Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supporting Information

for

Synergetic Impact of Nitrate-based Additives for Enhanced Solid Electrolyte Interphase Performance

Swastik Basu and Gyeong S. Hwang*

McKetta Department of Chemical Engineering, The University of Texas at Austin, Austin, Texas 78712, USA.

*Author to whom correspondence should be addressed:

Tel: 1-512-471-4847, Fax: 1-512-471-7060, E-mail: gshwang@che.utexas.edu

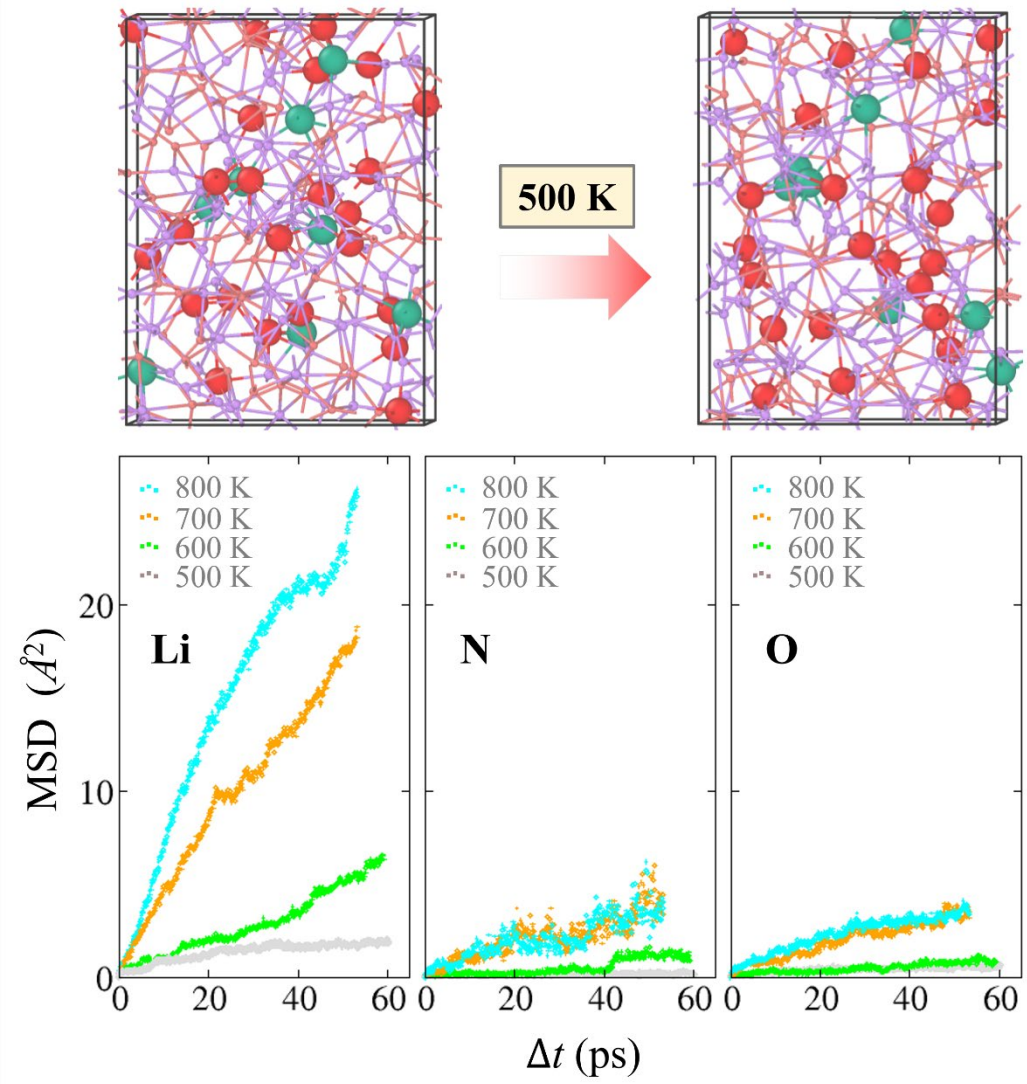

Figure S1: MSD-Δ*t* curves from high temperature AIMD simulations. Averaged MSD for Li, N, and O ions in a $Li_xLiF(NO_3)$ system ($x = 0.7$) equilibrated at 500 K, 600 K, 700 K, and 800 K are plotted, as functions of simulation time interval. The atomic structures at the beginning and after 60 ps of our chosen NVT run (at 500 K) are shown on top, where the small blue atoms represent Li, small pink atoms represent F, green atoms represent N, and the red atoms represent O.

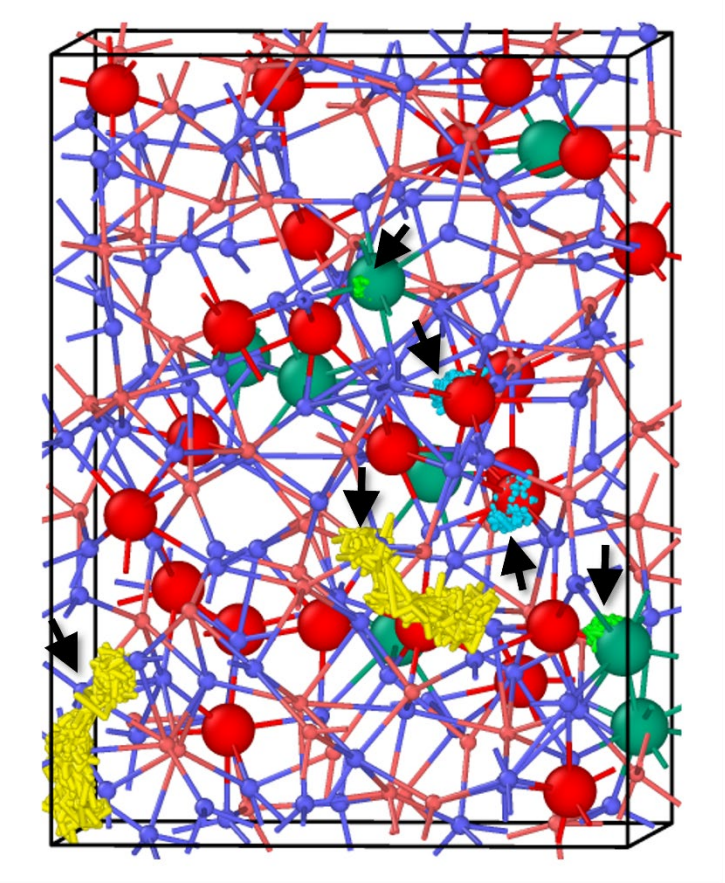

Figure S2: Evolution trajectory of representative Li, N, and O ions within a $Li_xLiF(NO_3)$ system (x = 0.7) at 500 K over 60 ps. The Li ion trajectory lines are drawn in yellow, N trajectory lines are in light green, and O trajectory lines are chosen as blue. The trajectory lines included here are further marked by arrows for ease of viewing. The small blue atoms represent Li, small pink atoms represent F, green atoms represent N, and the red atoms represent O.

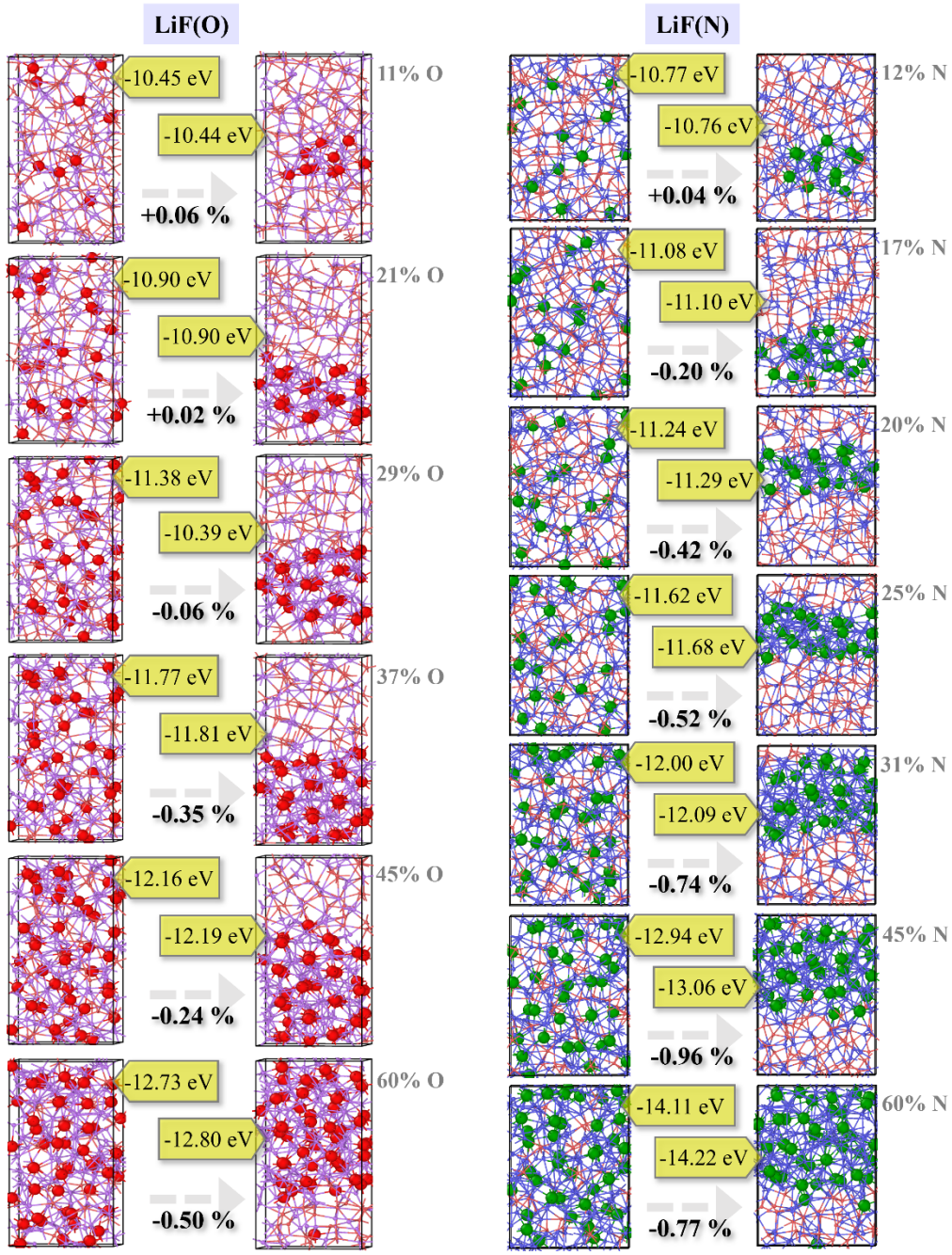

Figure S3: Relative configurational stabilities of alternative phase distributions in LiF(N) and LiF(O) systems. Snapshots represent amorphous LiF matrices mixed with varying concentrations of well-dispersed oxide phases, segregated oxide phases, well-dispersed nitride phases, and segregated nitride phases (from left to right). The total energy per formula unit (E) of each system is shown, along with the gap (%) in E between the dispersed and segregated structures. A positive (negative) value of the energy difference reflects higher (lower) energy of the segregated system, when compared to the well-dispersed one. The red and green balls represent O and N, respectively.

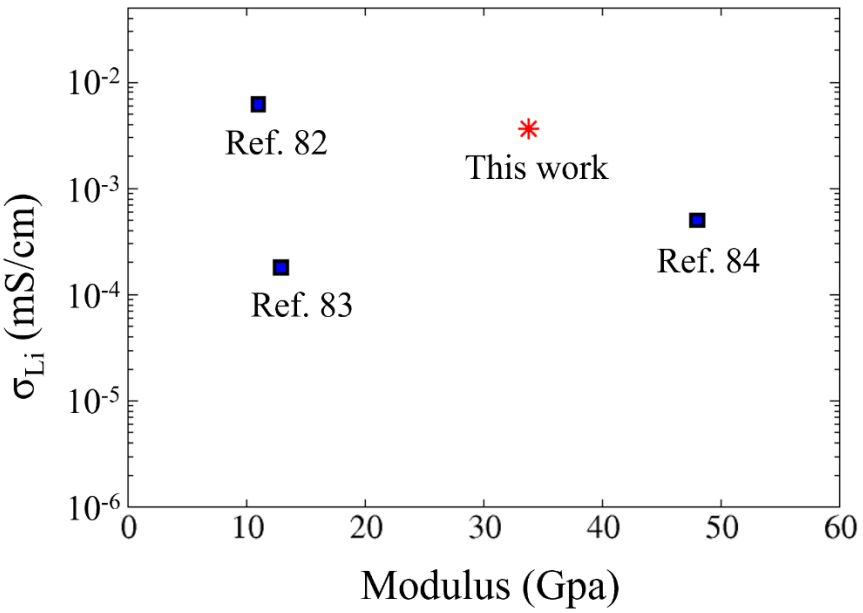

Figure S4: Comparison of Young's Modulus and ionic conductivity of our model LiF(N, O) system with related experimental works. Ref. 82 studied LiF-rich SEI without Li_3N; Ref. 83 examined LiF-Li_3N-Li_2O mixed SEI; Ref. 84 looked at plasma-activated Li_3N SEI.