Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supporting Information for: Materials Design Principles of Amorphous Cathode Coatings for Lithium-ion Battery Applications

Jianli Cheng,[†,‡] Kara D. Fong,[¶,‡] and Kristin A. Persson[*,†,‡]

†*Department of Materials Science and Engineering, University of California, Berkeley, CA 94720-1760, USA*

‡*Energy Storage and Distributed Resources Division, Lawrence Berkeley National Laboratory, Berkeley CA 94720, USA*

¶*Department of Chemical and Biomolecular Engineering, University of California, Berkeley, CA 94720-1760, USA*

E-mail: kapersson@lbl.gov

Overpotential (ΔV)

The relation between overpotential ΔV and $D_{\mathrm{rt}}^{\mathrm{Li}}$ can be derived from the Nernst-Planck equation for the flux of Li through the bulk electrolyte, J^{Li}:

$$J^{\mathrm{Li}} = -u^{\mathrm{Li}} c^{\mathrm{Li}} \frac{\mathrm{d}\phi}{\mathrm{d}x} - D_{\mathrm{rt}}^{\mathrm{Li}} \frac{\mathrm{d}c^{\mathrm{Li}}}{\mathrm{d}x} \ , \tag{1}$$

where u^{Li} is the electrophoretic mobility of the Li-ion and ϕ is the electric potential. From here, we assume (i) uniform concentration throughout the coating, such that $\frac{\mathrm{d}c^{\mathrm{Li}}}{\mathrm{d}x} = 0$, (ii) that the mobility and diffusion coefficient may be related by the Einstein relation ($D_{\mathrm{rt}}^{\mathrm{Li}} = \frac{u^{\mathrm{Li}} k_{\mathrm{B}} T}{q}$, where q is the elementary charge), and (iii) that the electric field in the coating is uniform such that $\frac{\mathrm{d}\phi}{\mathrm{d}x} = \Delta V / l_{\mathrm{c}}$, where l_{c} is the coating thickness. Eq. 1 thus reduces to

$$J^{\mathrm{Li}} = -\frac{q D_{\mathrm{rt}}^{\mathrm{Li}} c^{\mathrm{Li}} \Delta V}{k_{\mathrm{B}} T l_{\mathrm{c}}} \ . \tag{2}$$

Solving for the voltage difference ΔV yields

$$\Delta V = \frac{-J^{\mathrm{Li}} l_{\mathrm{c}} k_{\mathrm{B}} T}{D_{\mathrm{rt}}^{\mathrm{Li}} c^{\mathrm{Li}} q} \ . \tag{3}$$

Finally, we can relate the flux of Li-ions J^{Li} to the current density through the cathode coating J via $J = -q J^{\mathrm{Li}}$, giving

$$\Delta V = \frac{J l_{\mathrm{c}} k_{\mathrm{B}} T}{D_{\mathrm{rt}}^{\mathrm{Li}} c^{\mathrm{Li}} q^2} \ . \tag{4}$$

Electrochemical stability window

The electrochemical stability window consists of a reduction limit (V_{red}) at which the material starts lithiation during discharge and an oxidation limit ($-V_{\mathrm{ox}}$) at which the material starts delithiation/decomposition during charge. Here we take $LiAl_5O_8$, Al_2O_3 and B_2O_3 as examples to illustrate our method in calculating the electrochemical stability window of Li-containing and non-Li containing compounds. The lithiation compound of $LiAl_5O_8$ can

be directly identified from a Li-Al-O phase diagram, see Figure S1a. Its discharge reaction can be expressed as:

$$\frac{1}{3}\mathrm{LiAl_5O_8} + \mathrm{Li} \rightarrow \frac{4}{3}\mathrm{LiAlO_2} + \frac{1}{3}\mathrm{Al} \tag{5}$$

As all the reactants and products are in their solid phases, $V_{\mathrm{red}} = -\Delta G/zF = -\Delta H/zF =$ 0.8 V versus Li metal, where z is the number of electrons transferred in the reaction and F is the Faraday's constant. As $\mathrm{LiAl_5O_8}$ is a Li-containing compound, its delithiation takes place via a dissolution of $\mathrm{Li^+}$. From the Li-Al-O phase diagram, the delithiation reaction of $\mathrm{LiAl_5O_8}$ can be expressed as:

$$\mathrm{LiAl_5O_8} \rightarrow \mathrm{Li^+} + e^- + \frac{5}{2}\mathrm{Al_2O_3} + \frac{1}{4}\mathrm{O_2}(g) \tag{6}$$

As the reaction involves oxygen gas evolution, we include the entropy value of $\mathrm{O_2}$ taken from the JANAF tables.[1] Thus, $V_{\mathrm{ox}} = -\Delta G/zF = -(\Delta H - TS)/zF = -4.0$ V versus Li metal. Therefore, the electrochemical stability window of $\mathrm{LiAl_5O_8}$ can be estimated as: $[V_{\mathrm{red}}, -V_{\mathrm{ox}}]$=[0.8, 4.0].

Similar to $\mathrm{LiAl_5O_8}$, the lithiation compound of $\mathrm{Al_2O_3}$ can also be directly identified from a Li-Al-O phase diagram, see Figure S1b. Its discharge reaction can be expressed as:

$$\frac{8}{3}\mathrm{Al_2O_3} + \mathrm{Li} \rightarrow \mathrm{LiAl_5O_8} + \frac{1}{3}\mathrm{Al} \tag{7}$$

As all the reactants and products are in their solid phases, $V_{\mathrm{red}} = -\Delta G/zF = -\Delta H/zF =$ 1.3 V versus Li metal. As $\mathrm{Al_2O_3}$ is a non-Li containing compound, we assume its oxidation takes place via a dissolution of $\mathrm{Al^{3+}}$. From the Li-Al-O phase diagram, the decomposition reaction of $\mathrm{Al_2O_3}$ can be expressed as:

$$\mathrm{Al_2O_3} \rightarrow 2\mathrm{Al^{3+}} + 6e^- + \frac{3}{2}\mathrm{O_2}(g) \tag{8}$$

As the reaction involves oxygen gas evolution, we include the entropy value of $\mathrm{O_2}$. Thus,

$\Delta G_1 = \Delta H - TS = 16.18$ eV. Next, we add the standard free energy of Al^{3+} formation, ΔG_2, to ΔG_1.

$$Al \rightarrow Al^{3+} + 3e^- \tag{9}$$

$\Delta G_2 = -nFE^0_{Al^{3+}} = -4.99$ eV. n is the valence state of Al^{3+} and $E^0_{Al^{3+}}$ is the standard oxidation potential of Al^{3+} versus standard hydrogen electrode (SHE) taken from the IUPAC publication.[2]

$$Al_2O_3 \rightarrow 2Al^{3+} + 6e^- + \frac{3}{2}O_2(g) \tag{10}$$

$\Delta G_3 = \Delta G_1 + 2\Delta G_2 = 6.21$ eV. Next, we reference the above equation to Li/Li^+ to calculate the reaction potential with respect to the Li metal: $Li^+(aq) + e^- \rightarrow$Li:

$$Al_2O_3 + 6Li^+ \rightarrow 2Al^{3+} + 6Li + \frac{3}{2}O_2(g) \tag{11}$$

The standard oxidation potential of Li^+ is $E^0_{Li^+} = 3.04$ V versus SHE. Thus, $\Delta G_4 = \Delta G_3 + 6nFE^0_{Li^+} = 24.45eV$. Finally, the reaction potential V_{ox} can be obtained using the Nernst equation: $V_{ox} = -(\Delta G_4)/zF = -4.1$ V. Therefore, the electrochemical stability window of Al_2O_3 can be estimated as: $[V_{red}, -V_{ox}]$=[1.3, 4.1].

The lithiation compound of B_2O_3 can be directly identified from a Li-B-O phase diagram, see Figure S1c. Its discharge reaction can be expressed as:

$$\frac{97}{8}B_2O_3 + 3Li \rightarrow Li_3B_{11}O_{18} + \frac{9}{48}B_6O \tag{12}$$

As all the reactants and products are in their solid phases, $V_{red} = -\Delta G/zF = -\Delta H/zF =$ 2.2 V versus Li metal. As B_2O_3 is a non-Li containing compound, we assume its oxidation takes place via a dissolution of B^{3+}. However, B dissolution involves the presence of H_2O: $B(s)+3H_2O=B(OH)_3(aq)+3H^++3e^-$, which complicates the dissolution mechanism and requires additional assumptions, such as the abundance of H_2O in a battery cell. Therefore, the oxidation limit of B_2O_3 is estimated using the $|V_{ox}|$ value of $Li_3B_{11}O_{18}$. From the Li-B-O

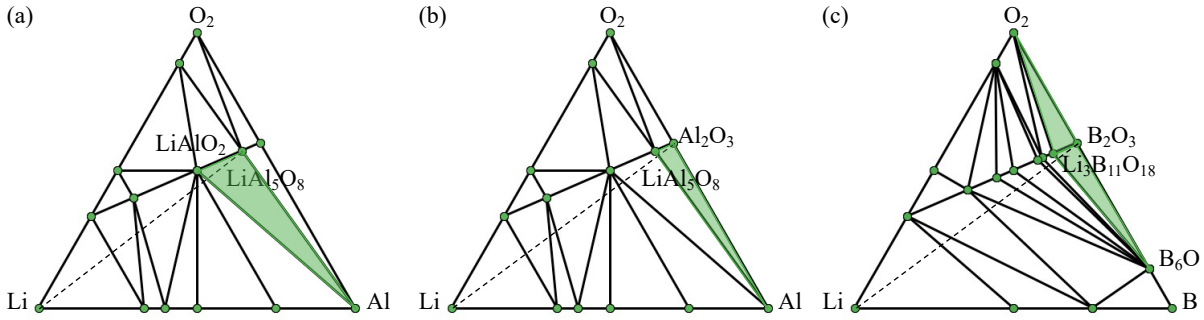

Figure S1: Li-Al-O phase diagrams. (a) The first phase-region (green triangle) formed by $LiAl_5O_8$, $LiAlO_2$ and Al for $LiAl_5O_8$ lithiation. The dash line represents the lithiation path of $LiAl_5O_8$. (b) The first phase-region (green triangle) formed by $LiAl_5O_8$, Al_2O_3 and Al for Al_2O_3 lithiation. The dash line represents the lithiation path of Al_2O_3. (c) The first phase-region (green triangle) formed by $Li_3B_{11}O_{18}$, B_2O_3 and B_6O for B_2O_3 lithiation. The dash line represents the lithiation path of B_2O_3.

phase diagram, the delithiation reaction of $Li_3B_{11}O_{18}$ can be expressed as:

$$LiB_{11}O_{18} \rightarrow 3Li^+ + 3e^- + \frac{11}{2}B_2O_3 + \frac{3}{4}O_2(g) \tag{13}$$

As the reaction involves oxygen gas evolution, we include the entropy value of O_2. Thus, $V_{ox} = -\Delta G/zF = -(\Delta H - TS)/zF = -4.3$ V versus Li metal. Therefore, the electrochemical stability window of B_2O_3 can be estimated as: $[V_{red}, -V_{ox}]$=[1.3, 4.3].

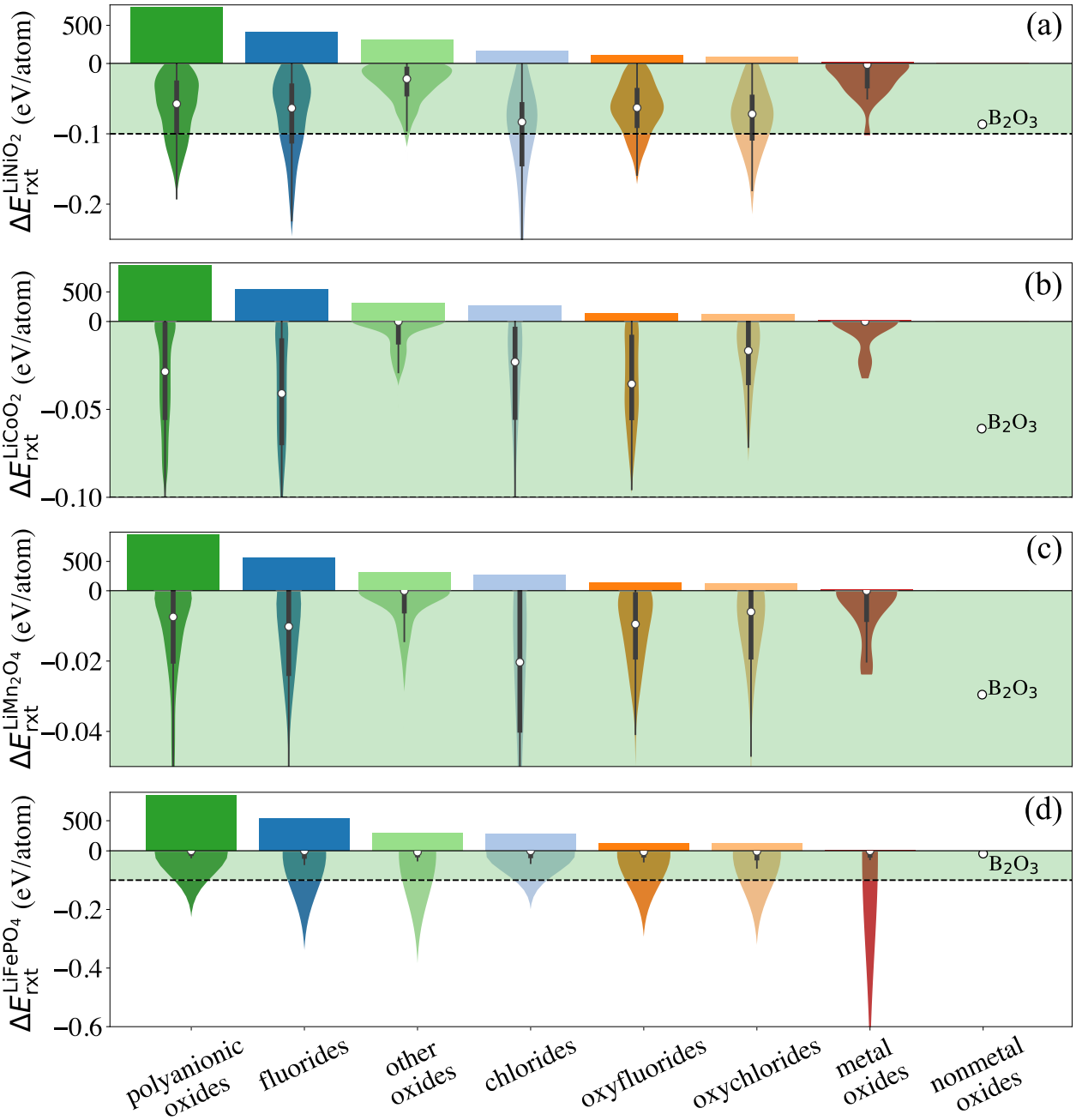

Figure S2: Distribution of the reaction energy ΔE_{rxt} with (a)$LiNiO_2$, (b)$LiCoO_2$, (c)$LiMn_2O_4$, and (d)$LiFeOP_4$ cathodes for each category that pass electrochemical stability descriptor. The horizontal dash lines represent the limits of ΔE_{rxt}. The histograms illustrate the numbers of compounds for each category that pass the descriptors, $\Delta E_{\text{rxt}} \geq -0.1$ eV/atom.

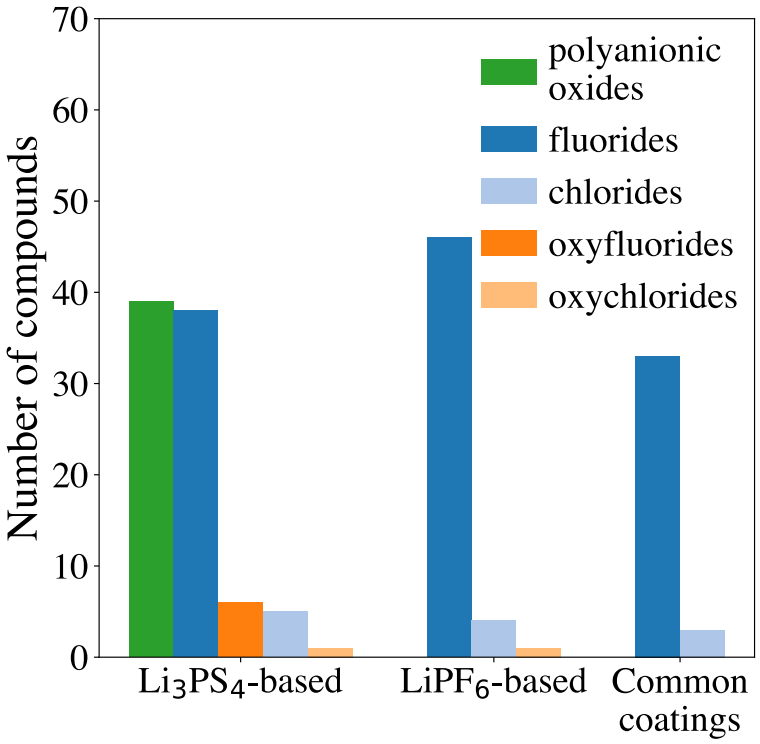

Figure S3: Histogram of the number of Li containing compounds for each category that pass the phase stability, electrochemical stability, and chemical stability descriptors in the computational screening.

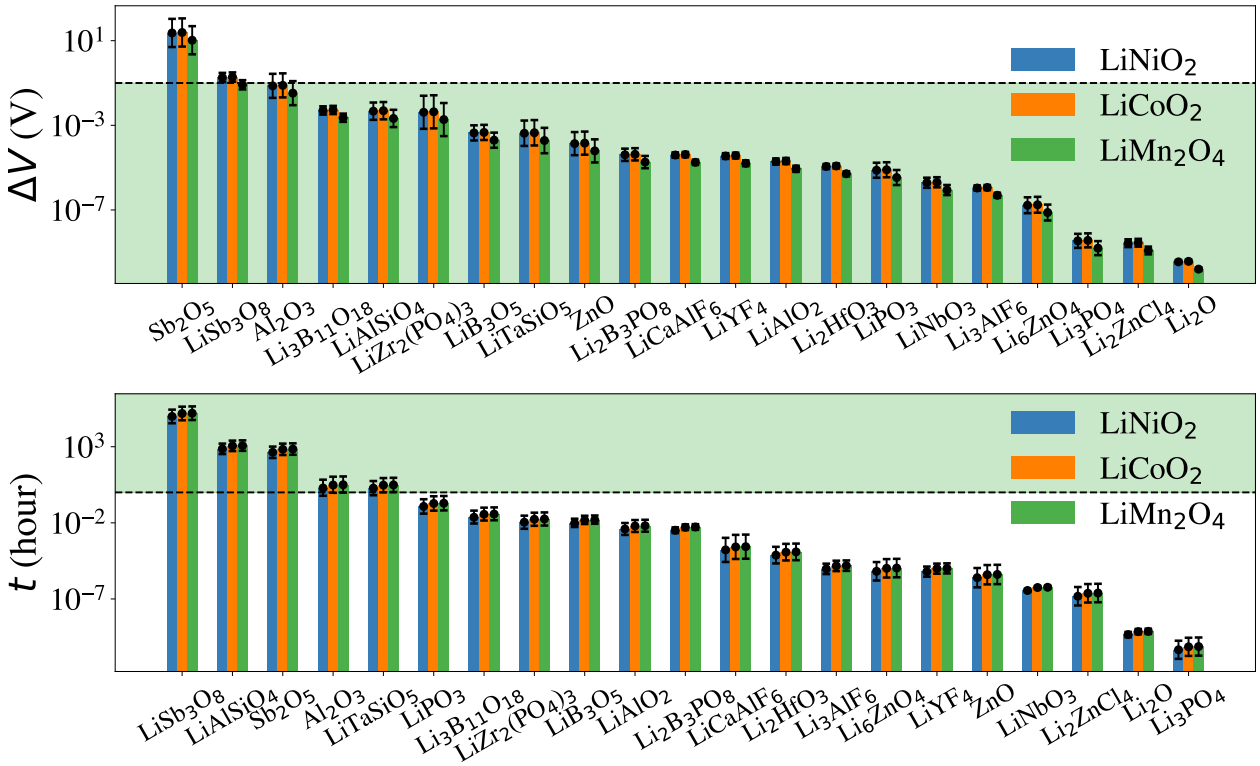

Figure S4: Calculated (a) overpotentials ΔV and (b) oxygen diffusion time t across room temperature 1 nm cathode coatings in $LiNiO_2$, $LiCoO_2$ and $LiMn_2O_4$ cathodes. The dashed lines in (a) and (b) represent$\Delta V = 0.1$ V and $t = 1$ h, respectively. We assume an $r = 1$ μm cathode particle and an $l_s = 2$ nm surface rocksalt phase.

Table S1: Calculated activation energy E_a, extrapolated room temperature diffusivity D_{rt}, conductivity C_{rt} and Onsager transport coefficient L^{LiLi} for Li^+ diffusion.

Composition	E_a^{Li} (eV)	$D_{\mathrm{rt}}^{\mathrm{Li}}$ (cm^2/s)	$D_{\mathrm{rt}}^{\mathrm{Li}}$ error bound	$C_{\mathrm{rt}}^{\mathrm{Li}}$ (mS/cm)	$C_{\mathrm{rt}}^{\mathrm{Li}}$ error bound	$L_{\mathrm{rt}}^{\mathrm{LiLi}}$ ($eV^{-1}cm^{-1}s^{-1}$)	$L_{\mathrm{rt}}^{\mathrm{LiLi}}$ error bound
Li_3AlF_6	0.48±0.02	1.96×10^{-11}	1.49×10^{-11}, 2.59×10^{-11}	4.01×10^{-3}	3.05×10^{-3}, 5.29×10^{-3}	2.30×10^{13}	1.74×10^{13}, 3.05×10^{13}
$LiCaAlF_6$	0.55±0.02	1.29×10^{-12}	9.69×10^{-13}, 1.71×10^{-12}	1.11×10^{-4}	8.33×10^{-5}, 1.47×10^{-4}	6.55×10^{11}	4.90×10^{11}, 8.74×10^{11}
Li_2ZnCl_4	0.3±0.03	2.41×10^{-8}	1.58×10^{-8}, 3.69×10^{-8}	1.63	1.07, 2.48	1.02×10^{16}	5.96×10^{15}, 1.76×10^{16}
$LiYF_4$	0.55±0.02	1.14×10^{-12}	8.32×10^{-13}, 1.55×10^{-12}	1.23×10^{-4}	9.03×10^{-5}, 1.69×10^{-4}	7.54×10^{11}	5.47×10^{11}, 1.04×10^{12}
$LiAlSiO_4$	0.68±0.06	1.16×10^{-14}	4.52×10^{-15}, 2.97×10^{-14}	9.37×10^{-7}	3.66×10^{-7}, 2.40×10^{-6}	5.77×10^{9}	2.37×10^{9}, 1.40×10^{10}
$Li_3B_{11}O_{18}$	0.68±0.03	1.42×10^{-14}	9.04×10^{-15}, 2.22×10^{-14}	8.67×10^{-7}	5.54×10^{-7}, 1.36×10^{-6}	5.79×10^{9}	3.94×10^{9}, 8.50×10^{9}
$LiZr_2(PO_4)_3$	0.64±0.11	3.75×10^{-14}	6.20×10^{-15}, 2.27×10^{-13}	1.06×10^{-6}	1.75×10^{-7}, 6.39×10^{-6}	5.84×10^{9}	9.49×10^{8}, 3.60×10^{10}
Li_3PO_4	0.32±0.04	6.51×10^{-9}	3.03×10^{-9}, 1.40×10^{-8}	1.26	5.87×10^{-1}, 2.7	7.29×10^{15}	3.25×10^{15}, 1.63×10^{16}
LiB_3O_5	0.61±0.05	1.36×10^{-13}	5.94×10^{-14}, 3.09×10^{-13}	9.98×10^{-6}	4.37×10^{-6}, 2.28×10^{-5}	5.92×10^{10}	2.60×10^{10}, 1.35×10^{11}
$Li_2B_3PO_8$	0.55±0.04	1.25×10^{-12}	6.39×10^{-13}, 2.43×10^{-12}	1.08×10^{-4}	5.54×10^{-5}, 2.11×10^{-4}	6.63×10^{11}	3.50×10^{11}, 1.26×10^{12}
$LiPO_3$	0.51±0.05	5.54×10^{-12}	2.45×10^{-12}, 1.26×10^{-11}	5.80×10^{-4}	2.56×10^{-4}, 1.31×10^{-3}	3.57×10^{12}	1.57×10^{12}, 8.11×10^{12}
$LiAlO_2$	0.54±0.02	1.51×10^{-12}	1.08×10^{-12}, 2.11×10^{-12}	2.25×10^{-4}	1.61×10^{-4}, 3.14×10^{-4}	1.26×10^{12}	9.21×10^{11}, 1.72×10^{12}
Li_6ZnO_4	0.44±0.05	8.31×10^{-11}	3.50×10^{-11}, 1.97×10^{-10}	2.62×10^{-2}	1.10×10^{-2}, 6.21×10^{-2}	1.60×10^{14}	6.74×10^{13}, 3.82×10^{14}
$LiNbO_3$	0.47±0.03	2.23×10^{-11}	1.28×10^{-11}, 3.86×10^{-11}	2.26×10^{-3}	1.30×10^{-3}, 3.93×10^{-3}	1.38×10^{13}	7.92×10^{12}, 2.39×10^{13}
Li_2HfO_3	0.53±0.02	2.19×10^{-12}	1.67×10^{-12}, 2.88×10^{-12}	3.85×10^{-4}	2.93×10^{-4}, 5.06×10^{-4}	2.42×10^{12}	1.84×10^{12}, 3.19×10^{12}
$LiSb_3O_8$	0.77±0.03	5.74×10^{-16}	3.46×10^{-16}, 9.50×10^{-16}	2.40×10^{-8}	1.45×10^{-8}, 3.98×10^{-8}	1.34×10^{8}	8.12×10^{7}, 2.21×10^{8}
$LiTaSiO_5$	0.6±0.08	1.60×10^{-13}	4.01×10^{-14}, 6.36×10^{-13}	1.03×10^{-5}	2.60×10^{-6}, 4.12×10^{-5}	6.91×10^{10}	1.71×10^{10}, 2.79×10^{11}
Li_2O	0.26±0.01	2.72×10^{-8}	2.25×10^{-8}, 3.29×10^{-8}	1.24×10^{1}	1.02×10^{1}, 1.50×10^{1}	7.27×10^{16}	5.93×10^{16}, 8.92×10^{16}
Al_2O_3	0.74±0.08	9.70×10^{-16}	2.62×10^{-16}, 3.59×10^{-15}	5.96×10^{-8}	1.61×10^{-8}, 2.21×10^{-7}	4.61×10^{8}	1.11×10^{8}, 1.92×10^{9}
ZnO	0.58±0.07	5.98×10^{-13}	1.70×10^{-13}, 2.10×10^{-12}	3.20×10^{-5}	9.10×10^{-6}, 1.12×10^{-4}	1.74×10^{11}	4.61×10^{10}, 6.60×10^{11}
Sb_2O_5	0.9±0.09	7.37×10^{-18}	1.59×10^{-18}, 3.41×10^{-17}	1.88×10^{-10}	4.07×10^{-11}, 8.72×10^{-10}	1.08×10^{6}	2.35×10^{5}, 5.01×10^{6}

Table S2: Calculated activation energy E_a, extrapolated room temperature diffusivity D_{rt}, conductivity C_{rt} and Onsager transport coefficient L^{OO} for O^{2-} diffusion.

Composition	E_a^{O} (eV)	$D_{\mathrm{rt}}^{\mathrm{O}}$ (cm^2/s)	$D_{\mathrm{rt}}^{\mathrm{O}}$ error bound	$C_{\mathrm{rt}}^{\mathrm{O}}$ (mS/cm)	$C_{\mathrm{rt}}^{\mathrm{O}}$ error bound	$L_{\mathrm{rt}}^{\mathrm{OO}}$ ($eV^{-1}cm^{-1}s^{-1}$)	$L_{\mathrm{rt}}^{\mathrm{OO}}$ error bound
Li_3AlF_6	0.61±0.04	3.79×10^{-14}	1.78×10^{-14}, 8.07×10^{-14}	9.68×10^{-6}	4.54×10^{-6}, 2.06×10^{-5}	3.58×10^{9}	1.63×10^{9}, 7.87×10^{9}
$LiCaAlF_6$	0.69±0.11	2.39×10^{-15}	3.86×10^{-16}, 1.49×10^{-14}	5.49×10^{-7}	8.85×10^{-8}, 3.41×10^{-6}	2.03×10^{8}	3.27×10^{7}, 1.26×10^{9}
Li_2ZnCl_4	0.5±0.08	7.19×10^{-12}	1.78×10^{-12}, 2.90×10^{-11}	6.25×10^{-4}	1.55×10^{-4}, 2.52×10^{-3}	2.25×10^{11}	5.57×10^{10}, 9.08×10^{11}
$LiYF_4$	0.59±0.04	6.65×10^{-14}	3.15×10^{-14}, 1.40×10^{-13}	1.44×10^{-5}	6.84×10^{-6}, 3.05×10^{-5}	5.43×10^{9}	2.53×10^{9}, 1.16×10^{10}
$LiAlSiO_4$	1.2±0.05	2.16×10^{-23}	9.99×10^{-24}, 4.65×10^{-23}	1.12×10^{-13}	5.17×10^{-14}, 2.41×10^{-13}	4.65×10^{1}	2.11×10^{1}, 1.03×10^{2}
$Li_3B_{11}O_{18}$	0.92±0.05	6.86×10^{-19}	2.76×10^{-19}, 1.70×10^{-18}	4.03×10^{-9}	1.63×10^{-9}, 1.00×10^{-8}	1.46×10^{6}	5.34×10^{5}, 3.74×10^{6}
$LiZr_2(PO_4)_3$	0.88±0.06	1.40×10^{-18}	5.23×10^{-19}, 3.77×10^{-18}	7.60×10^{-9}	2.83×10^{-9}, 2.04×10^{-8}	3.08×10^{6}	1.14×10^{6}, 8.33×10^{6}
Li_3PO_4	0.33±0.08	3.54×10^{-10}	9.11×10^{-11}, 1.38×10^{-9}	1.46	3.76×10^{-1}, 5.68	7.41×10^{14}	1.88×10^{14}, 2.92×10^{15}
LiB_3O_5	0.89±0.03	1.87×10^{-18}	1.20×10^{-18}, 2.90×10^{-18}	1.10×10^{-8}	7.08×10^{-9}, 1.71×10^{-8}	3.57×10^{6}	1.81×10^{6}, 6.36×10^{6}
$Li_2B_3PO_8$	0.86±0.03	4.97×10^{-18}	3.24×10^{-18}, 7.62×10^{-18}	2.75×10^{-8}	1.79×10^{-8}, 4.23×10^{-8}	1.04×10^{7}	6.73×10^{6}, 1.59×10^{7}
$LiPO_3$	0.96±0.06	1.50×10^{-19}	5.21×10^{-20}, 4.34×10^{-19}	7.55×10^{-10}	2.62×10^{-10}, 2.18×10^{-9}	2.83×10^{5}	9.51×10^{4}, 8.42×10^{5}
$LiAlO_2$	0.86±0.05	4.65×10^{-18}	1.89×10^{-18}, 1.14×10^{-17}	2.21×10^{-8}	9.01×10^{-9}, 5.44×10^{-8}	8.56×10^{6}	3.47×10^{6}, 2.11×10^{7}
Li_6ZnO_4	0.7±0.1	3.71×10^{-15}	6.99×10^{-16}, 1.97×10^{-14}	1.25×10^{-5}	2.35×10^{-6}, 6.63×10^{-5}	5.16×10^{9}	1.28×10^{9}, 2.08×10^{10}
$LiNbO_3$	0.61±0.02	4.95×10^{-14}	3.69×10^{-14}, 6.64×10^{-14}	2.42×10^{-4}	1.80×10^{-4}, 3.24×10^{-4}	9.41×10^{10}	7.47×10^{10}, 1.19×10^{11}
Li_2HfO_3	0.74±0.07	3.32×10^{-16}	1.05×10^{-16}, 1.05×10^{-15}	1.40×10^{-6}	4.44×10^{-7}, 4.41×10^{-6}	4.47×10^{8}	1.27×10^{8}, 1.57×10^{9}
$LiSb_3O_8$	1.39±0.06	1.87×10^{-25}	6.73×10^{-26}, 5.21×10^{-25}	1.00×10^{-15}	3.61×10^{-16}, 2.79×10^{-15}	3.47×10^{-1}	1.24×10^{-1}, 9.71×10^{-1}
$LiTaSiO_5$	1.03±0.07	9.29×10^{-21}	2.80×10^{-21}, 3.08×10^{-20}	4.81×10^{-11}	1.45×10^{-11}, 1.60×10^{-10}	1.78×10^{4}	6.06×10^{3}, 5.21×10^{4}
Li_2O	0.37±0.02	5.19×10^{-11}	3.48×10^{-11}, 7.75×10^{-11}	1.89×10^{-1}	1.27×10^{-1}, 2.82×10^{-1}	7.42×10^{13}	4.98×10^{13}, 1.11×10^{14}
Al_2O_3	1.04±0.07	9.02×10^{-21}	2.87×10^{-21}, 2.84×10^{-20}	4.88×10^{-11}	1.55×10^{-11}, 1.54×10^{-10}	1.74×10^{4}	4.95×10^{3}, 5.63×10^{4}
ZnO	0.67±0.09	9.00×10^{-15}	2.08×10^{-15}, 3.90×10^{-14}	3.59×10^{-5}	8.29×10^{-6}, 1.56×10^{-4}	1.36×10^{10}	3.14×10^{9}, 5.85×10^{10}
Sb_2O_5	1.23±0.05	4.08×10^{-23}	1.68×10^{-23}, 9.91×10^{-23}	2.17×10^{-13}	8.91×10^{-14}, 5.28×10^{-13}	7.85×10^{1}	3.31×10^{1}, 1.86×10^{2}

Table S3: Calculated voltage window [V_{red}, $-V_{\text{ox}}$] (V), reduction and oxidation reactions, and reaction energy (eV/atom) with Li_3PS_4 ($\Delta E_{\text{rxt}}^{\text{LPS}}$), HF ($\Delta E_{\text{rxt}}^{\text{HF}}$) and cathodes ($\Delta E_{\text{rxt}}^{\text{cathode}}$).

Composition	[V_{red}, $-V_{\text{ox}}$]	Reduction and oxidation reactions	$\Delta E_{\text{rxt}}^{\text{LPS}}$	$\Delta E_{\text{rxt}}^{\text{HF}}$	$\Delta E_{\text{rxt}}^{\text{cathode}}$
$BaLi(B_3O_5)_3$	[1.3, 4.7]	0.2292 $BaLi(B_3O_5)_3$ + Li → 0.1146 $Ba_2Li(BO_2)_5$ + 1.115 $LiBO_2$ + 0.0625 B_6O $BaLi(B_3O_5)_3$ → BaB_8O_{13} + 0.25 O_2 + 0.5 B_2O_3 + Li	-0.00	-0.19	-0.02
$BaLiAlF_6$	[1.0, 6.1]	0.3333 $BaLiAlF_6$ + Li → 1.333 LiF + 0.3333 BaF_2 + 0.3333 Al $BaLiAlF_6$ → $BaAlF_5$ + 0.5 F_2 + Li	-0.04	-0.09	-0.05
$Cs_2Li_2B_2P_4O_{15}$	[2.1, 4.3]	0.3 $Cs_2Li_2B_2P_4O_{15}$ + Li → 0.5 $CsPO_3$ + 0.1 $CsLi(B_3O_5)_2$ + 0.5 Li_3PO_4 + 0.2 P $Cs_2Li_2B_2P_4O_{15}$ → 2 $CsPO_3$ + 2 BPO_4 + 0.5 O_2 + 2 Li	-0.04	-0.16	-0.07
$Cs_2Li_3B_3P_6(PbO_{12})_2$	[2.1, 4.6]	0.186 $Cs_2Li_3B_3P_6(PbO_{12})_2$ + Li → 0.1674 $Cs_2Li_2B_2P_4O_{15}$ + 0.03721 $CsLi(B_3O_5)_2$ + 0.007309 P_7Pb + 0.3953 Li_3PO_4 + 0.3648 Pb $Cs_2Li_3B_3P_6(PbO_{12})_2$ → PbO_2 + 3 BPO_4 + 0.5 $P_2Pb_2O_7$ + 2 $CsPO_3$ + 0.25 O_2 + 3 Li	-0.06	-0.16	-0.08
$Cs_2LiAl_3F_{12}$	[1.1, 6.5]	0.3333 $Cs_2LiAl_3F_{12}$ + Li → 0.3333 Cs_2LiAlF_6 + 0.3333 Li_3AlF_6 + 0.3333 Al $Cs_2LiAl_3F_{12}$ → 2 $CsAlF_4$ + 0.5 F_2 + AlF_3 + Li	-0.02	-0.05	-0.05
Cs_2LiAlF_6	[0.8, 6.2]	Cs_2LiAlF_6 + Li → 0.6667 Cs_3AlF_6 + 2 LiF + 0.3333 Al Cs_2LiAlF_6 → 0.5 $CsAlF_4$ + 0.5 Cs_3AlF_6 + 0.5 F_2 + Li	-0.03	-0.10	-0.02
Cs_2LiGaF_6	[2.1, 6.1]	Cs_2LiGaF_6 + Li → 0.6667 Cs_3GaF_6 + 2 LiF + 0.3333 Ga Cs_2LiGaF_6 → 0.3333 Cs_3GaF_6 + 0.3333 $Cs_3Ga_2F_9$ + 0.5 F_2 + Li	-0.14	-0.09	-0.04
$Cs_2LiSmCl_6$	[0.5, 4.2]	0.3333 $Cs_2LiSmCl_6$ + Li → 0.6667 $CsLiCl_2$ + 0.6667 LiCl + 0.3333 Sm $Cs_2LiSmCl_6$ → 0.5 $CsSm_2Cl_7$ + 1.5 CsCl + 0.5 Cl_2 + Li	-0.02	-0.10	-0.08
$Cs_2LiTbCl_6$	[0.4, 4.2]	0.3333 $Cs_2LiTbCl_6$ + Li → 0.6667 $CsLiCl_2$ + 0.6667 LiCl + 0.3333 Tb $Cs_2LiTbCl_6$ → 0.6 Cs_3TbCl_6 + 0.2 $CsTb_2Cl_7$ + 0.5 Cl_2 + Li	-0.01	-0.10	-0.09
$Cs_2Sr_2Li_3B_3(PO_4)_6$	[2.1, 4.4]	0.2207 $Cs_2Sr_2Li_3B_3(PO_4)_6$ + Li → 0.1655 $Cs_2SrP_2O_7$ + 0.1379 $Sr_2P_2O_7$ + 0.5172 Li_3PO_4 + 0.1103 $CsLi(B_3O_5)_2$ + 0.2 P $Cs_2Sr_2Li_3B_3(PO_4)_6$ → $SrBPO_5$ + 2 $CsPO_3$ + 0.5 $Sr_2P_2O_7$ + 2 BPO_4 + 0.75 O_2 + 3 Li	-0.03	-0.16	-0.06
$Cs_4KLiFe_2F_{12}$	[2.7, 6.4]	1.25 $Cs_4KLiFe_2F_{12}$ + Li → 0.25 $Cs_7Fe_4F_{15}$ + 1.25 Cs_2KFeF_6 + 0.25 Cs_3FeF_6 + 2.25 LiF $Cs_4KLiFe_2F_{12}$ → 0.5 Cs_2KFeF_6 + 1.5 Cs_2FeF_5 + 0.5 KF_3 + Li	-0.14	-0.10	-0.03
$Cs_4KLiGa_2F_{12}$	[1.9, 6.5]	$Cs_4KLiGa_2F_{12}$ + Li → 0.6667 Cs_3GaF_6 + Cs_2KGaF_6 + 2 LiF + 0.3333 Ga $Cs_4KLiGa_2F_{12}$ → 0.5 Cs_3GaF_6 + 0.5 $Cs_3Ga_2F_9$ + 0.5 KF_3 + 0.5 Cs_2KGaF_6 + Li	-0.13	-0.09	-0.04
$CsBaLiP_2O_7$	[1.8, 4.0]	1.395 $CsBaLiP_2O_7$ + Li → 0.02632 Cs_3P_7 + 0.6579 $Cs_2BaP_2O_7$ + 0.7982 Li_3PO_4 + 0.2456 $Ba_3(PO_4)_2$ $CsBaLiP_2O_7$ → 0.5 $Ba_2P_2O_7$ + $CsPO_3$ + 0.25 O_2 + Li	-0.07	-0.17	-0.03
$CsLi(B_3O_5)_2$	[1.2, 4.3]	0.3438 $CsLi(B_3O_5)_2$ + Li → 0.332 $CsLi_4(BO_2)_5$ + 0.003906 $Cs_3Li_4(BO_2)_7$ + 0.0625 B_6O $CsLi(B_3O_5)_2$ → 0.25 CsB_9O_{14} + 0.75 CsB_5O_8 + 0.25 O_2 + Li	-0.00	-0.20	-0.01
$CsLi(PO_3)_2$	[2.3, 5.0]	0.8 $CsLi(PO_3)_2$ + Li → 0.8 $CsPO_3$ + 0.6 Li_3PO_4 + 0.2 P $CsLi(PO_3)_2$ → $CsPO_3$ + 0.5 P_2O_5 + 0.25 O_2 + Li	-0.06	-0.16	-0.07
$CsLiBeF_4$	[0.7, 6.1]	$CsLiBeF_4$ + Li → 0.5 Cs_2BeF_4 + 2 LiF + 0.5 Be $CsLiBeF_4$ → $CsBeF_3$ + 0.5 F_2 + Li	-0.01	-0.08	-0.03
$CsLiF_2$	[0.6, 6.0]	$CsLiF_2$ + Li → Cs + 2 LiF $CsLiF_2$ → 0.5 F_2 + CsF + Li	-0.05	-0.18	-0.04
$K_2Li_3B(P_2O_7)_2$	[2.2, 4.2]	0.4 $K_2Li_3B(P_2O_7)_2$ + Li → 0.4 $K_2LiB(PO_4)_2$ + 0.6 Li_3PO_4 + 0.2 P $K_2Li_3B(P_2O_7)_2$ → $KLi(PO_3)_2$ + KPO_3 + BPO_4 + 0.5 O_2 + 2 Li	-0.03	-0.16	-0.07
K_2LiAlF_6	[0.8, 6.4]	K_2LiAlF_6 + Li → 0.6667 K_3AlF_6 + 2 LiF + 0.3333 Al K_2LiAlF_6 → 0.5 K_2AlF_5 + 0.5 $KAlF_4$ + 0.5 KF_3 + Li	-0.03	-0.10	-0.02
$K_2LiB(PO_4)_2$	[2.0, 4.2]	0.7458 $K_2LiB(PO_4)_2$ + Li → 0.01316 KP_{15} + 0.03925 $K_5B_{19}O_{31}$ + 0.4274 $K_3LiP_2O_7$ + 0.4395 Li_3PO_4 $K_2LiB(PO_4)_2$ → 1.833 KPO_3 + 0.1667 BPO_4 + 0.1667 KB_5O_8 + 0.25 O_2 + Li	-0.05	-0.18	-0.05
$K_2LiBiCl_6$	[2.4, 4.0]	0.3333 $K_2LiBiCl_6$ + Li → 1.333 LiCl + 0.6667 KCl + 0.3333 Bi $K_2LiBiCl_6$ → 2 KCl + 0.5 Cl_2 + $BiCl_3$ + Li	-0.08	-0.09	-0.10
K_2LiGaF_6	[2.0, 6.4]	0.3333 K_2LiGaF_6 + Li → 0.6667 KF + 1.333 LiF + 0.3333 Ga K_2LiGaF_6 → KF_2 + $KGaF_4$ + Li	-0.10	-0.09	-0.05
K_2LiInF_6	[2.4, 6.0]	K_2LiInF_6 + Li → 0.6667 K_3InF_6 + 2 LiF + 0.3333 In K_2LiInF_6 → 0.3333 KF_2 + 0.3333 $K_5In_3F_{14}$ + 0.6667 LiF + 0.3333 Li	-0.13	-0.10	-0.04
K_2LiScF_6	[0.4, 6.2]	0.2 K_2LiScF_6 + Li → 1.2 LiF + 0.4 K + 0.2 Sc K_2LiScF_6 → 0.25 $KScF_4$ + 0.25 $K_5Sc_3F_{14}$ + 0.5 KF_3 + Li	-0.03	-0.11	-0.02
$K_2LiTa_6(PO_8)_3$	[1.9, 4.3]	0.1625 $K_2LiTa_6(PO_8)_3$ + Li → 0.125 $K_2Ta_4O_{11}$ + 0.075 KTa_5O_{13} + 0.3875 Li_3PO_4 + 0.1 TaP $K_2LiTa_6(PO_8)_3$ → 1.75 KTa_2PO_8 + 0.25 KTa_5O_{13} + 1.25 $TaPO_5$ + 0.25 O_2 + Li	-0.05	-0.19	-0.05
$K_3LiP_2O_7$	[1.7, 4.2]	0.7586 $K_3LiP_2O_7$ + Li → 0.01724 K_3P_{11} + 0.7414 K_3PO_4 + 0.5862 Li_3PO_4 $K_3LiP_2O_7$ → 0.5 $K_4P_2O_7$ + KPO_3 + 0.25 O_2 + Li	-0.07	-0.18	-0.02
$K_5Li_2NdF_{10}$	[0.4, 5.9]	0.25 $K_5Li_2NdF_{10}$ + Li → 0.25 $KNdF_4$ + 1.5 LiF + K $K_5Li_2NdF_{10}$ → K_2NdF_5 + 2 KF_2 + KF + 2 Li	-0.09	-0.16	-0.02
$K_5Li_2PrF_{10}$	[0.4, 5.9]	0.25 $K_5Li_2PrF_{10}$ + Li → 0.25 $KPrF_4$ + 1.5 LiF + K $K_5Li_2PrF_{10}$ → 2 KF_2 + $KPrF_4$ + 2 KF + 2 Li	-0.08	-0.16	-0.02
$KLi(PO_3)_2$	[2.3, 4.9]	1.4 $KLi(PO_3)_2$ + Li → 0.6 $Li_4P_2O_7$ + 1.4 KPO_3 + 0.2 P $KLi(PO_3)_2$ → KPO_3 + 0.5 P_2O_5 + 0.25 O_2 + Li	-0.05	-0.16	-0.09
$KLiBeF_4$	[0.8, 6.4]	$KLiBeF_4$ + Li → 0.5 K_2BeF_4 + 2 LiF + 0.5 Be $KLiBeF_4$ → 0.75 $KBeF_3$ + 0.25 Li_2BeF_4 + 0.25 KF_3 + 0.5 Li	-0.02	-0.09	-0.03
$KLiZnP_2O_7$	[2.4, 4.2]	1.333 $KLiZnP_2O_7$ + Li → 0.08333 ZnP_2 + 0.6667 $K_2ZnP_2O_7$ + 0.5833 $Li_4Zn(PO_4)_2$ $KLiZnP_2O_7$ → 0.3333 $K_2Zn_3(P_2O_7)_2$ + 0.3333 $KLi(PO_3)_2$ + 0.1667 O_2 + 0.6667 Li	-0.09	-0.15	-0.06
$Li_2Al(BO_2)_5$	[1.3, 4.1]	0.3438 $Li_2Al(BO_2)_5$ + Li → $LiBO_2$ + 0.3437 Li_2AlBO_4 + 0.0625 B_6O $Li_2Al(BO_2)_5$ → 0.4091 $Li_3B_{11}O_{18}$ + 0.25 $Al_4B_2O_9$ + 0.1932 O_2 + 0.7727 Li	-0.00	-0.21	-0.02
$Li_2B_3O_4F_3$	[1.9, 4.3]	$Li_2B_3O_4F_3$ + Li → 0.4375 $Li_2B_6O_9F_2$ + 0.0625 B_6O + 2.125 LiF $Li_2B_3O_4F_3$ → 0.3913 LiB_6O_9F + 0.6522 $LiBF_4$ + 0.2391 O_2 + 0.9565 Li	0.00	-0.17	-0.07
$Li_2B_3PO_8$	[2.2, 4.1]	0.7 $Li_2B_3PO_8$ + Li → 0.3 $Li_3B_7O_{12}$ + 0.5 Li_3PO_4 + 0.2 P $Li_2B_3PO_8$ → 0.1818 $Li_3B_{11}O_{18}$ + BPO_4 + 0.3636 O_2 + 1.455 Li	0.00	-0.18	-0.06
$Li_2B_6O_9F_2$	[1.9, 4.1]	0.6736 $Li_2B_6O_9F_2$ + Li → 0.3333 $Li_3B_{11}O_{18}$ + 0.0625 B_6O + 1.347 LiF $Li_2B_6O_9F_2$ → 0.8 LiB_6O_9F + 0.4 $Li_2B_3O_4F_3$ + 0.1 O_2 + 0.4 Li	-0.00	-0.18	-0.06
Li_2BeF_4	[0.9, 6.1]	0.5 Li_2BeF_4 + Li → 0.5 Be + 2 LiF Li_2BeF_4 → BeF_2 + F_2 + 2 Li	0.00	-0.06	-0.05
Li_2CaHfF_8	[1.0, 6.3]	0.25 Li_2CaHfF_8 + Li → 1.5 LiF + 0.25 CaF_2 + 0.25 Hf Li_2CaHfF_8 → F_2 + CaF_2 + HfF_4 + 2 Li	0.00	-0.05	-0.06
$Li_2InP_2HO_8$	[2.3, 4.1]	0.3333 $Li_2InP_2HO_8$ + Li → 0.1667 $LiP(HO_2)_2$ + 0.5 Li_3PO_4 + 0.3333 In $Li_2InP_2HO_8$ → $LiInP_2O_7$ + 0.25 O_2 + 0.5 H_2O + Li	-0.08	-0.15	-0.06

Composition	$[V_{red}, -V_{ox}]$	Reduction and oxidation reactions	ΔE_{rxt}^{LPS}	ΔE_{rxt}^{HF}	$\Delta E_{rxt}^{cathode}$
Li_2NiF_4	[2.8, 5.6]	0.5 Li_2NiF_4 + Li → 0.5 Ni + 2 LiF Li_2NiF_4 → 0.5 Li_3NiF_6 + 0.5 NiF_2 + 0.5 Li	-0.19	-0.08	-0.06
$Li_2ScP_2HO_8$	[2.3, 4.1]	1.5 $Li_2ScP_2HO_8$ + Li → 0.5833 $Li_3Sc_2(PO_4)_3$ + 0.1667 $Sc_2P_3(HO_3)_3$ + 0.75 Li_3PO_4 + 0.5 H_2O $Li_2ScP_2HO_8$ → $LiScP_2O_7$ + 0.25 O_2 + 0.5 H_2O + Li	-0.01	-0.16	-0.05
$Li_2Ta_2(OF_2)_3$	[1.7, 4.7]	0.25 $Li_2Ta_2(OF_2)_3$ + Li → 0.15 Ta_2O_5 + 1.5 LiF + 0.2 Ta $Li_2Ta_2(OF_2)_3$ → 0.3529 Ta_3O_7F + 0.9412 $LiTaF_6$ + 0.2647 O_2 + 1.059 Li	-0.04	-0.15	-0.07
$Li_2TiCr(PO_4)_3$	[2.2, 4.3]	0.3 $Li_2TiCr(PO_4)_3$ + Li → 0.2 $Li_2CrP_2O_7$ + 0.1 CrP + 0.4 Li_3PO_4 + 0.3 TiO_2 $Li_2TiCr(PO_4)_3$ → 0.5 $LiTi_2(PO_4)_3$ + 0.75 $LiCrP_2O_7$ + 0.05 Cr_5O_{12} + 0.075 O_2 + 0.75 Li	-0.03	-0.14	-0.10
Li_2TiF_6	[1.9, 6.4]	Li_2TiF_6 + Li → Li_3TiF_6 Li_2TiF_6 → TiF_4 + F_2 + 2 Li	-0.05	-0.02	-0.10
Li_2ZrF_6	[1.2, 6.2]	Li_2ZrF_6 + Li → 0.75 Li_4ZrF_8 + 0.25 Zr Li_2ZrF_6 → 0.25 $Li_3Zr_4F_{19}$ + 0.625 F_2 + 1.25 Li	-0.03	-0.03	-0.07
Li_3AlF_6	[1.1, 6.1]	0.3333 Li_3AlF_6 + Li → 0.3333 Al + 2 LiF Li_3AlF_6 → AlF_3 + 1.5 F_2 + 3 Li	0.00	-0.06	-0.05
$Li_3B_{11}O_{18}$	[1.8, 4.3]	0.6771 $Li_3B_{11}O_{18}$ + Li → 1.01 $Li_3B_7O_{12}$ + 0.0625 B_6O $Li_3B_{11}O_{18}$ → 5.5 B_2O_3 + 0.75 O_2 + 3 Li	0.00	-0.19	-0.03
Li_3GaF_6	[2.2, 6.2]	0.3333 Li_3GaF_6 + Li → 0.3333 Ga + 2 LiF Li_3GaF_6 → GaF_3 + 1.5 F_2 + 3 Li	-0.09	-0.06	-0.08
Li_3PO_4	[0.7, 4.0]	0.125 Li_3PO_4 + Li → 0.5 Li_2O + 0.125 Li_3P Li_3PO_4 → 0.5 $Li_4P_2O_7$ + 0.25 O_2 + Li	-0.00	-0.17	-0.00
$Li_3Sc_2(PO_4)_3$	[1.8, 4.1]	0.2667 $Li_3Sc_2(PO_4)_3$ + Li → 0.6 Li_3PO_4 + 0.2667 Sc_2O_3 + 0.2 P $Li_3Sc_2(PO_4)_3$ → $LiScP_2O_7$ + $ScPO_4$ + 0.5 O_2 + 2 Li	-0.00	-0.17	-0.05
$Li_3Zr_4F_{19}$	[1.5, 6.3]	0.3 $Li_3Zr_4F_{19}$ + Li → 0.95 Li_2ZrF_6 + 0.25 Zr $Li_3Zr_4F_{19}$ → 4 ZrF_4 + 1.5 F_2 + 3 Li	-0.04	-0.02	-0.09
$Li_4Be_3P_3BrO_{12}$	[1.7, 4.5]	0.2667 $Li_4Be_3P_3BrO_{12}$ + Li → 0.6 Li_3PO_4 + 0.8 BeO + 0.2667 LiBr + 0.2 P $Li_4Be_3P_3BrO_{12}$ → 0.5 Br_2O_3 + 1.5 BeO + 1.5 $Be(PO_3)_2$ + 4 Li	0.00	-0.15	-0.05
$Li_4Be_3P_3ClO_{12}$	[1.7, 4.6]	0.2667 $Li_4Be_3P_3ClO_{12}$ + Li → 0.6 Li_3PO_4 + 0.8 BeO + 0.2667 LiCl + 0.2 P $Li_4Be_3P_3ClO_{12}$ → 0.75 ClO_2 + 1.5 BeO + 1.5 $Be(PO_3)_2$ + 0.125 Cl_2 + 4 Li	0.00	-0.15	-0.07
$Li_4P_2O_7$	[2.3, 4.1]	0.8 $Li_4P_2O_7$ + Li → 1.4 Li_3PO_4 + 0.2 P $Li_4P_2O_7$ → 2 $LiPO_3$ + 0.5 O_2 + 2 Li	-0.01	-0.16	-0.06
Li_4ZrF_8	[1.2, 6.0]	0.25 Li_4ZrF_8 + Li → 0.25 Zr + 2 LiF Li_4ZrF_8 → Li_2ZrF_6 + F_2 + 2 Li	-0.02	-0.06	-0.06
$Li_9Cr_3P_8O_{29}$	[2.5, 4.1]	0.3333 $Li_9Cr_3P_8O_{29}$ + Li → $Li_2CrP_2O_7$ + 0.6667 Li_3PO_4 $Li_9Cr_3P_8O_{29}$ → $Li_4P_2O_7$ + 3 $LiCrP_2O_7$ + 0.5 O_2 + 2 Li	-0.00	-0.15	-0.10
$LiB_5H_2O_9$	[1.9, 4.5]	0.7143 $LiB_5H_2O_9$ + Li → 0.2143 $Li_3B_5(HO_5)_2$ + 0.3571 $Li_3B_7O_{12}$ + 0.5 H_2 $LiB_5H_2O_9$ → 2 BHO_2 + 1.5 B_2O_3 + 0.25 O_2 + Li	0.00	-0.18	-0.03
LiB_6O_9F	[1.9, 4.7]	1.347 LiB_6O_9F + Li → 0.6736 $Li_2B_6O_9F_2$ + 0.3333 $Li_3B_{11}O_{18}$ + 0.0625 B_6O LiB_6O_9F → 0.25 $LiBF_4$ + 2.875 B_2O_3 + 0.1875 O_2 + 0.75 Li	0.00	-0.19	-0.06
$LiBiF_4$	[2.6, 5.3]	0.3333 $LiBiF_4$ + Li → 0.3333 Bi + 1.333 LiF $LiBiF_4$ → 0.3333 $LiBiF_6$ + 0.6667 BiF_3 + 0.6667 Li	-0.14	-0.04	-0.08
$LiCaAlF_6$	[1.1, 6.3]	0.3333 $LiCaAlF_6$ + Li → 1.333 LiF + 0.3333 CaF_2 + 0.3333 Al $LiCaAlF_6$ → $CaAlF_5$ + 0.5 F_2 + Li	0.00	-0.05	-0.05
$LiCaGaF_6$	[2.4, 6.5]	$LiCaGaF_6$ + Li → 0.6667 Li_3GaF_6 + CaF_2 + 0.3333 Ga $LiCaGaF_6$ → CaF_2 + 0.5 F_2 + GaF_3 + Li	-0.11	-0.05	-0.09
$LiClO_4$	[2.9, 4.5]	0.125 $LiClO_4$ + Li → 0.5 Li_2O + 0.125 LiCl $LiClO_4$ → 0.5 Cl_2O_7 + 0.25 O_2 + Li	-1.06	-0.09	-0.06
LiF	[-0.0, 6.0]	Li → Li LiF → 0.5 F_2 + Li	0.00	-0.11	-0.00
$LiInF_4$	[2.5, 6.1]	0.3333 $LiInF_4$ + Li → 0.3333 In + 1.333 LiF $LiInF_4$ → InF_3 + 0.5 F_2 + Li	-0.16	-0.04	-0.10
$LiInP_2O_7$	[2.4, 4.5]	0.2353 $LiInP_2O_7$ + Li → 0.05882 InP + 0.4118 Li_3PO_4 + 0.1765 In $LiInP_2O_7$ → 0.5 $InPO_4$ + 0.5 $In(PO_3)_3$ + 0.25 O_2 + Li	-0.09	-0.14	-0.08
$LiLuF_4$	[0.3, 6.3]	0.3333 $LiLuF_4$ + Li → 0.3333 Lu + 1.333 LiF $LiLuF_4$ → LuF_3 + 0.5 F_2 + Li	0.00	0.00	-0.03
$LiMg_3P_3O_{11}$	[2.3, 4.2]	0.8 $LiMg_3P_3O_{11}$ + Li → 1.8 $LiMgPO_4$ + 0.2 $Mg_3(PO_4)_2$ + 0.2 P $LiMg_3P_3O_{11}$ → 1.5 $Mg_2P_2O_7$ + 0.25 O_2 + Li	-0.01	-0.16	-0.05
$LiMgAlF_6$	[1.2, 6.2]	$LiMgAlF_6$ + Li → 0.6667 Li_3AlF_6 + MgF_2 + 0.3333 Al $LiMgAlF_6$ → MgF_2 + 0.5 F_2 + AlF_3 + Li	0.00	-0.02	-0.06
$LiMgPO_4$	[1.6, 4.0]	0.8 $LiMgPO_4$ + Li → 0.6 Li_3PO_4 + 0.8 MgO + 0.2 P $LiMgPO_4$ → 0.3333 $LiMg_3P_3O_{11}$ + 0.1667 O_2 + 0.6667 Li	0.00	-0.17	-0.03
$LiP(HO_2)_2$	[2.3, 4.4]	0.75 $LiP(HO_2)_2$ + Li → 0.25 $LiP(HO)_2$ + 0.5 Li_3PO_4 + 0.5 H_2O $LiP(HO_2)_2$ → 0.6667 PH_3O_4 + 0.3333 $LiPO_3$ + 0.1667 O_2 + 0.6667 Li	-0.02	-0.13	-0.07
$LiScP_2O_7$	[2.3, 4.4]	0.8 $LiScP_2O_7$ + Li → 0.4 $Li_3Sc_2(PO_4)_3$ + 0.2 Li_3PO_4 + 0.2 P $LiScP_2O_7$ → 0.5 $Sc(PO_3)_3$ + 0.5 $ScPO_4$ + 0.25 O_2 + Li	-0.01	-0.15	-0.07
$LiTb_6B_3O_{14}$	[0.9, 4.2]	0.225 $LiTb_6B_3O_{14}$ + Li → 0.4083 Li_3BO_3 + 0.06667 TbB_4 + 0.6417 Tb_2O_3 $LiTb_6B_3O_{14}$ → 3 $TbBO_3$ + 0.25 O_2 + 1.5 Tb_2O_3 + Li	-0.08	-0.34	-0.07
$LiTi_2(PO_4)_3$	[2.2, 4.5]	$LiTi_2(PO_4)_3$ + Li → $Li_2Ti_2(PO_4)_3$ $LiTi_2(PO_4)_3$ → 0.1667 $Ti_5(PO_5)_4$ + 1.167 TiP_2O_7 + 0.25 O_2 + Li	-0.03	-0.14	-0.08
$LiYF_4$	[0.4, 6.2]	0.3333 $LiYF_4$ + Li → 0.3333 Y + 1.333 LiF $LiYF_4$ → YF_3 + 0.5 F_2 + Li	0.00	-0.03	-0.03
$LiYbAlF_6$	[1.0, 6.5]	0.3333 $LiYbAlF_6$ + Li → 1.333 LiF + 0.3333 YbF_2 + 0.3333 Al $LiYbAlF_6$ → YbF_3 + AlF_3 + Li	0.00	-0.00	-0.04
$LiZnP_2HO_7$	[2.6, 4.5]	1.167 $LiZnP_2HO_7$ + Li → 0.5833 $LiP(HO_2)_2$ + 1.083 $LiZnPO_4$ + 0.08333 ZnP_2 + 0.5 $LiPO_3$ $LiZnP_2HO_7$ → 0.1667 $Zn_2P_2O_7$ + 0.6667 $Zn(PO_3)_2$ + 0.3333 PH_3O_4 + 0.25 O_2 + Li	-0.08	-0.13	-0.09
$LiZr_2(PO_4)_3$	[2.0, 4.5]	0.2 $LiZr_2(PO_4)_3$ + Li → 0.4 Li_3PO_4 + 0.4 ZrO_2 + 0.2 P $LiZr_2(PO_4)_3$ → 0.5 $Zr_2P_2O_9$ + ZrP_2O_7 + 0.25 O_2 + Li	-0.01	-0.15	-0.06

Composition	$[V_{red}, -V_{ox}]$	Reduction and oxidation reactions	ΔE_{rxt}^{LPS}	ΔE_{rxt}^{HF}	$\Delta E_{rxt}^{cathode}$
$Na_2LiB_5(PO_7)_2$	[2.1, 4.3]	0.4571 $Na_2LiB_5(PO_7)_2$ + Li → 0.2286 $Na_3B_6PO_{13}$ + 0.1143 $Na_2B_8O_{13}$ + 0.4857 Li_3PO_4 + 0.2 P $Na_2LiB_5(PO_7)_2$ → 0.05556 $Na_3B(PO_4)_2$ + 0.6111 $Na_3B_6PO_{13}$ + 1.278 BPO_4 + 0.25 O_2 + Li	-0.01	-0.17	-0.06
$Na_2LiBe_2F_7$	[1.1, 6.1]	2 $Na_2LiBe_2F_7$ + Li → 1.5 Li_2BeF_4 + 2 Na_2BeF_4 + 0.5 Be $Na_2LiBe_2F_7$ → Na_2BeF_4 + 0.5 F_2 + BeF_2 + Li	-0.02	-0.06	-0.05
$Na_3Li_3Al_2F_{12}$	[0.9, 6.3]	0.1667 $Na_3Li_3Al_2F_{12}$ + Li → 0.5 NaF + 1.5 LiF + 0.3333 Al $Na_3Li_3Al_2F_{12}$ → 0.5 $Na_5Al_3F_{14}$ + 0.5 $NaAlF_4$ + 1.5 F_2 + 3 Li	-0.00	-0.05	-0.03
$Na_3Li_3Fe_2F_{12}$	[2.8, 6.4]	0.5 $Na_3Li_3Fe_2F_{12}$ + Li → $NaFeF_3$ + 0.5 NaF + 2.5 LiF $Na_3Li_3Fe_2F_{12}$ → Na_3FeF_6 + FeF_6 + 3 Li	-0.11	-0.05	-0.06
$Na_3Li_3In_2F_{12}$	[2.3, 6.2]	0.1667 $Na_3Li_3In_2F_{12}$ + Li → 0.5 NaF + 1.5 LiF + 0.3333 In $Na_3Li_3In_2F_{12}$ → Na_3InF_6 + 1.5 F_2 + InF_3 + 3 Li	-0.10	-0.07	-0.06
$Na_3Li_3Sc_2F_{12}$	[0.4, 6.2]	0.1111 $Na_3Li_3Sc_2F_{12}$ + Li → 1.333 LiF + 0.3333 Na + 0.2222 Sc $Na_3Li_3Sc_2F_{12}$ → Na_3ScF_6 + 1.5 F_2 + ScF_3 + 3 Li	-0.00	-0.08	-0.03
$Na_3LiP_2O_7$	[2.3, 4.0]	3.2 $Na_3LiP_2O_7$ + Li → 2.4 $Na_4P_2O_7$ + 1.4 Li_3PO_4 + 0.2 P $Na_3LiP_2O_7$ → 0.6 $Na_5P_3O_{10}$ + 0.2 Li_3PO_4 + 0.1 O_2 + 0.4 Li	-0.05	-0.18	-0.04
$Na_3LiTi_2F_{12}$	[1.7, 6.4]	2 $Na_3LiTi_2F_{12}$ + Li → Li_3TiF_6 + 3 Na_2TiF_6 $Na_3LiTi_2F_{12}$ → 1.5 Na_2TiF_6 + 0.5 TiF_4 + 0.5 F_2 + Li	-0.04	-0.00	-0.08
$Na_3LiY_3P_3CO_{15}F_2$	[2.1, 4.0]	0.25 $Na_3LiY_3P_3CO_{15}F_2$ + Li → 0.04167 $Na_3Y(PO_4)_2$ + 0.625 $NaLi_2PO_4$ + 0.04167 YPO_4 + 0.5 YOF + 0.08333 Y_2O_3 + 0.25 C $Na_3LiY_3P_3CO_{15}F_2$ → $NaYCO_3F_2$ + 2 YPO_4 + 0.5 $Na_4P_2O_7$ + 0.25 O_2 + Li	-0.06	-0.17	-0.02
$NaLi_2B(PO_4)_2$	[2.3, 4.1]	0.8667 $NaLi_2B(PO_4)_2$ + Li → 0.2 $Na_3B(PO_4)_2$ + 0.1333 $Na_2LiB_5(PO_7)_2$ + 0.8667 Li_3PO_4 + 0.2 P $NaLi_2B(PO_4)_2$ → $NaPO_3$ + BPO_4 + 0.5 O_2 + 2 Li	-0.02	-0.16	-0.07
$NaLiEr_2F_8$	[0.3, 6.2]	0.1429 $NaLiEr_2F_8$ + Li → 1.143 LiF + 0.1429 Na + 0.2857 Er $NaLiEr_2F_8$ → $NaErF_4$ + 0.5 F_2 + ErF_3 + Li	-0.00	-0.04	-0.03
$NaLiHo_2F_8$	[0.3, 6.2]	0.1429 $NaLiHo_2F_8$ + Li → 1.143 LiF + 0.1429 Na + 0.2857 Ho $NaLiHo_2F_8$ → $NaHoF_4$ + 0.5 F_2 + HoF_3 + Li	0.00	-0.04	-0.03
$NaLiLu_2F_8$	[0.5, 6.7]	$NaLiLu_2F_8$ + Li → 2 $LiLuF_4$ + Na $NaLiLu_2F_8$ → NaF + 0.5 F_2 + 2 LuF_3 + Li	-0.02	-0.01	-0.03
$NaLiMgPO_4F$	[1.5, 4.1]	1.917 $NaLiMgPO_4F$ + Li → 0.02778 NaP_7 + 0.3889 $NaMgF_3$ + 0.75 Na_2MgPO_4F + 0.9722 Li_3PO_4 + 0.7778 MgO $NaLiMgPO_4F$ → 0.03704 $LiMg_3P_3O_{11}$ + 0.1111 $Na_3Mg_2P_5O_{16}$ + 0.3333 Na_2MgPO_4F + 0.3333 MgF_2 + 0.2407 O_2 + 0.963 Li	-0.02	-0.17	-0.02
$NaLiTm_2F_8$	[0.3, 9.4]	0.1429 $NaLiTm_2F_8$ + Li → 1.143 LiF + 0.1429 Na + 0.2857 Tm $NaLiTm_2F_8$ → NaF + 0.5 F_2 + 2 TmF_3 + Li	0.00	0.00	-0.03
$Rb_2Li_3B(P_2O_7)_2$	[2.1, 4.3]	0.4222 $Rb_2Li_3B(P_2O_7)_2$ + Li → 0.7333 $RbPO_3$ + 0.02222 $Rb_5B_{19}O_{31}$ + 0.7556 Li_3PO_4 + 0.2 P $Rb_2Li_3B(P_2O_7)_2$ → $LiPO_3$ + 2 $RbPO_3$ + BPO_4 + 0.5 O_2 + 2 Li	-0.04	-0.15	-0.06
$Rb_2LiBiCl_6$	[2.3, 4.3]	0.3333 $Rb_2LiBiCl_6$ + Li → 1.333 LiCl + 0.6667 RbCl + 0.3333 Bi $Rb_2LiBiCl_6$ → 0.6667 Rb_3BiCl_6 + 0.5 Cl_2 + 0.3333 $BiCl_3$ + Li	-0.06	-0.04	-0.08
Rb_2LiGaF_6	[2.0, 6.2]	Rb_2LiGaF_6 + Li → 0.6667 Rb_3GaF_6 + 2 LiF + 0.3333 Ga Rb_2LiGaF_6 → 0.5 Rb_3GaF_6 + 0.5 RbF_3 + 0.5 GaF_3 + Li	-0.12	-0.04	-0.05
$Rb_2LiInCl_6$	[2.1, 4.4]	0.5 $Rb_2LiInCl_6$ + Li → 1.5 LiCl + RbCl + 0.5 InCl $Rb_2LiInCl_6$ → 0.6667 Rb_3InCl_6 + 0.3333 $InCl_3$ + 0.5 Cl_2 + Li	-0.05	-0.03	-0.09
Rb_2LiInF_6	[2.2, 6.0]	0.3333 Rb_2LiInF_6 + Li → 0.6667 RbF + 1.333 LiF + 0.3333 In Rb_2LiInF_6 → 0.3571 Rb_3InF_6 + 0.2143 $Rb_2In_3F_{11}$ + 0.5 RbF_3 + Li	-0.13	-0.05	-0.03
$Rb_2LiRhCl_6$	[2.7, 4.4]	0.3333 $Rb_2LiRhCl_6$ + Li → 0.6667 RbCl + 1.333 LiCl + 0.3333 Rh $Rb_2LiRhCl_6$ → $RhCl_3$ + 2 RbCl + 0.5 Cl_2 + Li	-0.13	-0.04	-0.10
Rb_2LiScF_6	[0.5, 5.7]	Rb_2LiScF_6 + Li → 0.6667 Rb_3ScF_6 + 2 LiF + 0.3333 Sc Rb_2LiScF_6 → 0.75 $RbScF_4$ + 0.25 Rb_3ScF_6 + 0.5 RbF_3 + Li	-0.05	-0.08	-0.02
Rb_2LiYF_6	[0.5, 5.8]	0.5 Rb_2LiYF_6 + Li → 0.5 $LiYF_4$ + LiF + Rb Rb_2LiYF_6 → 0.5714 Rb_3YF_6 + 0.4286 $LiYF_4$ + 0.2857 RbF_3 + 0.5714 Li	-0.09	-0.09	-0.02
$Rb_4LiZr_3H_2F_{19}$	[2.4, 6.9]	0.5 $Rb_4LiZr_3H_2F_{19}$ + Li → 0.3333 $Rb_5Zr_4F_{21}$ + 0.1667 Rb_2ZrF_6 + 1.5 LiF + 0.5 H_2 $Rb_4LiZr_3H_2F_{19}$ → 0.7 $Rb_5Zr_4F_{21}$ + 0.5 RbF_3 + 0.2 ZrF_4 + 2 HF + Li	-0.07	0.00	-0.06
$RbLi_2Be_2F_7$	[0.8, 6.1]	0.3333 $RbLi_2Be_2F_7$ + Li → 0.1667 Rb_2BeF_4 + 1.667 LiF + 0.5 Be $RbLi_2Be_2F_7$ → RbF_3 + 2 BeF_2 + 2 Li	-0.01	-0.04	-0.05
$SrLi(B_3O_5)_3$	[1.6, 4.4]	0.8553 $SrLi(B_3O_5)_3$ + Li → 0.6184 $Li_3B_7O_{12}$ + 0.2138 $Sr_4B_{14}O_{25}$ + 0.0625 B_6O $SrLi(B_3O_5)_3$ → SrB_8O_{13} + 0.25 O_2 + 0.5 B_2O_3 + Li	-0.01	-0.20	-0.03
$SrLiAlF_6$	[1.0, 6.3]	0.3333 $SrLiAlF_6$ + Li → 1.333 LiF + 0.3333 SrF_2 + 0.3333 Al $SrLiAlF_6$ → $SrAlF_5$ + 0.5 F_2 + Li	-0.01	-0.02	-0.05
$SrLiGaF_6$	[2.3, 6.7]	$SrLiGaF_6$ + Li → 0.6667 Li_3GaF_6 + SrF_2 + 0.3333 Ga $SrLiGaF_6$ → SrF_3 + GaF_3 + Li	-0.10	-0.00	-0.08

References

(1) Chase, M. W.; Curnutt, J. L.; Downey, J. R.; Mcdonald, R. A.; Syverud, A. N.; Valenzuela, E. A. JANAF Thermochemical Tables, 1982 Supplement. *Journal of Physical and Chemical Reference Data* **1982**, *11*, 695–940.

(2) Bard, A. J.; Parsons, R.; Jordan, J. Standard Potentials in Aqueous Solution. *Standard Potentials in Aqueous Solution* **2017**,