SUPPLEMENTARY INFORMATION

First-Principles Study on a New Chloride Solid Lithium-Ion Conductor Material with High Ionic Conductivity

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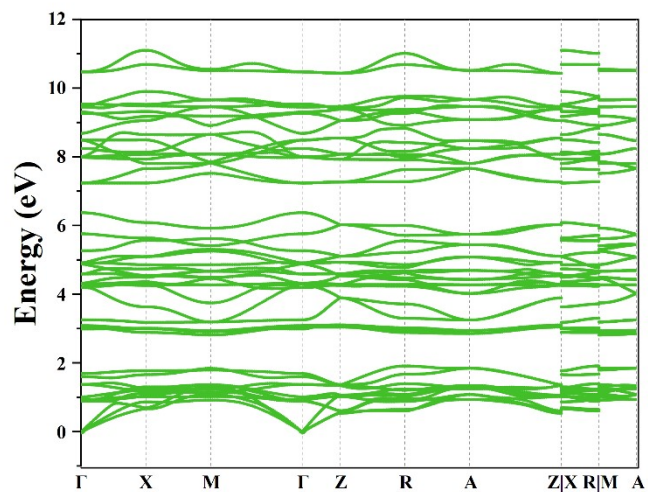
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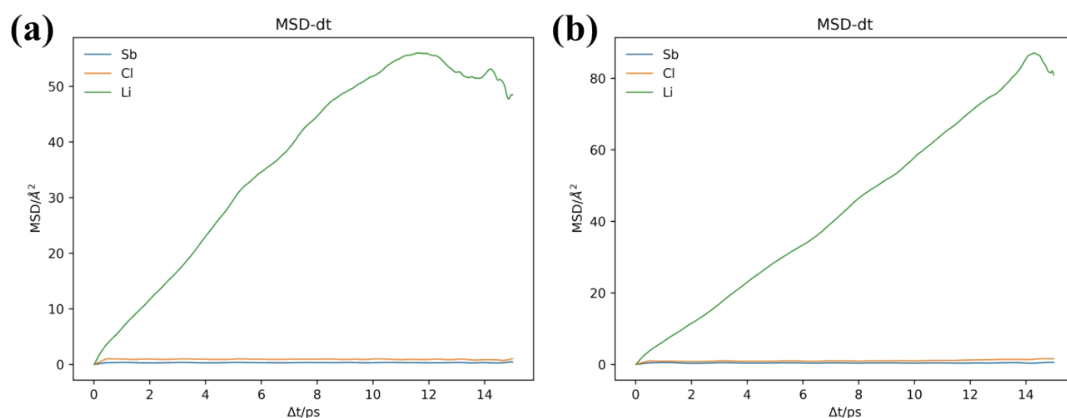**Fig. S1.** The phonon energy spectrum of LSC calculated using the DFPT method.

Fig. S2. MSD plots of 600K AIMD simulations in (a) 2×2×1 supercell and (b) 2×2×2 supercell of LSC, respectively.
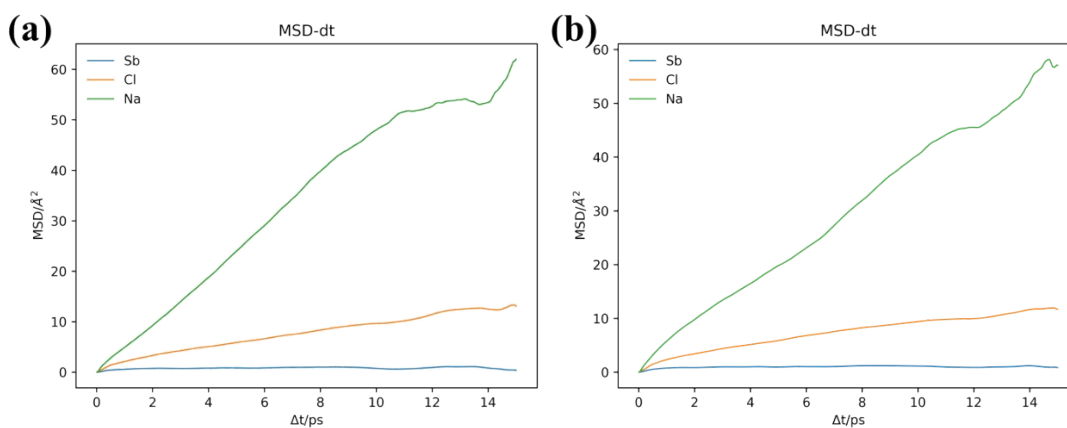
Fig. S3. MSD plots of 800K AIMD simulations in (a) 2×2×1 supercell and (b) 2×2×2 supercell of NSC, respectively.
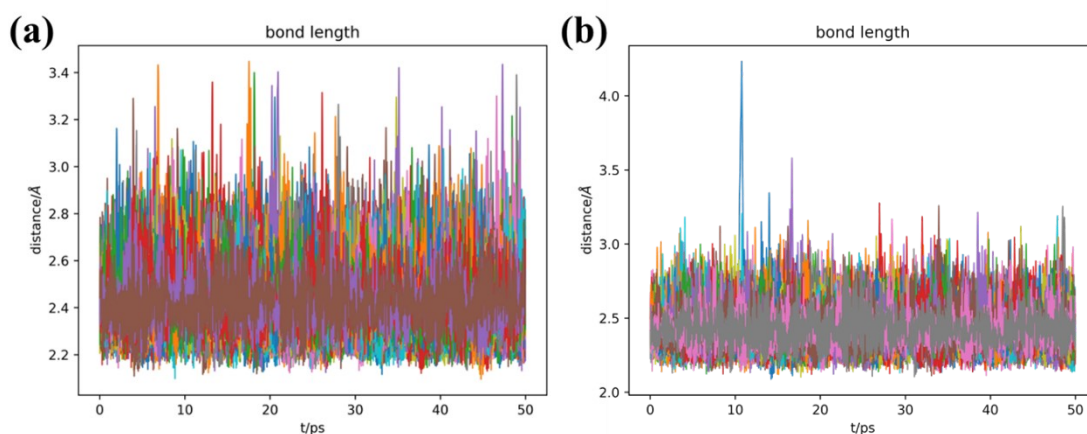

Fig. S4. Bond length analysis of 1000K AIMD simulations for all the Sb-Cl bonds in (a) LSC and (b) NSC
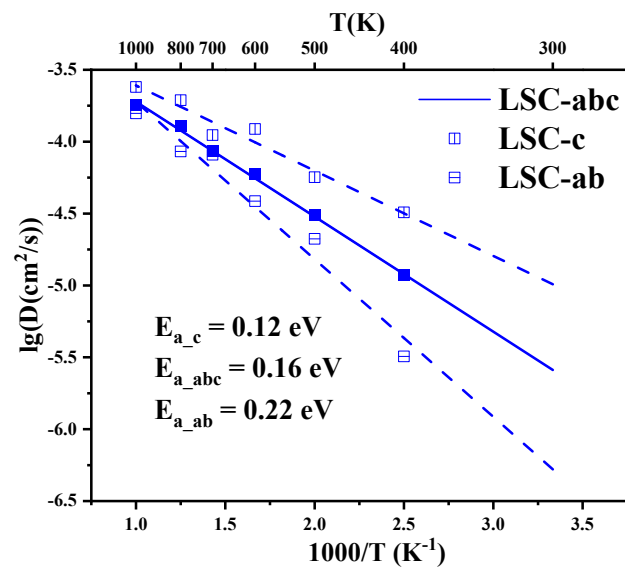
Fig. S5. The projected Arrhenius plots of diffusivity in LSC, along [001] direction, marked as LSC-c, and (001) planes, marked as LSC-ab.

Table S1. DFT fully relaxed LSC structural parameters, with interstitial sites denoted as Li_i. Space group: $P4_2/m$ (No. 84); Cell parameters: a = b = 6.4443 Å, c = 11.0519 Å.

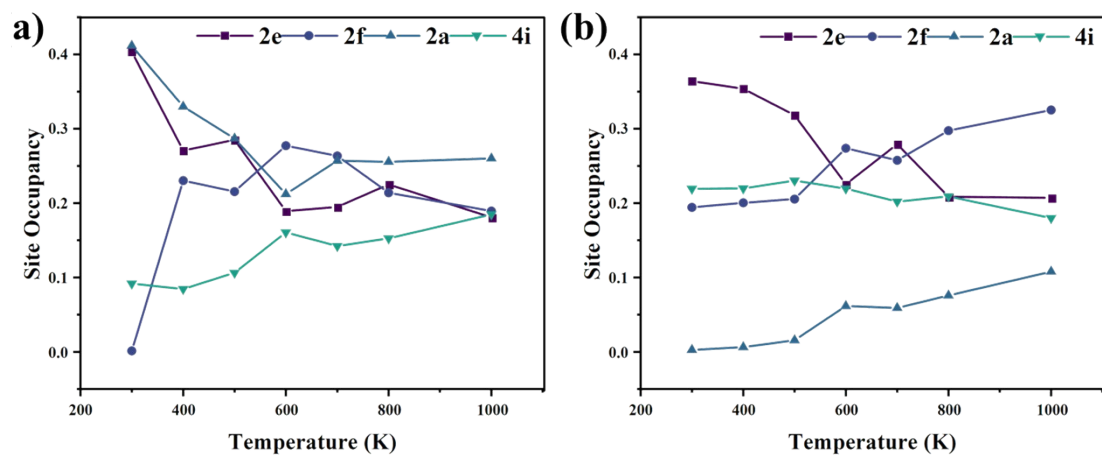| Atom	Wyckoff Site	x	y	z	Occupancy
Sb	2c	0.5000	0.0000	0.5000	1.0
Cl	4j	0.2587	0.2780	0.5000	1.0
Cl	8k	0.7006	0.1782	0.3441	1.0
Li	2e	0.0000	0.0000	0.7500	1.0
Li_i	2f	0.5000	0.5000	0.2500	-
Li_i	2a	0.0000	0.0000	0.0000	-
Li_i	4i	0.5000	0.0000	0.1500	-

Fig. S6. Site occupancy analysis for (a) Li of LSC and (b) Na of NSC in AIMD simulations at temperatures from 300K to 1000K

Table S2. The minimum distance between 2e Li sites and interstitial sites in LSC calculated by BV method.

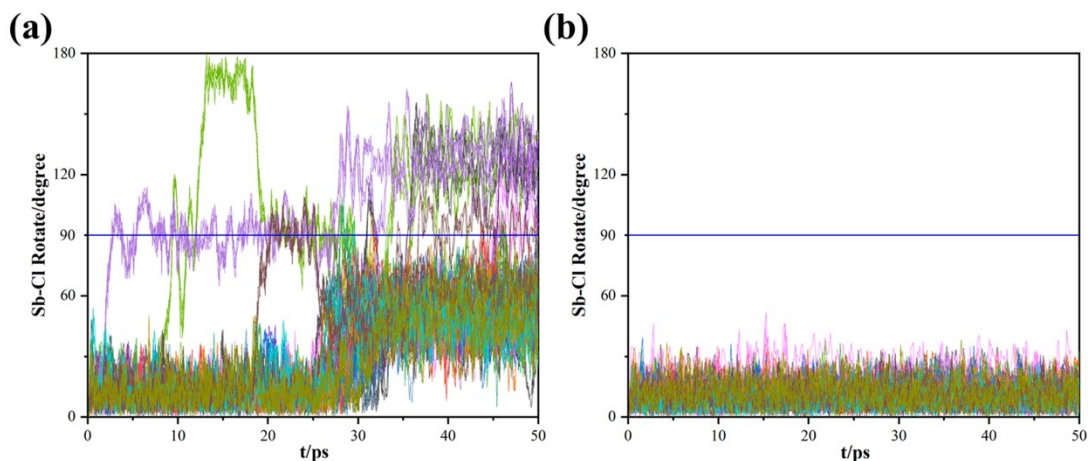| Sites	2e(self)	2a	2f	4i
Distance /Å	5.53	2.76	4.56	3.41

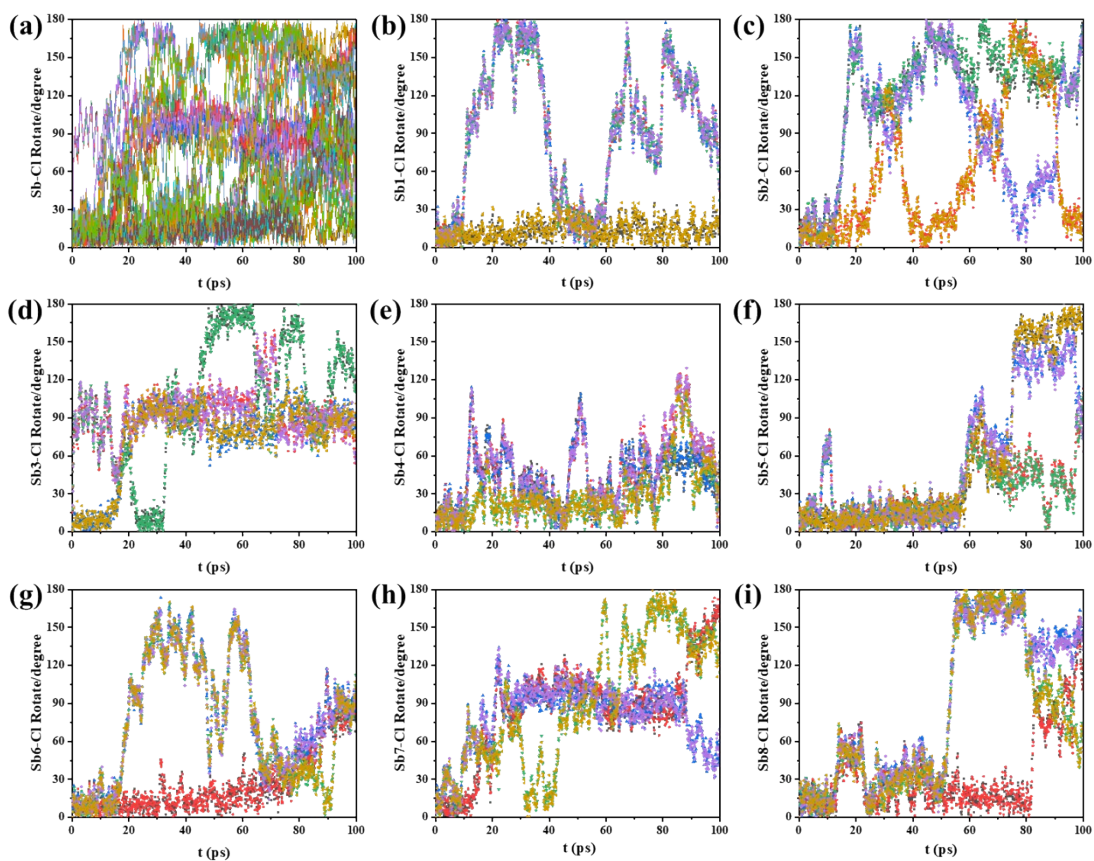**Fig. S7**. Sb-Cl bond rotate angle in LSC AIMD simulation at (a) 800K and (b) 400K.

Fig. S8. Sb-Cl bond rotate angle in NSC AIMD simulation at 500K, (a) for all bonds and (b-i) for each Sb centre, respectively.
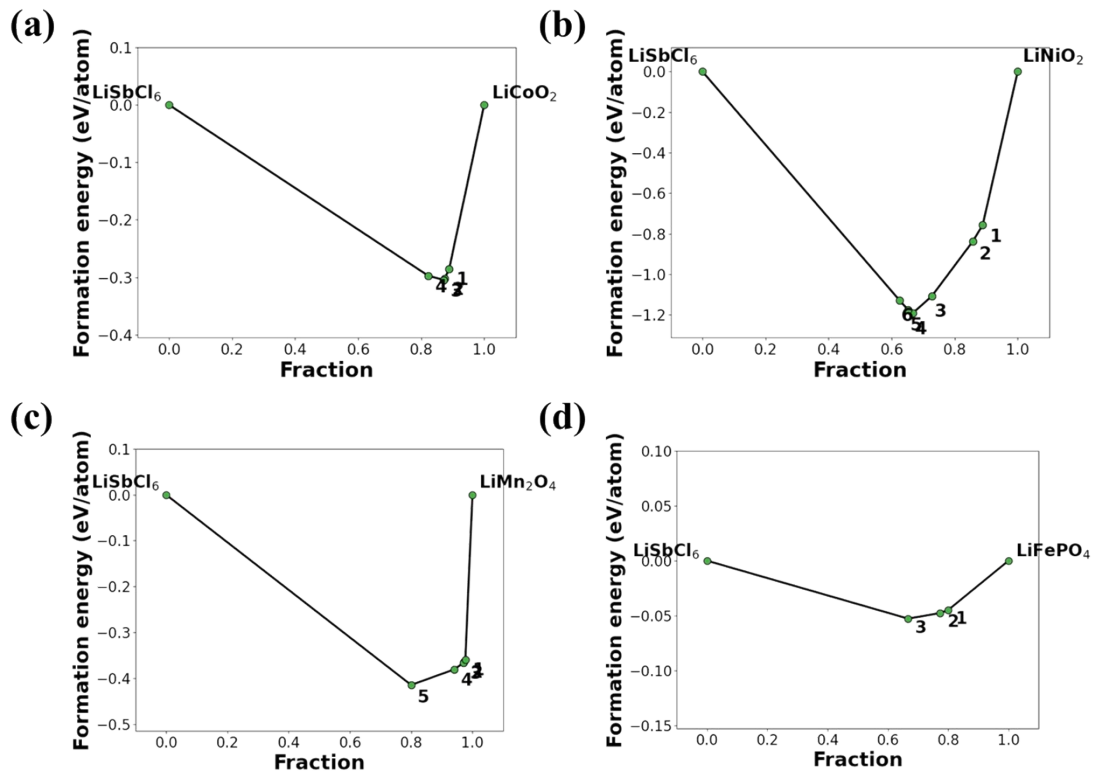
Fig. S9. Reaction phase diagrams between LSC and (a)LiCoO$_2$, (b)LiNiO$_2$, (c)LiMn$_2$O$_4$ and (d)LiFePO$_4$. Calculated with data from Materials Project.

Table S3. The independent elastic constants C_{ij} (GPa), bulk modulus B (GPa), shear modulus G (GPa), Young's modulus E (GPa), Poisson's ratio μ, and B/G ratio of LSC and NSC.

	C_{11}	C_{44}	C_{12}	B	G	E	μ	B/G
LSC	13.048	5.459	0.550	6.447	4.367	10.689	0.224	1.476
NSC	11.073	2.873	3.258	7.035	2.897	7.641	0.319	2.429