

## **Supplementary Material**

# **Lithium Ion Transport in Solid Polymer Electrolyte Filled with Alumina Nanoparticles**

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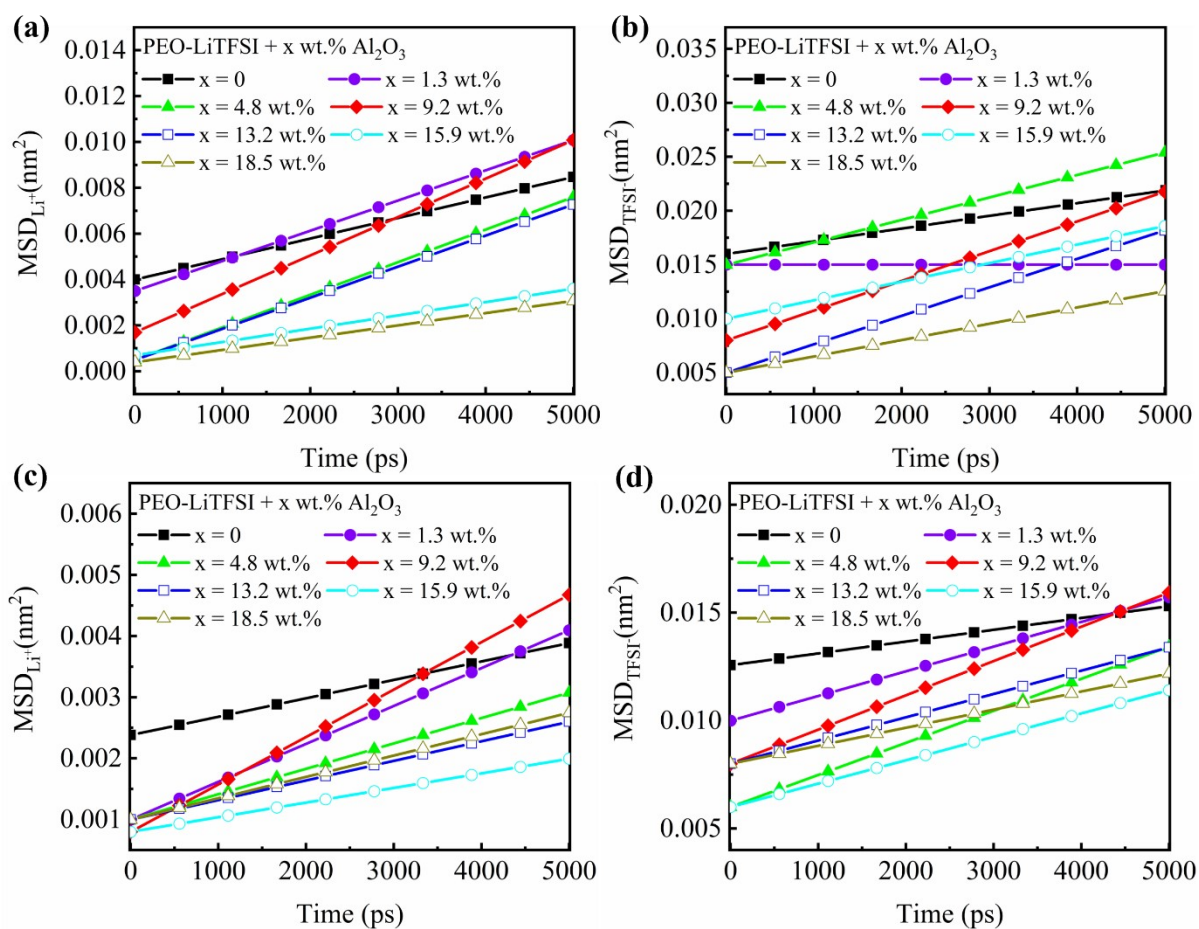


Figure S1. Mean square displacement (MSD) functions of (a)  $\text{Li}^+$  at 333 K, (b)  $\text{TFSI}^-$  at 333 K, (c)  $\text{Li}^+$  cations at 300 K, and (d)  $\text{TFSI}^-$  at 300 K in the SC system. PEO-LiTFSI + x wt.%  $\text{Al}_2\text{O}_3$  represents PEO-LiTFSI with x wt.%  $\text{Al}_2\text{O}_3$ . x is the mass fraction of  $\text{Al}_2\text{O}_3$ .

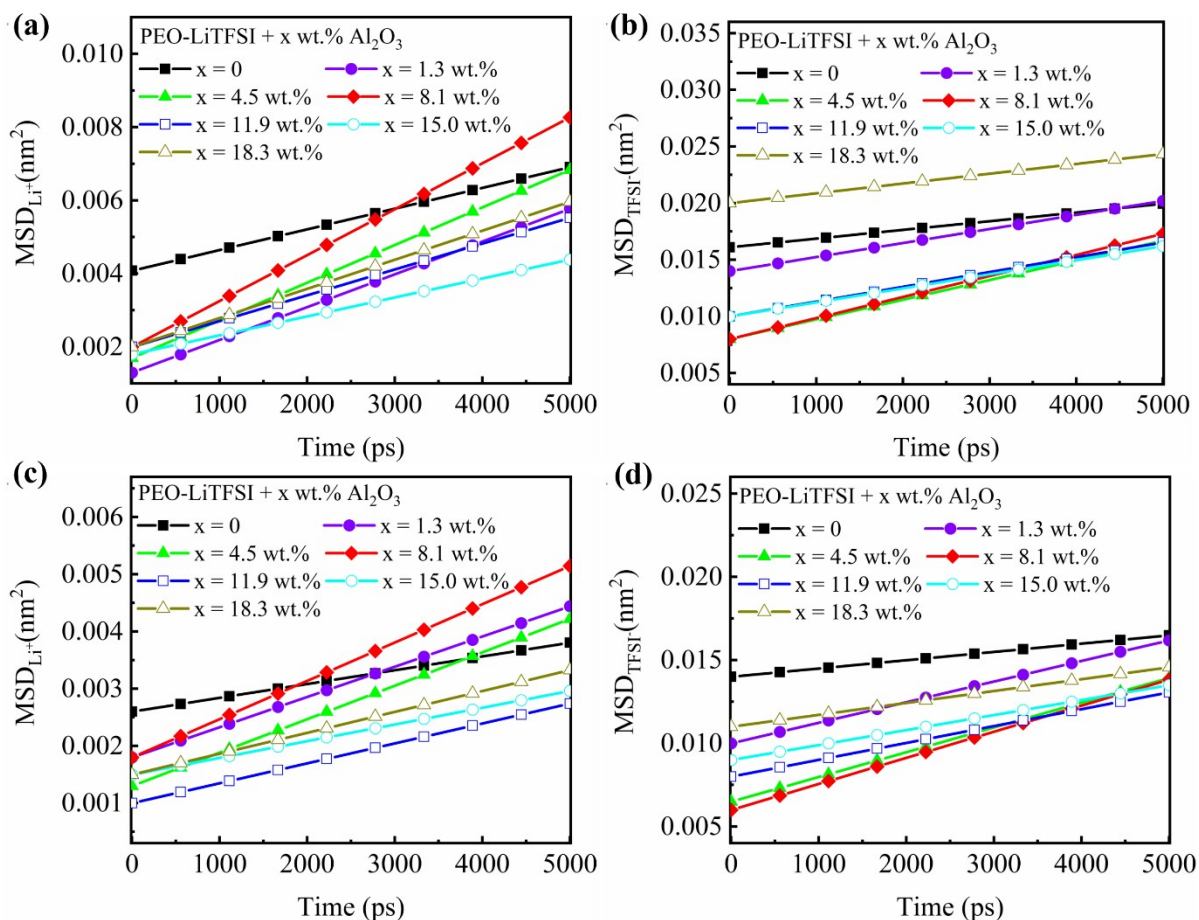


Figure S2. Mean square displacement (MSD) functions of (a)  $\text{Li}^+$  at 333 K, (b)  $\text{TFSI}^-$  at 333 K, (c)  $\text{Li}^+$  cations at 300 K, and (d)  $\text{TFSI}^-$  at 300 K in the LC system.

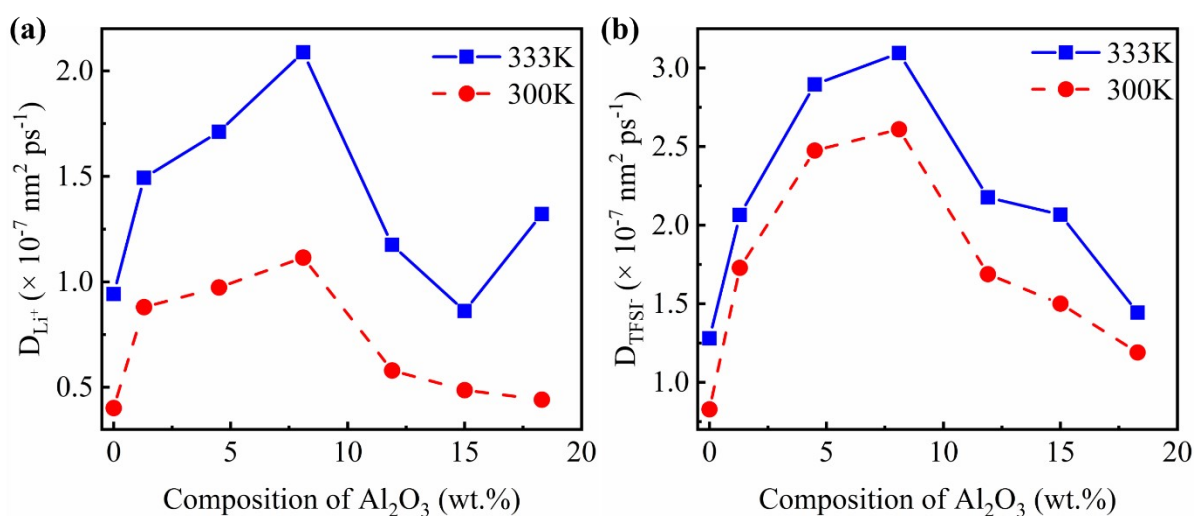


Figure S3. Diffusivities of (a)  $\text{Li}^+$  and (b)  $\text{TFSI}^-$  at different temperatures in the LC system.

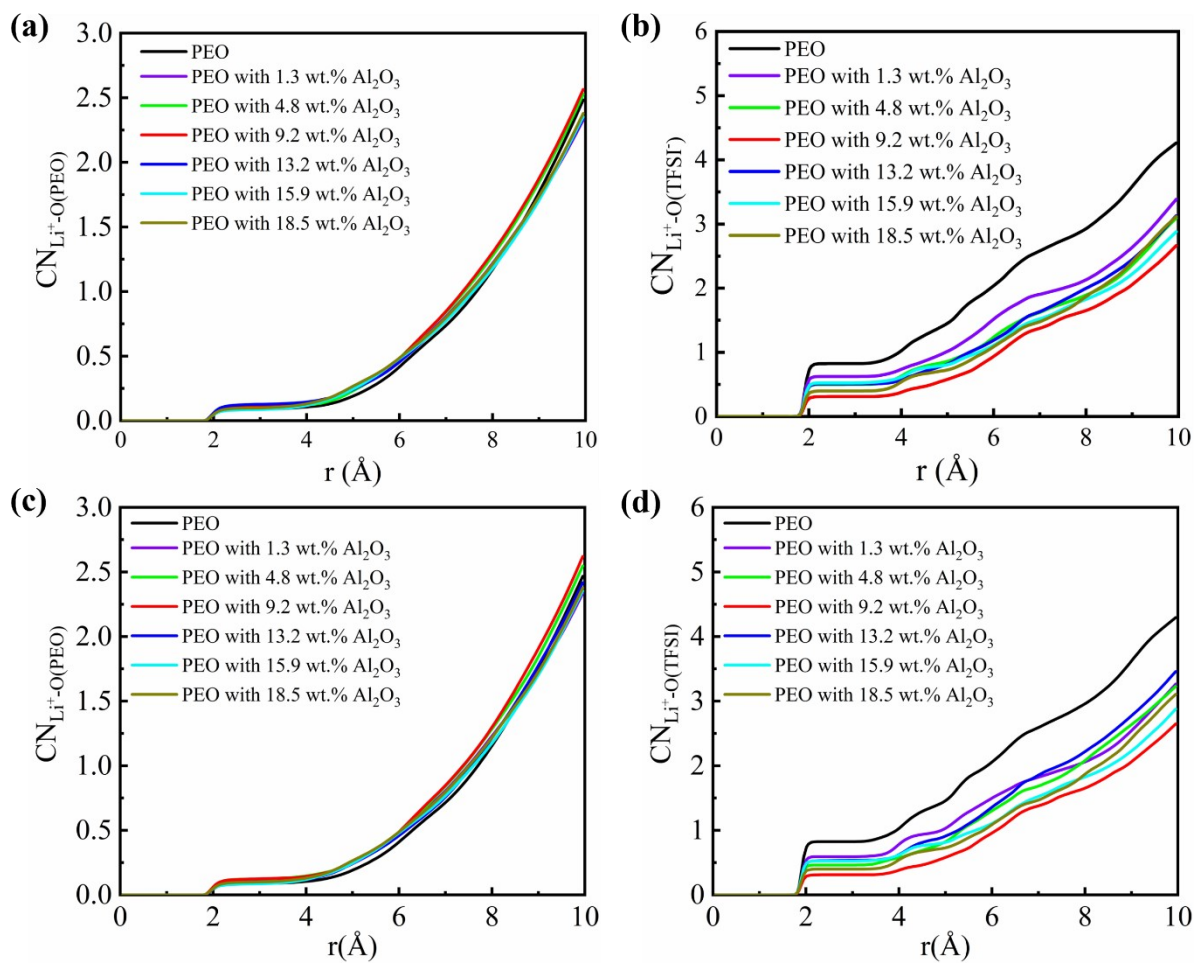


Figure S4. Coordination number (CN) for (a)  $\text{Li}^+\text{-O(PEO)}$  at 333 K, (b)  $\text{Li}^+\text{-O(TFSI)}$  at 333 K, (c)  $\text{Li}^+\text{-O(PEO)}$  at 300 K, and (d)  $\text{Li}^+\text{-O(TFSI)}$  at 300 K in the SC systems.

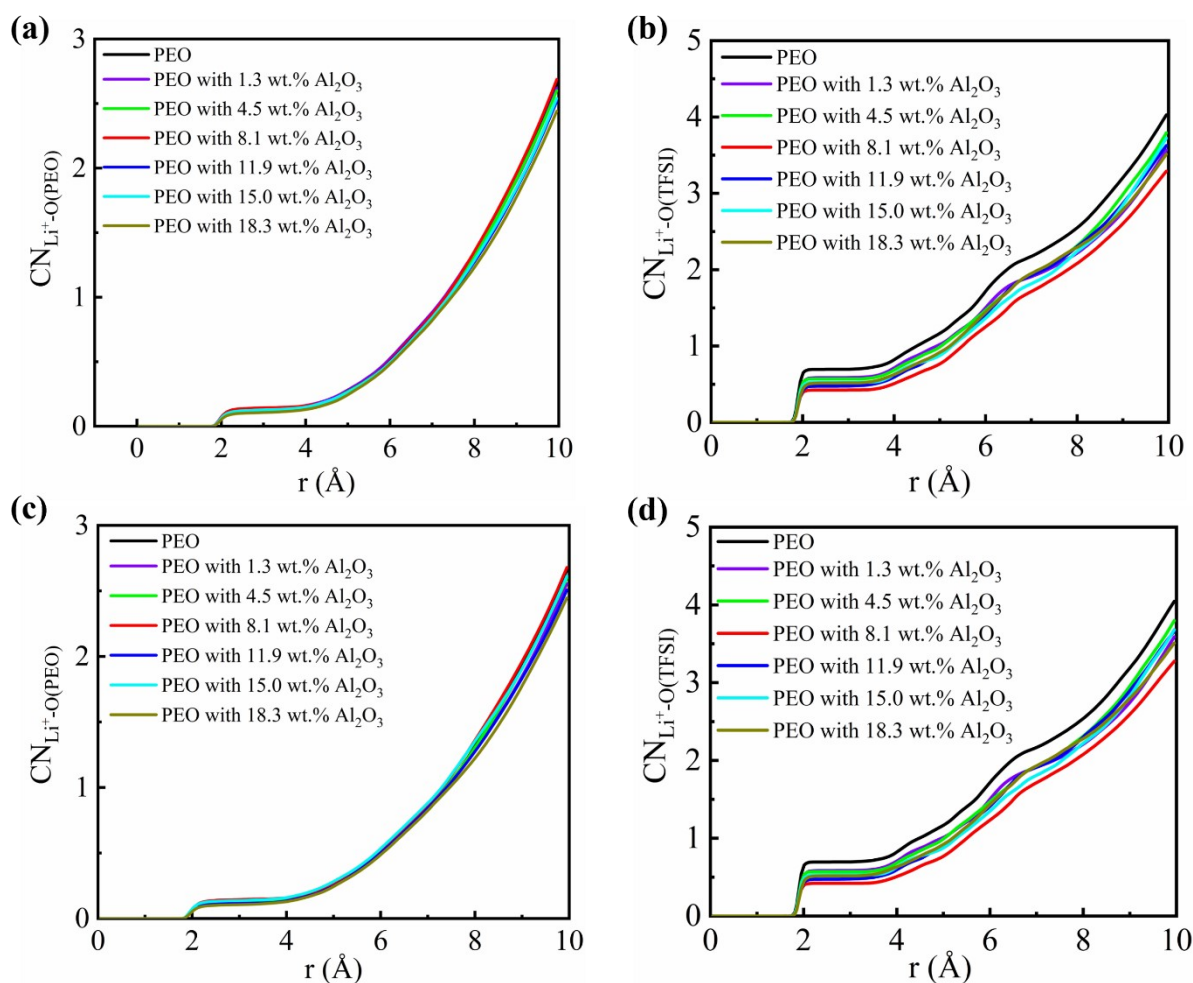


Figure S5. Coordination number (CN) for (a) Li<sup>+</sup>-O(PEO) at 333 K, (b) Li<sup>+</sup>-O(TFSI) at 333 K, (c) Li<sup>+</sup>-O(PEO) at 300 K, and (d) Li<sup>+</sup>-O(TFSI) at 300 K in the LC systems.

The CN of Li<sup>+</sup>-O (PEO) increases from 2.48 to 2.57 at 333 K and increases from 2.46 to 2.62 at 300 K in the SC system, which can explain the larger increase in the conductivity of SPE at 300 K than that at 333 K. The CN of Li<sup>+</sup>-O (PEO) increases from 2.61 to 2.67 at 333 K and increases from 2.60 to 2.72 at 300 K in the LC system.