Supplementary Information

High-Throughput Discovery of $Li_3Sc_2(PO_4)_3$ as a Protective Coating for Stabilizing Mid-Ni NCM Interfaces in All-Solid-State Batteries

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Supporting figures and notes

Ionic conductivity calculation

To obtain the Li-ion diffusivity, we should have Mean-Squared Displacement (MSD). The MSD of mobile ions can be calculated from the average displacements over time duration t, where $r_i(t)$ is the position of a mobile ion.

$$MSD = \frac{1}{N}\sum_i \langle [r_i(t + t_0)]^2 - [r_i(t_0)]^2 \rangle \quad \text{(eq1)}$$

The diffusivity (D) can be calculated the movement of mobile ions per time from trajectories generated as a result of AIMD simulations.

$$D = \frac{1}{2dt} MSD \quad \text{(eq2)}$$

We can calculate the Li-ion diffusivity of specific temperature because ion diffusivity follows an Arrhenius relationship in no phase transition solid. After attaining each diffusivity of calculated temperatures, we extrapolated the Li-ion diffusivity of specific temperature from an Arrhenius fitting using equation (3).

$$D = D_0 exp\left(-\frac{Ea}{kT}\right) \quad \text{(eq3)}$$

Here, D_0 is diffusivity at infinite temperature, E_a is the activation energy of diffusion, k is the Boltzmann constant and T is the calculated temperature. E_a can calculate from the linear fitting of $\log(D)$ versus $1/T$. The ionic conductivity σ_T of a specific temperature can be obtained using the Li-ion diffusivity of specific temperatures from the Nernst-Einstein relation:

$$\sigma_T = \frac{\rho z^2 F^2}{RT} D_T \quad \text{(eq4)}$$

where ρ is the molar density of mobile ions in a unit cell, z is the charge of mobile ions, F is Faraday's constant, R is the gas constant, T is temperature and D_T is the Li-ion diffusivity of a specific temperature.

Electrochemical stability window calculation

The electrochemical stability window was determined using a methodology consistent with previous first-principles studies on solid-state electrolytes (SSEs).[1, 2] In this approach, electrochemical stability is evaluated by examining the phase behavior of the material under different lithium chemical potentials (μ_{li}), which correspond to a range of electrode voltage. To quantify this, we constructed grand potential phase diagrams at 0 K, which describe the thermodynamic stability of each compound in contact with lithium at a given chemical potential. For a given composition *c*, the grand potential Φ is defined as:

$$\Phi[\mathrm{c}, \mu_{li}] = E[c] - n_{Li}[c] \cdot \mu_{li} \quad \text{(eq5)}$$

where $E[c]$ is the DFT total energy of compound c, $n_{Li}[c]$ is the Li concentration of composition *c*. Phase stability is then evaluated by determining whether the compound lies on the lower convex hull of the grand potential diagram across a range of values (0 to -5 eV, corresponding to 0-7 V vs. Li/Li^+). Compounds that remain on the convex hull across a range of μ_{li} are considered stable within that interval. The upper and lower of this interval (μ_{ox}, μ_{red}) define the electrochemical stability window, which is converted to voltage using:

$$V_{red} = \frac{\mu^0_{Li} - \mu_{red}}{e} \quad \text{(eq6)}$$

$$V_{ox} = \frac{\mu^0_{Li} - \mu_{ox}}{e} \quad \text{(eq7)}$$

where μ^0_{Li} is the chemical potential of lithium metal and *e* is the elementary charge.

Chemical mixing reaction energy calculation

To evaluate the chemical compatibility between coating materials and SSEs or cathode interfaces, we calculated the chemical mixing reaction energy (ΔE_{mix}).[3] This thermodynamic descriptor quantifies the driving force for interfacial chemical reactions and indicates whether a spontaneous reaction is expected upon contact.

For two reactant phases *A* and *B*, the reaction energy was determined by identifying the most stable combination of reaction products that could form from their mixture. The mixing ratio $x \in [0, 1]$ was varied continuously, and the most favorable product configuration was obtained by minimizing the reaction energy:

$$\Delta E_{mix} = min_{x\in[0,1]}\{E_{pd}[xc_A + (1-x)c_B] - xE[c_A] - (1-x)E[c_B]\} \quad \text{(eq8)}$$

Here, c_A and c_B are the atomic compositions of materials *A* and *B*, normalized by the total number of atoms; $E[c_A]$ and $E[c_B]$ are their DFT total energies; and $E_{pd}[c]$ is the energy of the most stable decomposition phase (i.e., the convex hull energy) at composition *c*. The resulting ΔE_{mix} is expressed in units of eV/atom. A large negative ΔE_{mix} represents a strong thermodynamics tendency for reaction at the interface, potentially leading to the formation of electronically insulating or ion-blocking layers. Conversely, a value close to 0 suggests chemical compatibility.

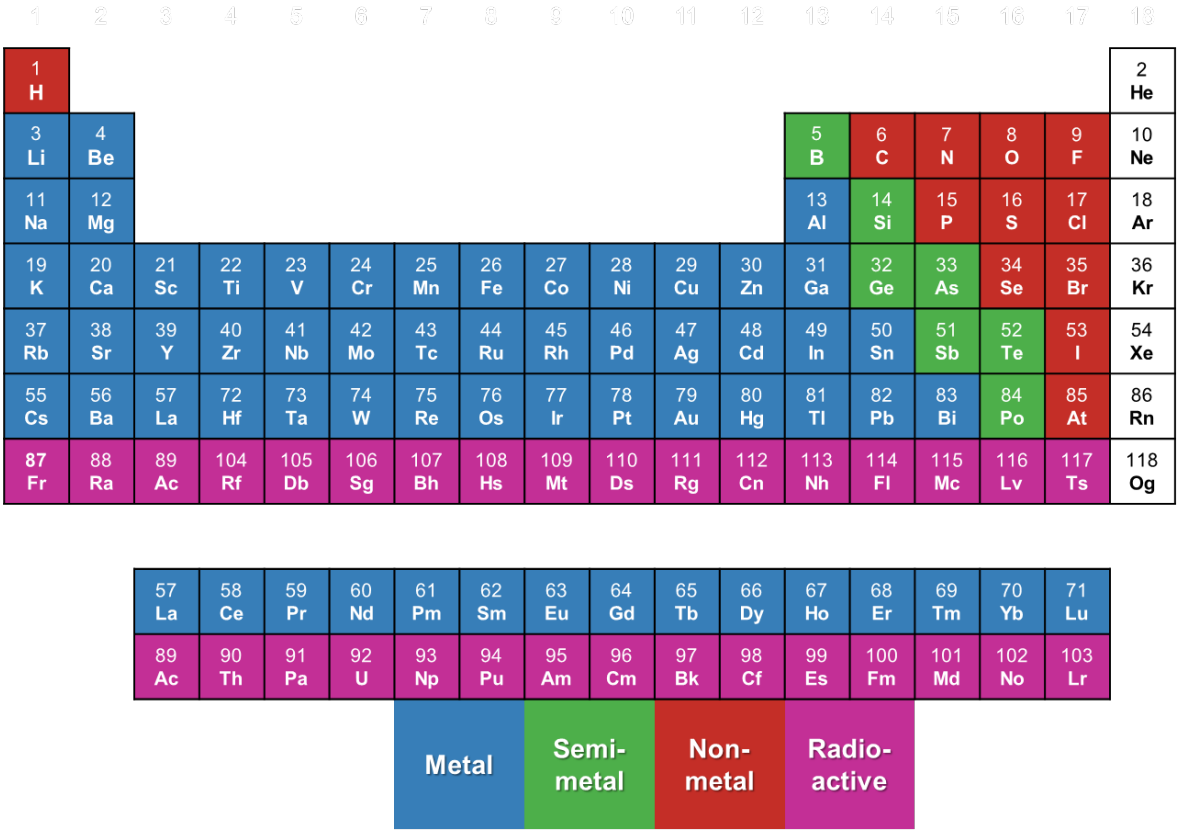

Figure S1. Categorized elements in the periodic table used for compositional classification in this study. Elements are grouped into four categories: metals (blue), semi-metals (green), non-metals (red), and radioactive elements (purple). Nobel gases are excluded from analysis due to their chemical inertness.

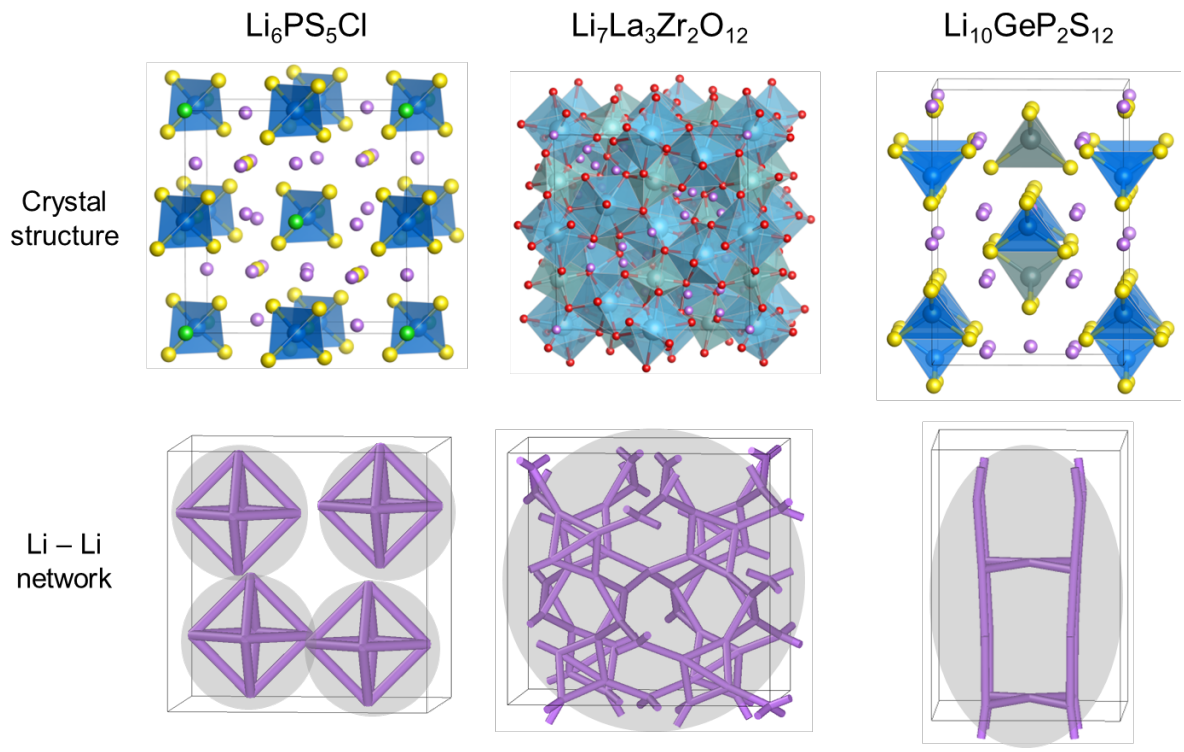

Figure S2. Representative solid-state electrolyte crystal structures (top) with high ionic conductivity and corresponding Li – Li connectivity networks (bottom): Li_6PS_5Cl, $Li_7La_3Zr_2O_{12}$, and $Li_{10}GeP_2S_{12}$. The Li–Li network is visualized to distinct ion transport pathway formed by Li–Li connections ($\leq$ 3.5 Å)

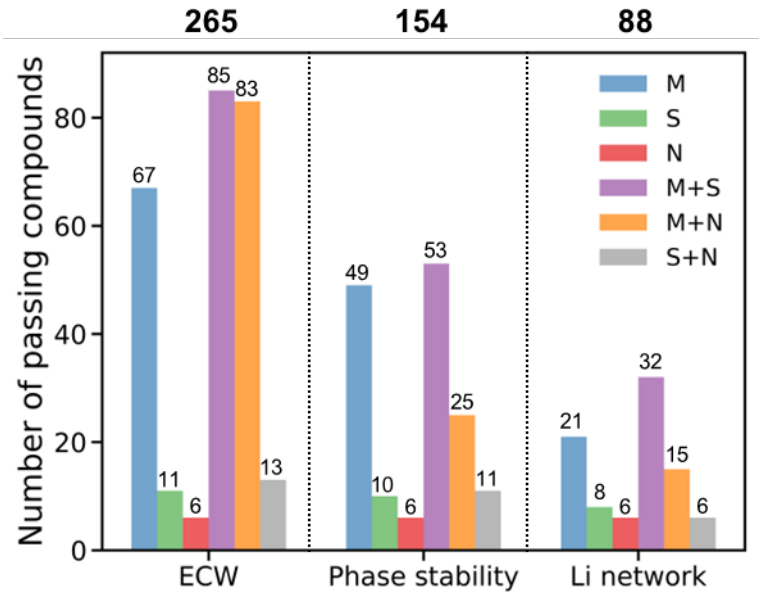

Figure S3. Histogram showing the number of candidates in each elemental category that pass through each filtering step in the high-throughput screening process. Blue, green, red, purple, orange, and gray bars represent materials containing metal (M), semi-metal (S), non-metal (N), metal + semi-metal (M+S), metal + non-mental (M+N), and semi-metal + non-metal (S+N), respectively, excluding Li and O.

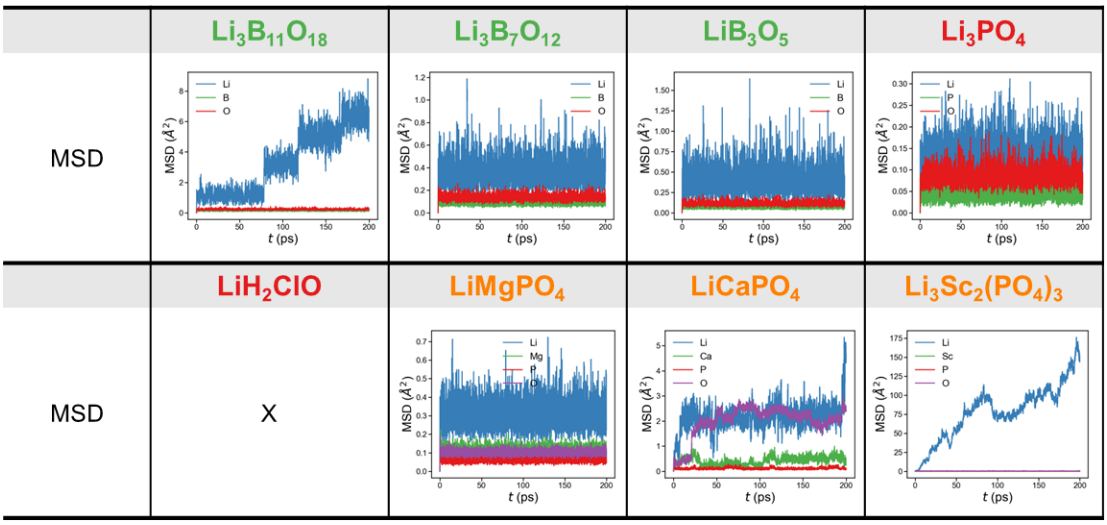

Figure S4. Mean squared displacement (MSD) of Li and framework atoms for 8 representative crystal structures, obtained from AIMD simulations during 200 ps at 1000 K. LiH_2ClO was excluded from the evaluation due to the detachment of H from H_2O.

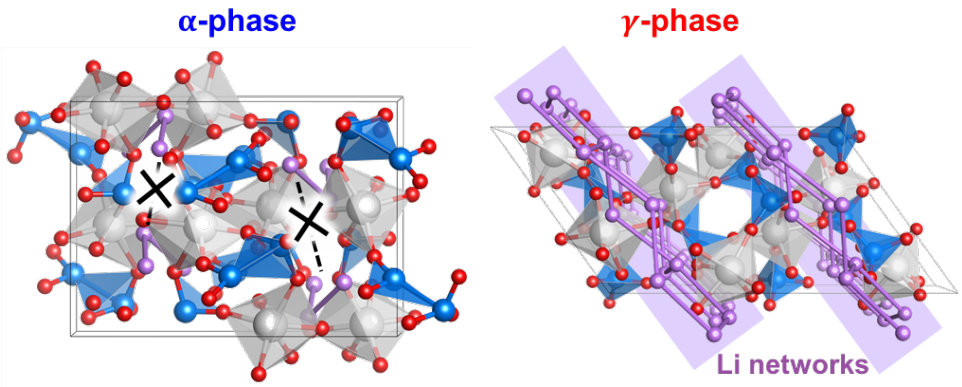

Figure S5. Li-ion networks pathway in two crystal structures for α- and γ-phases. The purple shaded regions highlight Li–Li networks within 3.5 Å.

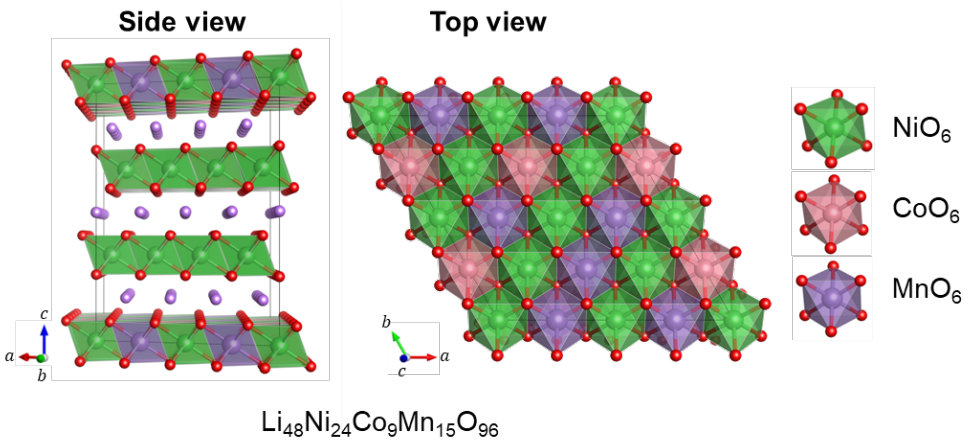

Figure S6. Crystal structure of $LiNi_{0.5}Co_{0.2}Mn_{0.3}O_2$ (NCM523) used in this study for molecular dynamics simulations, according to viewing perspective.

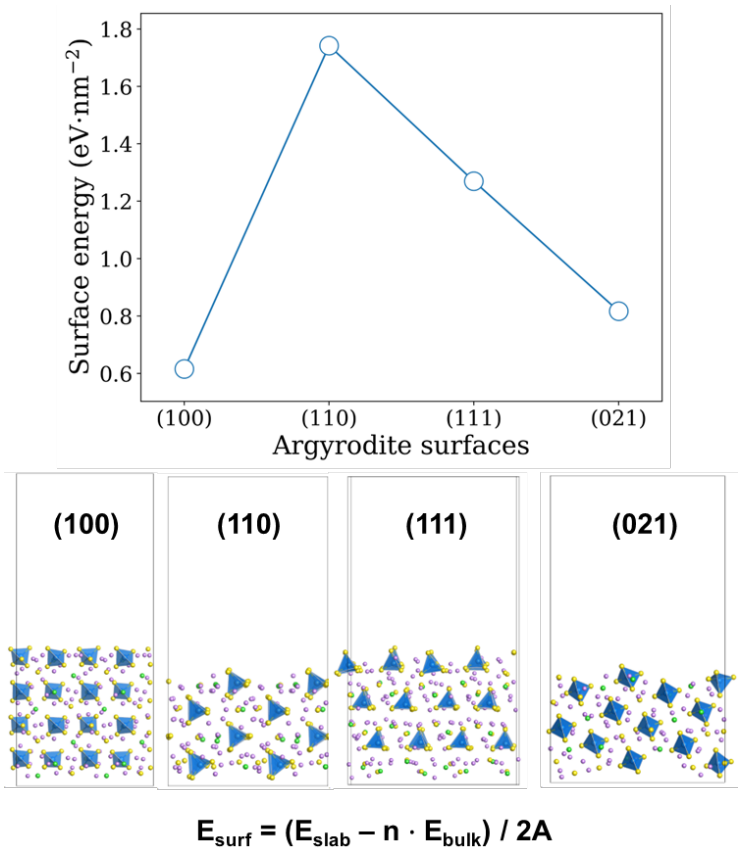

Figure S7. Calculated surface energies and models of Li_6PS_5Cl according to its surface indices.

Table S1. Representative 88 crystal structures screened in high-throughput screening process along with their database source, electrochemical window, interfacial stability, band gap, number of Li–Li networks, and max number of containing Li. Each category represents metal (M), semi-metal (S), non-metal (N), metal + semi-metal (M+S), metal + non-mental (M+N), and semi-metal + non-metal (S+N), respectively, excluding Li and O.

Composition	*Category*	*mp-ID*	*v1 (V)*	*v2 (V)*	*ECW (V)*	*ΔE_{rxn} NCM523 (meV/atom)*	*ΔE_{rxn} LPSC (meV/atom)*	*Band gap (eV)*	*Li networks (count)*	*Max number of Li (count)*
$Li_2BaTi_6O_{14}$	M	558083	*1.47*	*3.85*	*2.38*	*-7.56*	*-68.35*	*2.94*	*4*	*2*
$Li_2SrTa_2O_7$	M	558054	*1.09*	*3.55*	*2.46*	*0*	*-52.59*	*2.27*	*1*	*4*
$Li_2CaTa_2O_7$	M	1194523	*1.05*	*3.57*	*2.52*	*0*	*-50.15*	*2.81*	*2*	*4*
Li_2TiO_3	M	2931	*0.50*	*3.68*	*3.18*	*0*	*-60.12*	*3.03*	*1*	*8*
Li_3TaO_4	M	3151	*0.55*	*3.57*	*3.02*	*0*	*-47.80*	*4*	*1*	*12*
Li_3NbO_4	M	31488	*0.96*	*3.60*	*2.65*	*0*	*-96.12*	*3.84*	*1*	*12*
$Li_4Ti_5O_{12}$	M	685194	*1.74*	*3.68*	*1.94*	*-15.43*	*-64.44*	*2.72*	*1*	*8*
$Li_2Ti_4O_9$	M	772151	*1.74*	*3.68*	*1.94*	*-17.62*	*-65.98*	*2.89*	*2*	*2*
$Li_2Ti_3O_7$	M	1190132	*1.74*	*3.68*	*1.94*	*-16.45*	*-65.10*	*2.98*	*1*	*4*
$LiNdTiO_4$	M	10520	*0.55*	*3.54*	*2.99*	*0*	*-78.02*	*2.28*	*1*	*2*
$Li_{15}Ti_{11}Nb_5O_{42}$	M	767393	*1.82*	*3.68*	*1.87*	*-11.68*	*-82.74*	*2.27*	*2*	*4*

$LiLaTiO_4$	M	6521	*0.50*	*3.53*	*3.03*	*-78.45*	*-81.32*	*2.26*	*1*	*2*
$Li_2Ti_2O_5$	M	756294	*1.74*	*3.68*	*1.94*	*-7.84*	*-63.55*	*3.80*	*1*	*4*
$Li_7Ti_{12}Nb_{O_{30}}$	M	767146	*1.82*	*3.68*	*1.87*	*-10.84*	*-71.19*	*2.62*	*1*	*2*
$Li_4Ti_9O_{20}$	M	772090	*1.74*	*3.68*	*1.94*	*-11.95*	*-66.30*	*3.13*	*2*	*4*
$Li_{10}Ti_{11}Nb_{6}O_{42}$	M	767498	*1.82*	*3.68*	*1.87*	*0*	*-88.70*	*2.19*	*1*	*2*
$Li_4Ti_{11}O_{24}$	M	766548	*1.74*	*3.68*	*1.94*	*0*	*-66.77*	*2.57*	*1*	*3*
$Li_4Ba_4Ti_{19}O_{44}$	M	762032	*1.75*	*3.85*	*2.10*	*-1.43*	*-72.60*	*2.33*	*1*	*3*
$Li_7Ti_7Nb_5O_{30}$	M	767392	*1.82*	*3.68*	*1.87*	*0*	*-98.34*	*2.12*	*1*	*2*
$Li_4Ti_3O_8$	M	755266	*1.74*	*3.68*	*1.94*	*0*	*-62.23*	*2.17*	*1*	*4*
$Li_3Ta_7O_{19}$	M	772220	*1.59*	*3.93*	*2.34*	*-21.46*	*-45.05*	*2.87*	*2*	*3*
$Li_2Si_2O_5$	S	4117	*1.26*	*3.77*	*2.50*	*-14.85*	*0*	*5.15*	*1*	*4*
Li_2SiO_3	S	5012	*0.76*	*3.72*	*2.96*	*0*	*0*	*5.08*	*1*	*4*
$Li_3B_{11}O_{18}$	S	1020014	*1.93*	*4.41*	*2.48*	*-28.29*	*0*	*5.68*	*2*	*2*
$Li_3B_7O_{12}$	S	16828	*1.30*	*4.22*	*2.92*	*-11.70*	*0*	*5.70*	*2*	*3*
$LiBO_2$	S	14232	*1.07*	*3.66*	*2.59*	*0*	*0*	*7.28*	*1*	*2*
$Li_2B_4O_7$	S	4779	*1.29*	*3.66*	*2.37*	*-10.78*	*0*	*5.81*	*2*	*4*
$Li_2Si_3O_7$	S	555899	*1.32*	*3.77*	*2.45*	*-18.55*	*0*	*5.36*	*2*	*4*
LiB_3O_5	S	3660	*1.93*	*4.22*	*2.29*	*-21.15*	*0*	*6.48*	*2*	*2*

Li_3PO_4	N	13725	*0.69*	*4.19*	*3.51*	*0*	*0*	*5.82*	*1*	*6*
Li_2SO_4	N	4556	*1.63*	*4.65*	*3.02*	*0*	*-99.22*	*6.01*	*1*	*8*
Li_2CO_3	N	3054	*1.27*	*4.09*	*2.82*	*0*	*-83.80*	*5.06*	*1*	*4*
LiH_2BrO	N	754153	*1.55*	*3.68*	*2.12*	*-5.62*	*0*	*4.31*	*1*	*4*
$Li_2H_2SO_5$	N	23849	*1.99*	*4.40*	*2.41*	*0*	*-90.79*	*5.58*	*1*	*4*
LiH2ClO	N	760502	*1.54*	*4.07*	*2.53*	*0*	*-22.15*	*5.31*	*1*	*4*
$LiTmSiO_4$	M+S	15066	*0.84*	*3.65*	*2.81*	*0*	*0*	*4.87*	*2*	*2*
$LiYSiO_4$	M+S	558941	*0.74*	*3.61*	*2.87*	*0*	*-46.01*	*5.27*	*2*	*2*
$LiScSiO_4$	M+S	6224	*1.08*	*3.77*	*2.70*	*-3.15*	*0*	*4.61*	*2*	*2*
Li_2TiSiO_5	M+S	6332	*1.47*	*3.81*	*2.34*	*-7.0*	*0*	*3.22*	*1*	*4*
$LiSrBO_3$	M+S	10814	*0.32*	*3.54*	*3.23*	*0*	*-95.69*	*4.36*	*2*	*2*
$LiKSi_2O_5$	M+S	558102	*1.05*	*3.80*	*2.75*	*-6.02*	*0*	*4.71*	*1*	*2*
Li_3AlSiO_5	M+S	1020023	*0.64*	*3.62*	*2.98*	*0*	*0*	*4.94*	*1*	*12*
Li_2BeSiO_4	M+S	8070	*0.50*	*3.87*	*3.37*	*0*	*0*	*6.06*	*1*	*4*
$Li_3Gd(BO_3)_2$	M+S	559706	*0.78*	*3.52*	*2.74*	*0*	*-57.90*	*3.18*	*2*	*6*
Li_2MgSiO_4	M+S	11189	*0.52*	*3.71*	*3.20*	*0*	*0*	*4.76*	*1*	*8*
$Li_6Tm(BO_3)_3$	M+S	1211340	*0.88*	*3.51*	*2.63*	*0*	*-49.85*	*4.80*	*1*	*24*
$LiKB_4O_7$	M+S	6648	*1.16*	*3.74*	*2.58*	*-2.83*	*0*	*5.34*	*4*	*2*

$LiRbB_4O_7$	M+S	6787	*1.13*	*3.73*	*2.60*	*-2.77*	*0*	*5.14*	*4*	*2*
$Li_4Ca(BO_3)_2$	M+S	557467	*0.40*	*3.50*	*3.10*	*0*	*-73.07*	*4.73*	*2*	*4*
$Li_4Cs_3(BO_2)_7$	M+S	1019615	*0.91*	*3.59*	*2.68*	*0*	*-48.71*	*4.53*	*3*	*4*
$Li_3Sc(BO_3)_2$	M+S	557012	*0.95*	*3.56*	*2.61*	*0*	*-51.53*	*4.52*	*1*	*6*
$Li_4Cs(BO_2)_5$	M+S	1019716	*0.96*	*3.57*	*2.61*	*0*	*0*	*4.66*	*2*	*8*
$Li_5Cs_2(BO_2)_7$	M+S	1019607	*0.96*	*3.57*	*2.61*	*0*	*0*	*4.53*	*2*	*4*
$Li_6Rb_5(BO_2)_{11}$	M+S	1020620	*0.98*	*3.52*	*2.54*	*0*	*-59.13*	*4.51*	*1*	*6*
$Li_3Cs_2(BO_2)_5$	M+S	966802	*0.96*	*3.57*	*2.61*	*0*	*-48.20*	*4.54*	*2*	*3*
$Li_5Rb_2(BO_2)_7$	M+S	1020664	*1*	*3.54*	*2.54*	*0*	*0*	*4.63*	*2*	*4*
$Li_2Ca_2Si_5O_{13}$	M+S	560247	*1.32*	*3.77*	*2.45*	*-14.52*	*0*	*4.94*	*1*	*4*
$Li_2Ca_2Si_2O_7$	M+S	1020009	*0.81*	*3.56*	*2.74*	*0*	*-66.21*	*4.74*	*6*	*2*
$LiBeBO_3$	M+S	1020026	*1.07*	*3.66*	*2.59*	*-2.40*	*0*	*6.08*	*1*	*2*
Li_2AlBO_4	M+S	556655	*1.02*	*3.67*	*2.66*	*0*	*0*	*5.03*	*1*	*8*
$Li_5Al(SiO_4)_2$	M+S	1222486	*0.76*	*3.62*	*2.86*	*0*	*0*	*4.56*	*1*	*5*
$Li_2Mg_2Si_4O_{11}$	M+S	561336	*1.32*	*3.77*	*2.45*	*-16.81*	*0*	*5.13*	*2*	*2*
$Li_3Al(BO_3)_2$	M+S	6097	*1.07*	*3.66*	*2.59*	*0*	*0*	*4.82*	*1*	*6*
$Li_2Al_2SiO_6$	M+S	1222720	*1.10*	*3.68*	*2.58*	*0*	*0*	*4.63*	*1*	*2*
$Li_2Ti(BO_3)_2$	M+S	759926	*1.74*	*3.68*	*1.94*	*0*	*-42.51*	*2.95*	*2*	*4*

$Li_2MgSi_5O_{12}$	M+S	1222909	*1.32*	*3.77*	*2.45*	*0*	*-8.86*	*5.16*	*2*	*4*
$Li_3Co(BO_2)_5$	M+S	768669	*1.91*	*3.66*	*1.75*	*0*	*-39.91*	*3.05*	*2*	*4*
$Li_2Ta_2(OF_2)_3$	M+N	561011	*1.70*	*4.83*	*3.13*	*-57.34*	*-62.46*	*3.84*	*3*	*2*
$Li_3Sc_2(PO_4)_3$	M+N	6565	*1.86*	*4.19*	*2.33*	*-37.30*	*-24.69*	*4.76*	*2*	*6*
$LiMgPO_4$	M+N	9625	*1.58*	*4.18*	*2.61*	*-20.62*	*0*	*5.43*	*2*	*2*
Li_2NaPO_4	M+N	558045	*0.71*	*3.99*	*3.29*	*0*	*0*	*5.34*	*2*	*4*
$LiMnPO_4$	M+N	18997	*1.88*	*3.78*	*1.90*	*-64.81*	*-52.25*	*3.41*	*2*	*2*
$LiNa_5(PO_4)_2$	M+N	559452	*0.73*	*3.89*	*3.15*	*0*	*-74.06*	*4.52*	*4*	*2*
$LiCaPO_4$	M+N	16804	*1.17*	*4.08*	*2.91*	*0*	*-28.06*	*5.18*	*2*	*3*
$Li_3V(H_6O_5)_2$	M+N	1193122	*1.88*	*3.94*	*2.06*	*0*	*-90.80*	*4.07*	*1*	*3*
$Li_4Mn(PO_4)_2$	M+N	26081	*1.88*	*3.78*	*1.90*	*-44.07*	*0*	*4.13*	*1*	*16*
$Li_3Na_5Ti_5O_{14}$	M+N	774609	*1.40*	*3.60*	*2.20*	*0*	*-96.10*	*3.14*	*1*	*3*
$LiMn_4(PO_4)_3$	M+N	26393	*1.97*	*3.78*	*1.81*	*-76.64*	*-74.53*	*3.37*	*2*	*2*
$Li_5Mn_2(PO_4)_3$	M+N	849398	*1.88*	*3.78*	*1.90*	*-51.91*	*-41.63*	*4.11*	*1*	*20*
$Li_6Mn_9(PO_4)_8$	M+N	25923	*1.97*	*3.78*	*1.81*	*-69.51*	*-65.12*	*3.13*	*2*	*2*
$Li_4Mn_7(PO_4)_6$	M+N	849324	*1.97*	*3.78*	*1.81*	*-71.05*	*-67.11*	*2.98*	*1*	*3*
$Li_6Mn_3(PO_4)_4$	M+N	780723	*1.88*	*3.78*	*1.90*	*-55.39*	*-48.27*	*3.37*	*1*	*18*
$Li_2B_3O_4F_3$	S+N	1196457	*1.87*	*4.44*	*2.57*	*-62.11*	*0*	*6.57*	*2*	*4*

$Li_3B_5(HO_5)_2$	S+N	1199091	*1.66*	*3.86*	*2.20*	*-3.88*	*0*	*5.83*	*2*	*6*
$Li_{10}B_{14}Cl_2O_{25}$	S+N	23122	*1.26*	*3.52*	*2.25*	*-17.02*	*0*	*6.40*	*1*	*10*
$Li_4B_7ClO_{12}$	S+N	1222565	*1.37*	*4*	*2.62*	*-21.62*	*0*	*5.87*	*2*	*4*
$Li_2B_4H_4O_9$	S+N	604459	*1.91*	*3.83*	*1.92*	*-5.41*	*0*	*5.15*	*1*	*14*
$LiB_2H_3O_5$	S+N	24560	*1.91*	*3.83*	*1.92*	*-4.74*	*0*	*5.02*	*4*	*2*

Table S2. Representative 8 crystal structures screened in high-throughput screening process along with their database source, electrochemical window, thermodynamic stability, band gap, and Li – Li networks.

	mp-ID	*[V1, V2] ECW*	ΔE_{rxn} *w/. NCM523 (meV)*	ΔE_{rxn} *w/. LPSC (meV)*	*Band gap (eV)*	*N of Li networks*	*Max N of Li networks*
$Li_3Sc_2(PO_4)_3$	*mp-6565*	*[1.86, 4.19] 2.33*	*-37.30*	*-24.69*	*4.76*	*2*	*6*
$LiCaPO_4$	*mp-16804*	*[1.17, 4.08] 2.91*	*0*	*-28.06*	*5.18*	*2*	*3*
$LiMgPO_4$	*mp-9625*	*[1.58, 4.18] 2.61*	*-20.62*	*0*	*5.43*	*2*	*2*
LiH_2ClO	*mp-760502*	*[1.54, 4.07] 2.53*	*0*	*-22.15*	*5.31*	*1*	*4*
Li_3PO_4	*mp-13725*	*[0.69, 4.19] 3.51*	*0*	*0*	*5.82*	*1*	*6*
LiB_3O_5	*mp-3660*	*[1.93, 4.22] 2.29*	*-21.15*	*0*	*6.48*	*2*	*2*
$Li_3B_7O_{12}$	*mp-16828*	*[1.30, 4.22] 2.92*	*-11.70*	*0*	*5.70*	*2*	*3*
$Li_3B_{11}O_{18}$	*mp-1020014*	*[1.93, 4.41] 2.48*	*-28.29*	*0*	*5.68*	*2*	*2*

Table S3. Chemical reaction products of 8 representative candidates from the most favorable reactions at NCM523 and LPSC interfaces.

	Reaction products	
	NCM523	LPSC
$Li_3Sc_2(PO_4)_3$	$Mn(Ni_3O_4)_2$, Ni_3O_4, $Li_4MnCo_5O_{12}$, $Li_2Mn_3NiO_8$, Li_3PO_4, Sc_2O_3	$LiScS_2$, Li_3PS_4, Li_3PO_4, LiCl
$LiCaPO_4$	Stable	Li_3PS_4, Li_3PO_4, CaS, LiCl
$LiMgPO_4$	$Li_2MgMn_3O_8$, Ni_3O_4, $Li_4MnCo_5O_{12}$, Mg_6MnO_8, NiO, Li_3PO_4	Stable
LiH_2ClO	Stable	Li_3PS_4, Li_3PO_4, LiHS, LiCl
Li_3PO_4	Stable	Stable
LiB_3O_5	LiO_8, $Li_4MnCo_5O_{12}$, $Li_2Mn_3NiO_8$, Ni_3BO_5, $LiBO_2$	Stable
$Li_3B_7O_{12}$	LiO_8, $Li_4MnCo_5O_{12}$, $Li_2Mn_3NiO_8$, Ni_3BO_5, $LiBO_2$	Stable
$Li_3B_{11}O_{18}$	LiO_8, $Li_2Mn_3NiO_8$, Ni_3BO_5, $Co_3(BO_3)_2$, $Li_3B_7O_{12}$	Stable

Table S4. Lattice parameters and energy/atom of $Li_3Sc_2(PO_4)_3$ according to crystal structure phases. The crystal structures are shown in Figure 4(a).

	α-phase	γ-phase
Energy/atom (eV/atom)	-7.205	-7.565
a (Å)	8.8483	8.8290
b (Å)	12.2737	8.7980
c (Å)	8.7959	15.0495
γ (°)	90	125.6
Space group	$P2_1/c$	$P2_1/c$

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