Two dimensional Li-ion conduction in a Ruddlesden-Popper phase of lithium-hydroxide-halide antiperovskites

(*Institute for Chemical Research, Kyoto University*) ○Anucha Koedtruad, Midori Amano Patino, Daisuke Kan, Yuichi Shimakawa

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Lithium-oxide-halide and lithium-hydroxide-halide antiperovskites were intensively studied for potential electrolytes in all-solid Li-ion batteries. In this work, Ruddlesden Popper (RP) phases of $LiX(Li_{3-p}OH_pX)_n$ antiperovskites with X = Br and Cl, n = 1, 2, and 3, and p = 0, 0.5, and 1, were explored. The n = 2 RP phase $LiBr(Li_2OHBr)_2$ was successfully obtained. The compound crystalizes in a tetragonal structure with space group *I*4/*mmm*. The crystal structure consists of double antiperovskite Li_2OHBr layers intercalated with rock-salt type LiBr layers. Li-ion vacancies are introduced selectively to the antiperovskite layers, and the rock-salt type LiBr layers are rigid. The RP $LiBr(Li_2OHBr)_2$ exhibits ionic conductivity of 1.27 x 10^{-7} S/cm at 30 ºC with an activation energy of 0.57 eV. The rigid rock-salt type LiBr layers contribute less in Li-ion hopping and thus the Li-ion conduction occurs through the Li-ion vacancies within the antiperovskite layers, resulting in the two-dimensional ion conduction. Cl-containing compounds, in contrast, cannot be crystallized with the RP phases due to the structural mismatch between the antiperovskite layers and the rock-salt type LiCl layers.

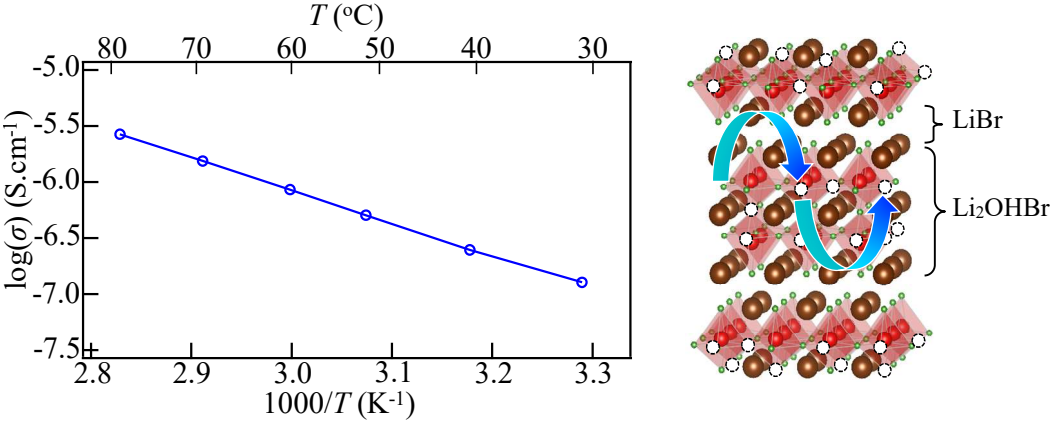

Figure 1 Temperature-dependent ionic conductivity (left) and two-dimensional Li-ion conduction (right) in the n = 2 RP phase $LiBr(Li_2OHBr)_2$.