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Supporting information:

First-Principles Study of Closo-Dodecaborates $M_2B_{12}H_{12}$ (M = Li, Na, K) as Solid-State Electrolyte Materials

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Figure S1- The HOMO and LUMO state of Li₂B₁₂H₁₂ (a), Na₂B₁₂H₁₂ (b) and K₂B₁₂H₁₂ (c) crystals, where the atomic orbitals in HOMO and LUMO levels are presented respectively by brown and blue colors. Green, pink, red, yellow and purple spheres represent B, H, Li, Na and K atoms respectively.



Figure S2 - Calculated heat capacity at constant volume as function of temperature.





Figure S3 - Molecular dynamic simulation of $Li_2B_{12}H_{12}$, $Na_2B_{12}H_{12}$ and $K_2B_{12}H_{12}$ structures at 300 K and 600 K.





Figure S4 - Molecular dynamic simulation of Kinetic energies of Li₂B₁₂H₁₂, Na₂B₁₂H₁₂ and K₂B₁₂H₁₂ structures at 300 K and 600 K.



Figure S5 - The direction of the reorientation anion $B_{12}H_{12}^{2-}$ in $Li_2B_{12}H_{12}$ structure at 0 K (a), 300 K (b) and 600 K (c) temperatures. The anion at 0 K was extracted from the relaxed system obtained by the PW-SCF calculation, while the anion at 300 K and 600 K was extracted by using the CP-NPT molecular dynamic simulation. The cubic unit cells are indicated by black boxes.



Figure S6 - The direction of the reorientation anion $B_{12}H_{12}^{2-}$ in $Na_2B_{12}H_{12}$ structure at 0 K (a), 300 K (b) and 600 K (c) temperatures. The anions at 0 K was extracted from the relaxed system obtained by the PW-SCF calculation, while the anion at 300 K and 600 K was explored using the CP-NPT molecular dynamic simulation. The unit cells indicated by black boxes have a monoclinic structure at 0 K and 300 K while at 600 K the system has a cubic structure.



Figure S7 - The direction of the reorientation anion $B_{12}H_{12}^{2-}$ in $K_2B_{12}H_{12}$ structure at 0 K (a), 300 K (b) and 600 K (c) temperatures. The anions at 0 K was extracted from the relaxed system obtained by the PW-SCF calculation, while the anion at 300 K and 600 K was explored using the CP-NPT molecular dynamic simulation. The cubic unit cells are indicated by black boxes.