$\label{eq:supplemental} \begin{array}{c} \text{Supplemental Material:} \\ \text{Role of Cation Size on Order-Disorder Phase Transition Temperature and Cation} \\ \text{Hopping Mechanism based on $LiCB_{11}H_{12}$} \end{array}$

Kartik Sau,^{1,2,*} Shigeyuki Takagi,³ Tamio Ikeshoji,² Kazuaki Kisu,³ Ryuhei Sato,¹ and Shin-ichi Orimo^{1,3,†}

¹Advanced Institute for Materials Research (WPI-AIMR),

Tohoku University, Aoba-ku, Sendai 980-8577, Japan

²Mathematics for Advanced Materials Open Innovation Laboratory (MathAM-OIL),

National Institute of Advanced Industrial Science and Technology (AIST),

c/o Advanced Institute for Materials Research (WPI-AIMR), Tohoku University, Sendai 980-8577, Japan

³Institute for Materials Research (IMR), Tohoku University, Sendai 980-8577, Japan

^{*} kartik.sau@gmail.com

[†] shin-ichi.orimo.a6@tohoku.ac.jp



FIG. S1. Angular auto-correlation function $\zeta(t')$ for anion from NVE-MD simulation at 475 K for three different cell volumes (small, medium, and large) cases.



FIG. S2. Isosurface density plots of the Li⁺ ion and H-atom for LiCB₁₁H₁₂ in a 2 × 2 × 2 supercell for three different cell volume cases (small, medium, and large). Three different isovalues are used for H (blue) for better visualization (a) 1.6×10^{-5} Å⁻³, (b) 6.5×10^{-5} Å⁻³, and (c) 6.0×10^{-5} Å⁻³. There is a transition of Li⁺ high densities area from the Oc-void to the Tt-void. The isovalues of 1.08×10^4 Å⁻³ (red) and 6.09×10^5 Å⁻³ (orange) are used for Li⁺ ion for all three cases.