Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A. This journal is © The Royal Society of Chemistry 2019

Supporting Information for:

Localized High Concentration Electrolyte Behavior Near a Lithium-Metal Anode Surface Yu Zheng^{1,3}, Fernando A. Soto¹, Victor Ponce^{1,2}, Jorge M. Seminario^{1,2,4}, Xia Cao⁵, Ji-Guang Zhang⁵, and Perla B. Balbuena^{1,2,3,*}

¹Department of Chemical Engineering, ²Department of Materials Science and Engineering, and ³Department of Chemistry, ⁴Department of Electrical Engineering, Texas A&M University, College Station, Texas 77843, United States; ⁵Energy and Environment Directorate, Pacific Northwest National Laboratory, Richland, Washington 99354, United States

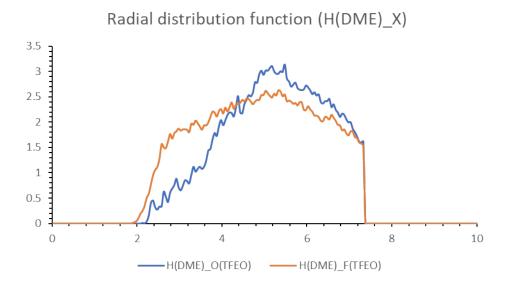


Figure S1. RDF profile for hydrogen atoms in DME and oxygen/fluorine atoms in TFEO obtained from AIMD simulations.

^{*}e-mail: balbuena@tamu.edu

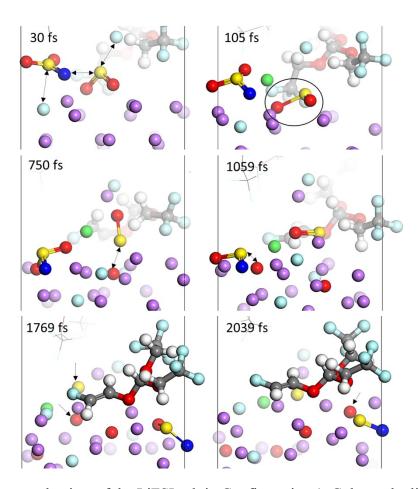


Figure S2. Reduction mechanism of the LiFSI salt in Configuration 1. Color code: lithium from the slab (salt), purple (green); oxygen, red; carbon, gray; fluorine, light blue; sulfur, yellow, nitrogen, blue; hydrogen, white.

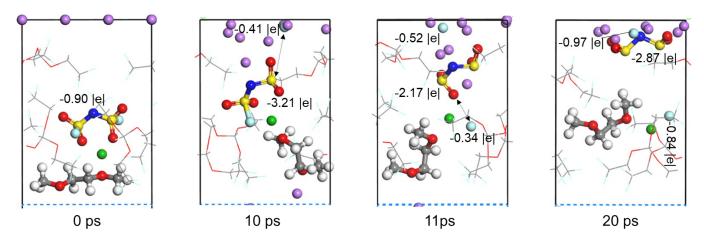
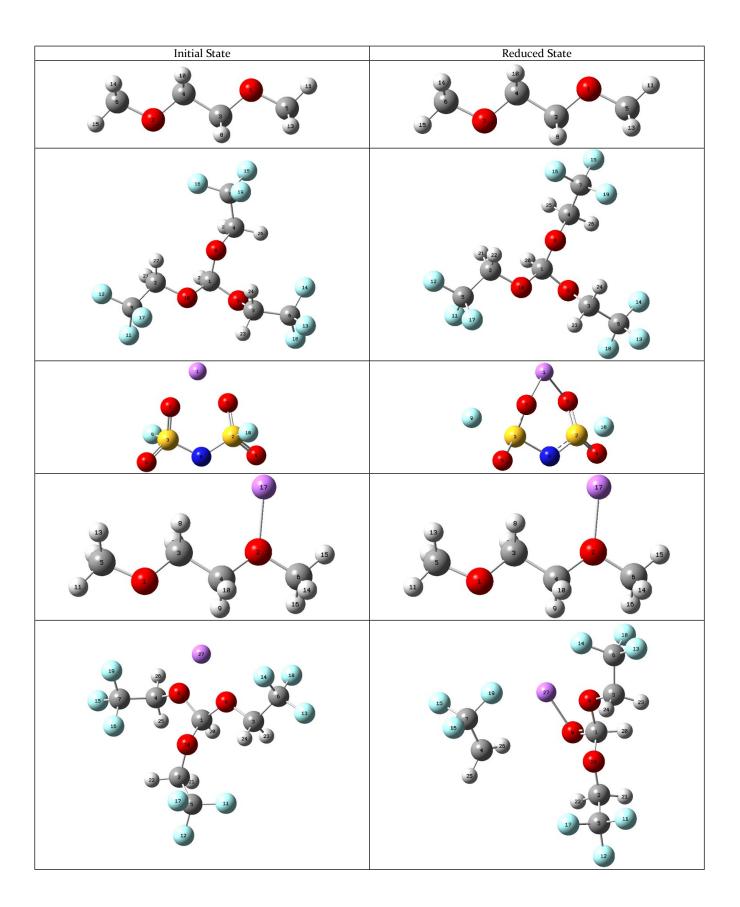
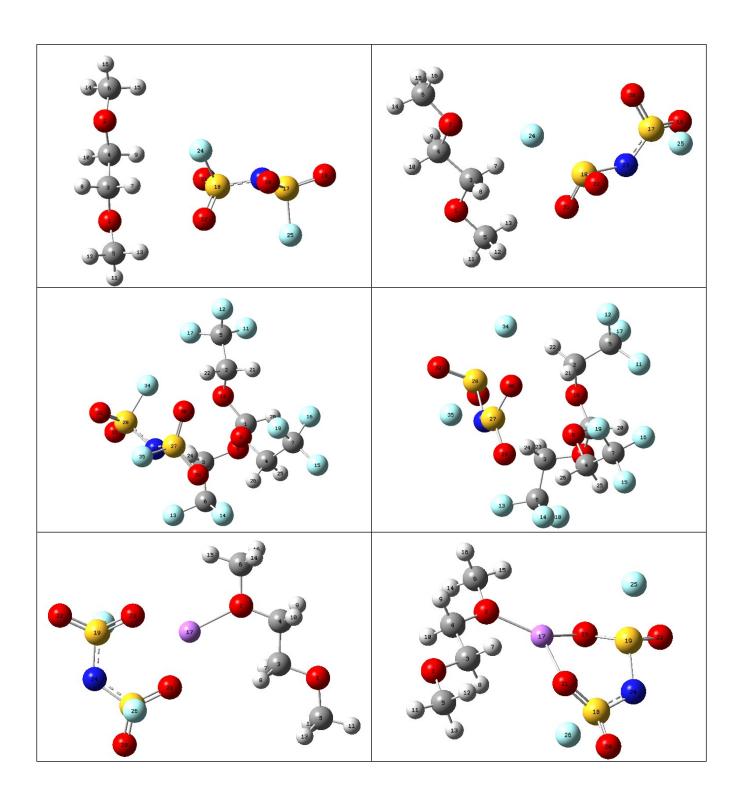


Figure S3. Reduction mechanism of the LiFSI salt in Configuration 2. Color code as in Figure S2.





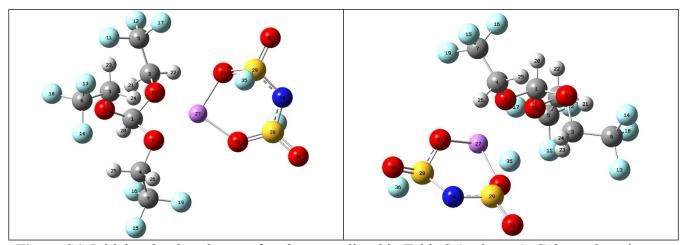


Figure S4. Initial and reduced state of each system listed in Table 2 (main text). Color code as in Figure S2.