Supporting Information

DFT-ReaxFF Hybrid Molecular Dynamics Investigation of the Decomposition Effects of Localized High-Concentration Electrolyte in Lithium Metal Batteries: LiFSI/DME/TFEO

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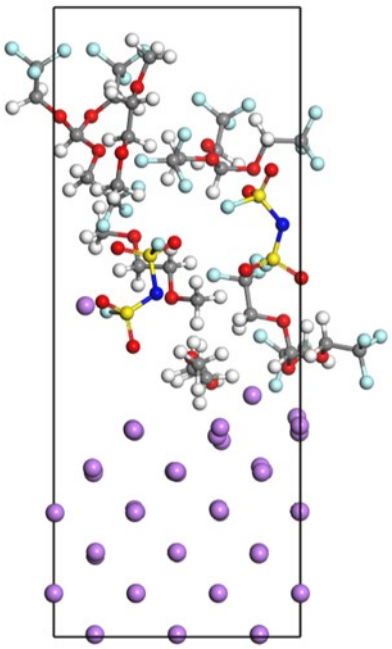

Figure 1. Initial model. Color: lithium, purple; oxygen, red; fluorine, cyan; carbon, gray; nitrogen, blue; sulfur, yellow, hydrogen, white.

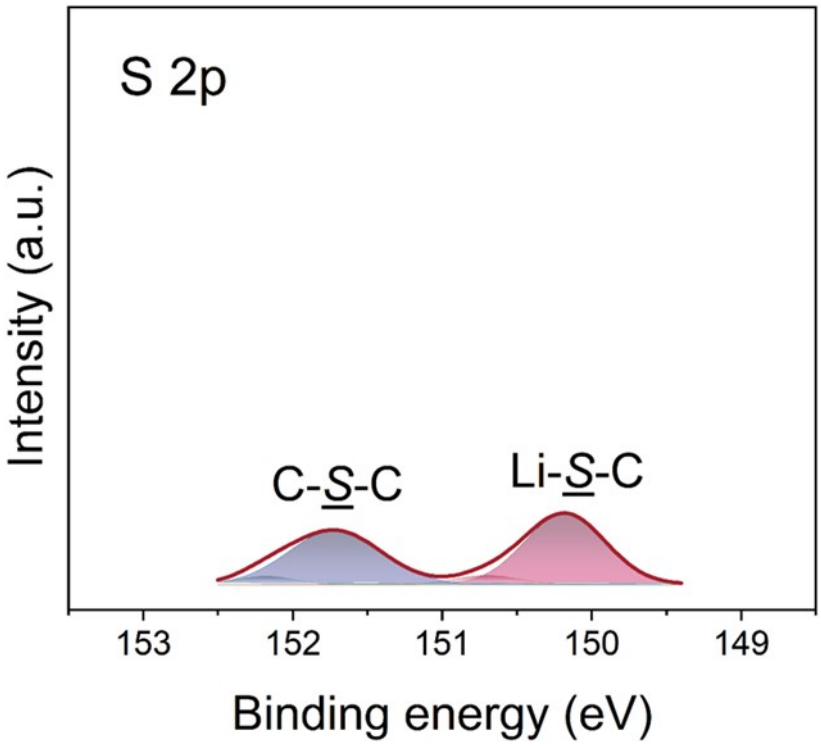

Figure 2. X-ray photoelectron spectroscopy (XPS) of S 2p of FSI-TFEO-DME

Time	Products
0ps	TFEO*3, DME*2, LiFSI*2
5.5ps	TFEO*3, DME*2, LiF*4, SO_2*2, NSO_2*2
11ps	TFEO*3, DME*2, LiF*4, SO_2, NSO_2, NSO, Li_2O*3, Li_2S
275ps	DME*2, LiF*20, C_2HOS, $SOCCH_2$, CHOS, C_2H_2N, NSCHO, CCH, CF_3CH_2O*3, CF_2CH_2O, CH_2CCHO, Li_2O*8, LiH*2
550ps	DME*2, LiF*29, $SNCCH_2$, $C_4H_2O_2S$, $CH_2CHCHCSO$, SH, CN, CO, CH_2CO_2, Polymer I, HF, HCO_2, LiH*2, Li_2O*7
1ns	DME*2, LiF*29, $C_4H_2O_2S$, SCO_2*2, NCCHCN, OH, Polymer II, Polymer III, $CHOCH_2F$, HF, LiH*3, Li_2O*6

Table S1. The products obtained from HAIR MD simulation for 1M LiFSI/TFEO/DME systems between 0-1000 ps.

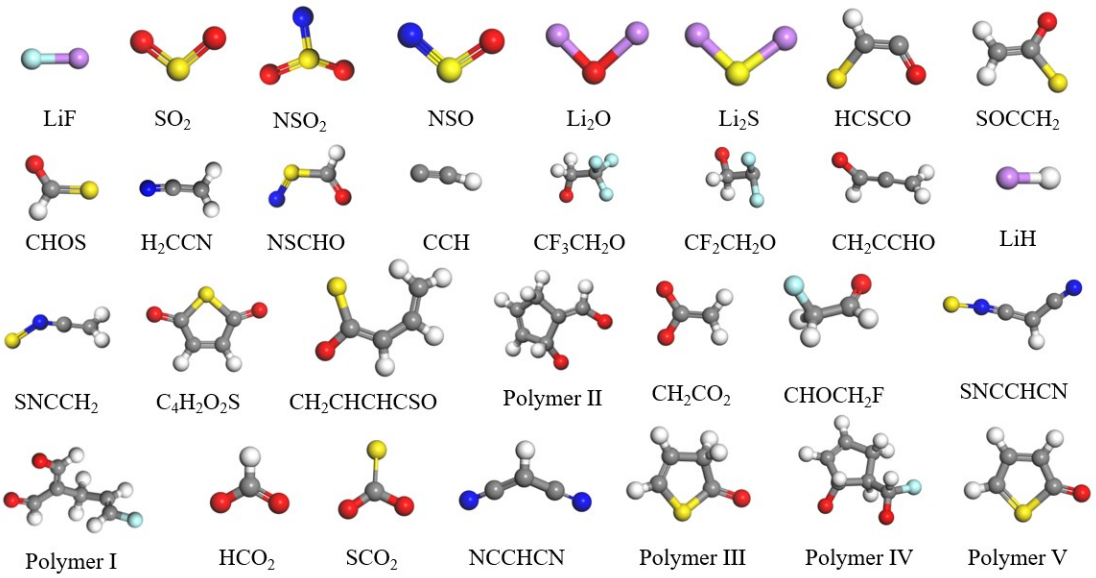

Figure S3. The geometries for main products in Table S1 obtained from MD simulations directly. Color code: lithium, purple; oxygen, red; carbon, gray; fluorine, cyan; sulfur, yellow, nitrogen, blue; hydrogen, white.