O	1.589376	-3.11022	0.833106
C	2.328009	-3.05247	2.056967
C	3.8309	-2.88436	1.823222
O	4.291118	-2.03181	2.85051
C	-1.15447	-3.46181	-1.87275
C	-2.42502	-3.06216	-1.15192
O	-2.04972	-2.11108	-0.15284
C	-3.15024	-1.53511	0.556551
C	-3.72129	-0.33283	-0.18157
O	-4.72831	0.167489	0.662829
F	1.128048	0.438736	2.673107
H	-2.88126	-3.93252	-0.66483
H	-3.14117	-2.62617	-1.85684
H	-2.77611	-1.21569	1.533309
H	-3.92903	-2.28832	0.721711
H	-4.12143	-0.63567	-1.15941
H	-2.92157	0.403874	-0.35195
H	-5.18362	0.909087	0.249753
H	3.708156	-0.36492	-0.9124
H	3.422935	0.101643	1.528625
H	-0.55968	-0.24645	-1.42579
H	-0.82261	0.273893	0.995533

H	1.166813	-0.75312	-4.78561
H	-0.11483	-0.2063	-3.57306
H	2.832059	-0.92091	-3.05043
H	1.485818	-3.27696	-1.84284
H	1.123123	-5.03329	-1.83653
H	2.93794	-4.34193	-0.17161
H	1.543032	-5.16378	0.589874
H	2.104732	-3.94203	2.658537
H	1.971647	-2.16987	2.592731
H	3.980233	-2.42997	0.8321
H	4.351135	-3.84953	1.844772
H	5.236245	-2.15171	2.993174
H	-1.33898	-4.31113	-2.54081
H	-0.74305	-2.62482	-2.45596

Li-PEO-FS-C3			
C	0.288473	-0.07817	-1.21858
C	-0.98345	0.03524	-0.65345
C	-1.10579	0.041584	0.736706
C	0.004039	-0.08443	1.568813
C	1.269331	-0.19782	0.982905
C	1.441805	-0.19734	-0.41566
F	-2.31869	0.143138	1.278893
C	2.802264	-0.32774	-0.97417
C	3.106199	-0.49033	-2.26389
Li	0.00645	-1.99487	0.129373
O	-0.33595	-3.78483	0.041017
C	-1.43478	-4.45256	0.675312
C	-2.33076	-3.38688	1.29281
O	-3.33457	-3.97084	2.075995
C	0.581405	-4.67197	-0.61206
C	1.694995	-3.81887	-1.19005
O	2.59299	-4.67463	-1.81946
C	3.685364	-3.99408	-2.41318
C	4.60195	-5.02712	-3.03614
O	5.65932	-4.31436	-3.62374
C	6.609495	-5.1595	-4.2454

C	7.692471	-4.28389	-4.84334
O	8.614545	-5.16599	-5.4491
H	0.983111	-5.38535	0.115202
H	0.061739	-5.2168	-1.40706
H	-1.0564	-5.12073	1.456334
H	-1.97465	-5.04379	-0.07398
H	-2.73937	-2.7331	0.506777
H	-1.7295	-2.76624	1.972423
H	-4.10382	-4.19427	1.540345
H	2.140526	-0.28947	1.625106
H	-0.1287	-0.0823	2.645719
H	0.378692	-0.0632	-2.29965
H	-1.87176	0.134183	-1.26842
H	4.140106	-0.57353	-2.58072
H	2.356183	-0.54355	-3.04857
H	3.606164	-0.2854	-0.2423
H	4.231861	-3.41517	-1.65437
H	3.325134	-3.29997	-3.18714
H	4.050972	-5.61303	-3.78678
H	4.968926	-5.71808	-2.26274
H	6.135777	-5.75605	-5.0379
H	7.052579	-5.84778	-3.51176
H	8.158595	-3.6891	-4.04665
H	7.242283	-3.59842	-5.57355
H	9.333064	-4.66653	-5.84958
H	1.276491	-3.08551	-1.908
H	2.195132	-3.24998	-0.38092

Li-PEO-FS-C4			
C	0.956847	2.171639	1.208355
C	2.042968	2.108902	0.357372
C	1.977199	2.310962	-1.00635
C	0.718371	2.558059	-1.55233
C	-0.43146	2.58505	-0.75026
C	-0.28836	2.414652	0.636103
C	-1.75155	2.793844	-1.37619
C	-2.90911	2.353953	-0.87633
F	3.2842	1.790967	0.909365

O	3.221436	-1.6123	-0.07558
C	4.297602	-2.55455	-0.0871
C	5.573636	-1.77787	-0.32406
O	5.551308	-0.67573	0.600523
C	1.931793	-2.23726	-0.15104
C	0.878621	-1.16767	0.056996
O	-0.36598	-1.80055	-0.00154
C	-1.43806	-0.88378	0.122141
C	-2.7397	-1.65812	0.104794
O	-3.76352	-0.70173	0.237091
C	-5.05637	-1.27098	0.299145
C	-6.05581	-0.13325	0.443658
O	-7.36776	-0.6251	0.605025
H	-2.76208	-2.37806	0.935929
H	-2.83837	-2.2153	-0.83833
H	-5.14229	-1.94813	1.160747
H	-5.25971	-1.851	-0.61548
H	-5.97203	0.544512	-0.41651
H	-5.82167	0.437435	1.34617
H	-7.71113	-0.92887	-0.24206
H	0.627191	2.720702	-2.62201
H	2.872794	2.286571	-1.61814
H	-1.16045	2.489752	1.27788
H	1.082602	2.044869	2.278446
H	-3.84096	2.539421	-1.39939
H	-2.97615	1.77333	0.040815
H	-1.74441	3.318815	-2.32927
H	1.023839	-0.68738	1.041592
H	0.964605	-0.38639	-0.71701
H	1.81638	-2.70674	-1.13357
H	1.849707	-3.00479	0.627339
H	4.14891	-3.28371	-0.89126
H	4.325731	-3.07844	0.876182
H	5.611009	-1.39272	-1.34793
H	6.440256	-2.41734	-0.13886
H	6.421571	-0.26817	0.681939
H	-1.42044	-0.15995	-0.70616
H	-1.35605	-0.32785	1.068909

Li	3.807169	0.012846	0.711857

Li-PEO-FS-C5			
C	-0.10697	2.420436	-1.01952
C	-0.70982	2.269937	0.213365
C	-0.03438	2.072841	1.398277
C	1.356101	2.00362	1.327272
C	2.034509	2.13987	0.108056
C	1.283234	2.348633	-1.05907
C	3.506563	2.042691	0.086314
C	4.298575	2.573958	-0.84678
F	-2.11433	2.289317	0.258157
O	-3.97608	-0.7374	-0.01407
C	-5.29407	-1.2476	-0.26346
C	-6.29685	-0.15794	0.070705
O	-7.52916	-0.61907	-0.40965
C	-2.95017	-1.74094	-0.09346
C	-1.63936	-1.00818	0.109258
O	-0.58335	-1.90497	0.00669
C	0.661427	-1.26796	0.258316
C	1.786441	-2.23421	-0.04526
O	2.973969	-1.51855	0.193715
C	4.141177	-2.25599	-0.11306
C	5.336618	-1.34369	0.115949
O	6.541655	-1.97691	-0.25205
H	1.727218	-2.56336	-1.09298
H	1.718878	-3.12193	0.600614
H	4.12786	-2.58502	-1.16178
H	4.205528	-3.15057	0.527075
H	5.350403	-1.00617	1.161376
H	5.236478	-0.4622	-0.52307
H	6.790458	-2.62516	0.415687
H	1.924806	1.839401	2.237508
H	-0.56651	1.977584	2.3388
H	1.786307	2.430346	-2.01679
H	-0.69712	2.578896	-1.91572
H	5.375569	2.459307	-0.7922
H	3.90996	3.153084	-1.6798

H	3.948609	1.502038	0.920776
H	-1.53872	-0.21797	-0.66282
H	-1.64123	-0.5167	1.102609
H	-3.10977	-2.49056	0.687701
H	-2.98041	-2.22259	-1.07644
H	-5.46425	-2.13001	0.361108
H	-5.38483	-1.52812	-1.31833
H	-5.99771	0.780216	-0.4351
H	-6.31068	0.018751	1.154866
H	-8.25515	-0.08458	-0.06942
H	0.713778	-0.94757	1.308524
H	0.766807	-0.37803	-0.37967
Li	-3.42056	1.016415	0.10187

Li-PEO-FS-C6			
C	4.797304	10.10067	5.148631
C	5.769748	9.161119	4.828151
C	5.899592	8.627105	3.550647
C	5.014806	9.044464	2.559322
C	4.007828	9.989771	2.846694
C	3.917401	10.51236	4.152065
C	2.98552	10.38505	1.84795
C	2.611831	9.632775	0.797735
F	6.616999	8.762574	5.777812
C	4.99871	13.32078	2.36714
C	3.749364	14.12046	2.65168
O	2.728187	13.25231	3.139163
O	4.78234	12.47256	1.258514
C	5.991166	11.99155	0.698305
C	5.711229	11.27427	-0.60558
O	5.45964	9.898386	-0.37689
C	5.106698	9.218858	-1.56689
C	5.276277	7.728908	-1.33457
O	4.819887	7.079012	-2.4844
C	5.076533	5.688941	-2.495
C	4.824896	5.159579	-3.88697
O	5.864984	5.634061	-4.71546
H	4.700612	7.407045	-0.44404

H	6.335611	7.503236	-1.13963
H	4.421738	5.177256	-1.77188
H	6.124433	5.494873	-2.22406
H	4.813419	4.061517	-3.84679
H	3.842162	5.510134	-4.22934
H	5.687416	5.398949	-5.63191
H	4.066921	9.445415	-1.84862
H	5.755939	9.522791	-2.39867
H	5.157676	8.710105	1.535231
H	6.697842	7.922712	3.343877
H	3.173098	11.27581	4.361443
H	4.747485	10.49783	6.156425
H	1.832652	9.963952	0.120796
H	3.143168	8.720806	0.511576
H	2.481747	11.32674	2.055775
H	4.846294	11.74739	-1.09303
H	6.580597	11.37033	-1.27083
H	6.658782	12.84245	0.500785
H	6.502734	11.30978	1.396523
H	5.812184	14.02823	2.147331
H	5.28905	12.73303	3.252952
H	3.424428	14.61393	1.728287
H	3.989108	14.884	3.401584
H	1.938473	13.77515	3.318882
Li	2.537522	8.390916	2.735463

Li-PEO-FS-C7			
C	-5.08858	1.251161	-0.51365
C	-4.6493	2.518329	-0.20391
C	-3.67362	2.827334	0.717596
C	-3.07795	1.753864	1.376435
C	-3.4577	0.432834	1.098938
C	-4.47355	0.196692	0.159249
C	-2.82387	-0.72156	1.764936
C	-1.57418	-0.74466	2.232603
F	-5.26853	3.606603	-0.88016
C	-1.9338	-2.38981	-0.964

C	-2.80549	-3.45416	-0.3221
O	-4.15863	-3.04389	-0.49634
O	-0.64146	-2.50773	-0.42611
C	0.199518	-1.44054	-0.79992
C	1.53051	-1.63615	-0.10294
O	2.331943	-0.52155	-0.40907
C	3.642203	-0.63523	0.106642
C	4.406012	0.612443	-0.28882
O	5.709808	0.473352	0.213724
C	6.543164	1.566036	-0.09943
C	7.962151	1.227177	0.291185
O	8.455681	0.282272	-0.63769
H	3.911564	1.503716	0.130239
H	4.415064	0.709685	-1.38497
H	6.210106	2.465225	0.443172
H	6.510312	1.775355	-1.17949
H	8.562136	2.148018	0.275303
H	7.959653	0.825314	1.312878
H	9.288084	-0.08133	-0.3202
H	3.621208	-0.72947	1.202469
H	4.146451	-1.52079	-0.3052
H	-2.32556	1.952175	2.132535
H	-3.40263	3.854728	0.933036
H	-4.76219	-0.82879	-0.06135
H	-5.87696	1.082976	-1.23896
H	-1.16697	-1.64138	2.686494
H	-0.90899	0.112112	2.154647
H	-3.43615	-1.62017	1.813751
H	1.370016	-1.7196	0.98366
H	2.001725	-2.56765	-0.44918
H	0.34471	-1.41552	-1.89
H	-0.24327	-0.48005	-0.48892
H	-1.91734	-2.50028	-2.05872
H	-2.35691	-1.40072	-0.72981
H	-2.54674	-3.51926	0.742533
H	-2.62531	-4.43142	-0.78239
H	-4.74191	-3.79998	-0.37317
Li	-5.45864	4.656411	-2.26972

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