Supplementary Information for

Ruddlesden-Popper phases of lithium-hydroxide-halide antiperovskites:
Two dimensional Li-ion conductors

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This supplementary information consists of (1) XRD patterns and refinement results of LiBr(Li3−pOHpBr)n (n = 1, 2, 3 and p = 0), (2) XRD patterns and refinement results of LiBr(Li3−pOHpBr)n (n = 1, 2, 3 and p = 0.5), (3) XRD patterns and refinement results of LiBr(Li3−pOHpBr)n (n = 1, 2, 3 and p = 0.5), (4) XRD patterns of LiCl(Li3−pOHpCl)n (n = 1 and p = 0, 0.5, 1), (5) Temperature-dependent SXRD patterns of the n = 2 RP phase of LiBr(Li2OHBr)2, and (6) DC polarization current of the n = 2 RP phase of LiBr(Li2OHBr)2 at 30 °C.

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Figure S1a. XRD patterns and refinement results of the samples synthesized with the compositions of LiBr(Li$_{3}$OBr)$_n$ ($n = 1, 2, 3$ and $p = 0$). The red markers and green solid line represent observed and calculated patterns, respectively. The blue line below is the difference between the observed and calculated intensities. The green, purple and pink ticks are the allowed Bragg reflection positions for the $n = 2$ RP, LiBr and Li$_2$O phases, respectively. Fraction of each phase is also presented in the figure.
Figure S1b. XRD patterns and refinement results of the samples synthesized with the compositions of LiBr(Li_{3-p}OH_pBr)_n (n = 1, 2, 3 and p = 0.5). The red markers and green solid line represent observed and calculated patterns, respectively. The blue line below is the difference between the observed and calculated intensities. The green and purple ticks are the allowed Bragg reflection positions for the n = 2 RP and antiperovskite phases, respectively. Fraction of each phase is also presented in the figure.
Figure S1c. XRD patterns and refinement results of the samples synthesized with the compositions of LiBr(Li$_3$OHBr)$_n$ ($n = 1, 2, 3$ and $p = 1$). The red markers and green solid line represent observed and calculated patterns, respectively. The blue line below is the difference between the observed and calculated intensities. The green, purple and pink ticks are the allowed Bragg reflection positions for the $n = 2$ RP, antiperovskite and LiBr phases, respectively. Fraction of each phase is also presented in the figure.

Figure S2. XRD patterns of the samples synthesized with the compositions of LiCl(Li$_3$OHCl)$_n$ ($n = 1$ and $p = 0, 0.5, 1$).
Figure S3. Temperature-dependent SXRD patterns of the \( n = 2 \) RP phase of LiBr(Li\(_2\)OHBr).2.

Figure S4. DC polarization current of the \( n = 2 \) RP phase of LiBr(Li\(_2\)OHBr)\(_2\) at 30 °C. When the applied voltage was set to zero after 30 minutes, the spike inverse current was observed, also confirming the ionic conduction in the sample.