Supporting Information

Ionic Conductivity of LiSiON and the Effect of Amorphization / Heterovalent Doping on Li^+ Diffusion

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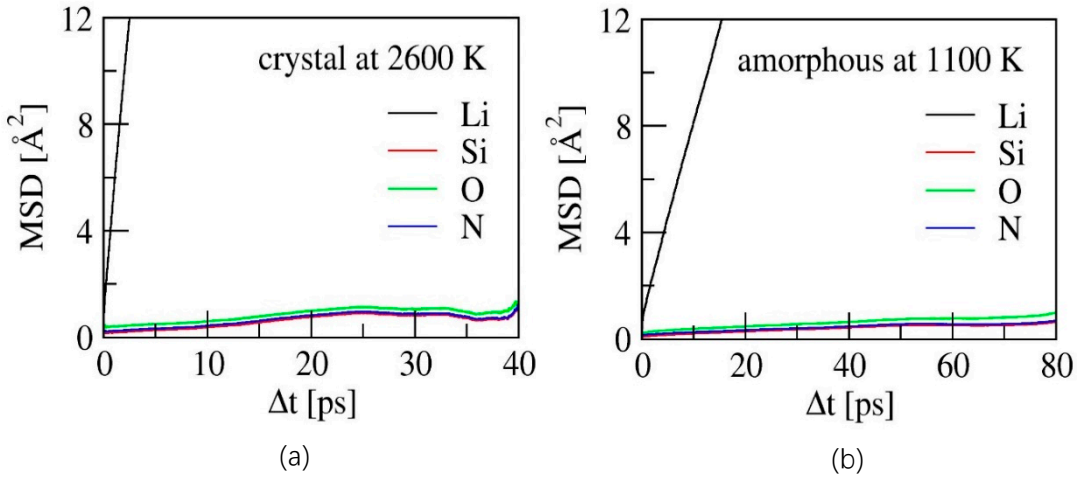

Figure S1. The mean-squared-displacements (MSD) for Li^{+}, Si^{4+}, O^{2-} and N^{3-} ions simulated by AIMD (a) for α-LiSiON at 2600 K and (b) for amorphous-LiSiON at 1100 K.

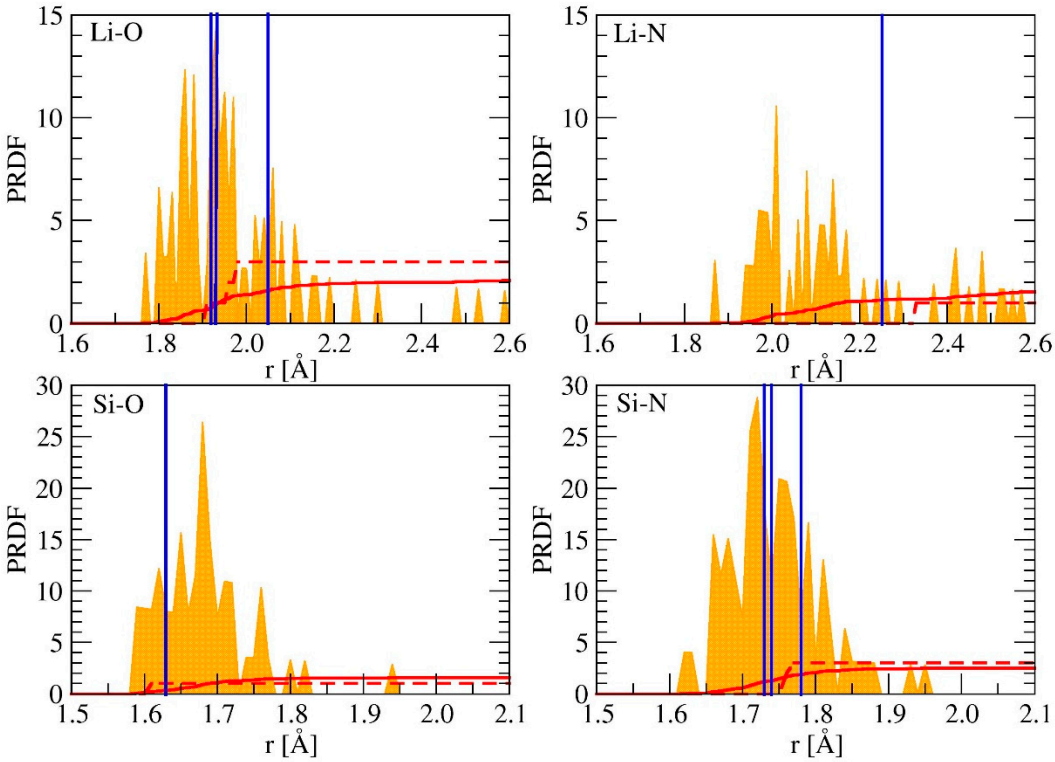

Figure S2. The partial radial distribution function (PRDF) for Li-O, Li-N, Si-O and Si-N pairs in amorphous-LiSiON. The pair correlation functions are shown in orange color and the integrated values for the PRDF are shown in red solid curves. For comparison, the integrated PRDFs for crystal α-LiSiON are given in red dashed curves, and the bond lengths appear in the crystal phase are labelled by perpendicular blue lines.

Table S1. The total energies (E_{tot}) of 16 configurations for $Li_{0.75}Si_{0.75}P_{0.25}ON$ and the Li^+ ion diffusion barriers evaluated by BV method (E_a by BV).

Configuration No.	E_{tot} [eV/f.u.]	E_a by BV [eV]	Configuration No.	E_{tot} [eV/f.u.]	E_a by BV [eV]
1	-26.679	0.72	9	-26.678	0.73
2	-26.670	0.80	10	-26.686	0.92
3	-26.678	0.73	11	-26.687	0.73
4	-26.686	0.92	12	-26.670	0.81
5	-26.670	0.80	13	-26.661	0.93
6	-26.680	0.73	14	-26.671	0.72
7	-26.676	0.91	15	-26.654	0.81
8	-26.678	0.73	16	-26.687	0.73

Table S2. The total energies (E_{tot}) of 12 configurations for $Li_{0.5}Si_{0.5}P_{0.5}ON$ and the Li^+ ion diffusion barriers evaluated by BV method (E_a by BV).

Configuration No.	E_{tot} [eV/f.u.]	E_a by BV [eV]	Configuration No.	E_{tot} [eV/f.u.]	E_a by BV [eV]
1	-25.164	0.88	7	-25.166	0.94
2	-25.163	0.97	8	-25.162	0.94
3	-25.142	1.05	9	-25.029	1.07
4	-25.121	0.93	10	-25.081	0.94
5	-25.166	1.21	11	-25.164	0.95
6	-25.150	1.02	12	-25.050	0.91

Table S3. The total energies (E_{tot}) of 4 configurations for $Li_{0.25}Si_{0.25}P_{0.75}ON$ and the Li^+ ion diffusion barriers evaluated by BV method (E_a by BV).

Configuration No.	E_{tot} [eV/f.u.]	E_a by BV [eV]	Configuration No.	E_{tot} [eV/f.u.]	E_a by BV [eV]
1	-23.373	1.20	3	-23.374	1.10
2	-23.367	1.34	4	-23.385	1.05

Table S4. The estimated value for the ionic conductivities at 300 K for crystal α-LiSiON, amorphous-LiSiON and P-doped LiSiON ($Li_{0.75}Si_{0.75}P_{0.25}ON$) according to the Arrhenius plot of diffusion coefficients represented in Figures 4b, 6b and 8, respectively.

Configurations	E_a [eV]	E_a error [eV]	Conductivity at 300K [mS/cm]
crystal α-LiSiON	1.59	0.24	2.5×10^{-20}
amorphous-LiSiON	0.18	0.08	8.1
P-doped LiSiON	0.44	0.16	3.9×10^{-3}