Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Cell Volume-Wise Dopant Screening for Amorphous LiPON Solid State Electrolyte toward Improved Li-ion Mobility: An ab initio study

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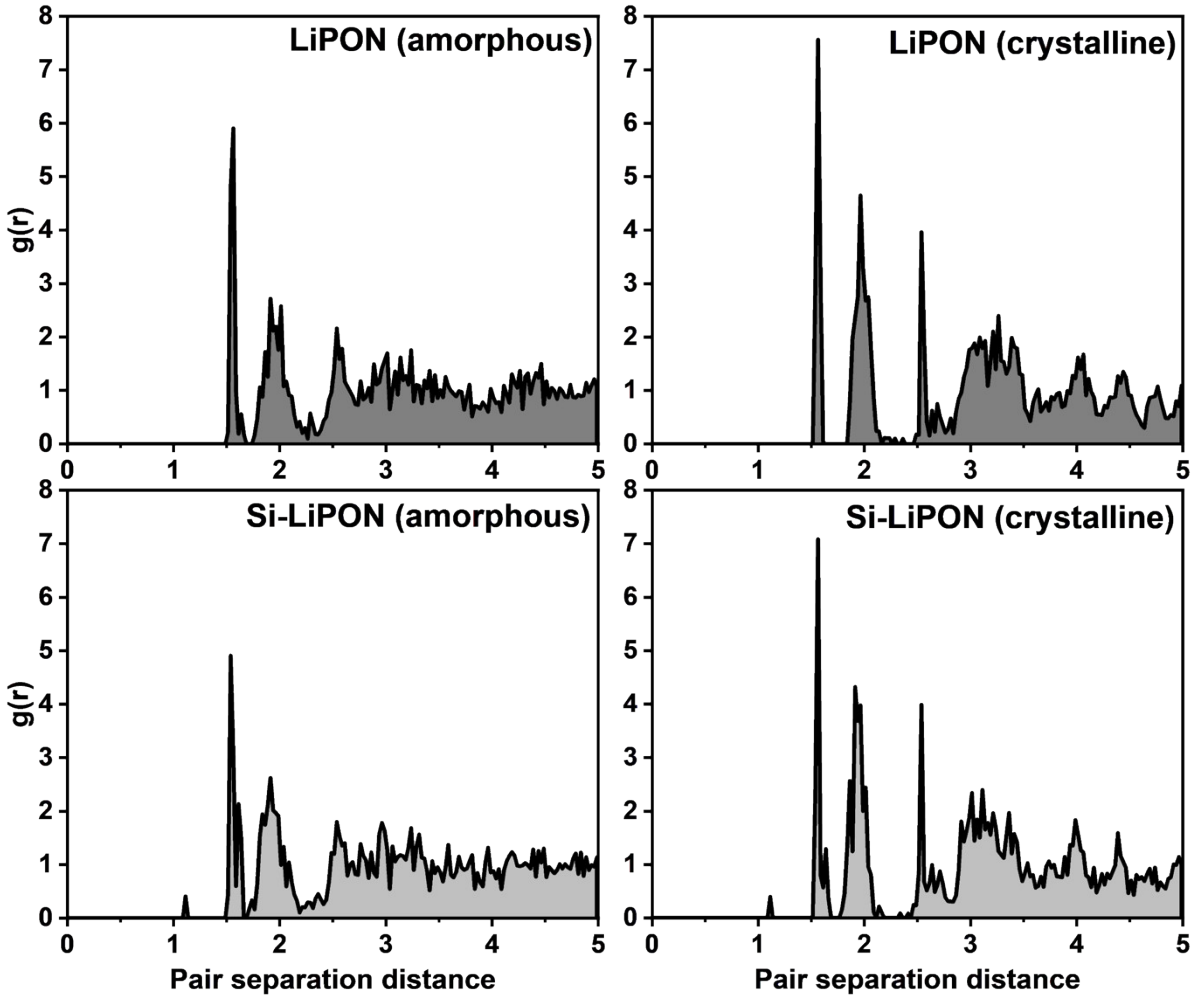

Figure S1. The radial distribution function g(r) of amorphous LiPON, Si-LiPON and crystalline LiPON, Si-LiPON.

The radial distribution function g(r) represents the mean number of atoms in a shell of width dr at distance r can be obtained by using following equation,

$$g(r) = p(r)(\rho 4\pi r^2\, dr)$$

where p(r) is the pair correlation function and ρ represent the atom density.[1] Crystalline LiPON and Si-LiPON showed more sharp lines than amorphous LiPON and Si-LiPON, indicating amorphization was well performed after ab initio molecular dynamics (AIMD) simulations at 3000 K.

Reference

(1) Lee, I.-H.; Chang, K. J. Crystal Structure Prediction in a Continuous Representative Space. *Computational Materials Science* **2021**, *194*, 110436. https://doi.org/10.1016/j.commatsci.2021.110436.